SYMPOSIUM A

Amorphous and Heterogeneous Silicon-Based Films–2001

April 16 – 20, 2001

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TUTORIAL

ST A: AMORPHOUS AND POLY-SILICON MATERIALS AND DEVICES FOR LARGE AREA ELECTRONICS
Monday, April 16, 2001
9:00 a.m. - 4:00 p.m.
Nob Hill A/B (Marriott)

Hydrogenated amorphous silicon (a-Si:H) and micro- or poly-crystalline silicon (μc-Si, poly-Si) are important technological materials for large-area electronics, with applications to thin film solar cells, active matrix liquid crystal displays (AM-LCDs), optical scanners, and radiation imaging. The course describes the growth and preparation, basic material properties, device physics and state-of-the-art processing issues of modern large-area-array technology based on amorphous or heterogeneous thin silicon films. Special emphasis will be on the relation between material properties and device performance.

Instructors:
Robert A. Street, Xerox Palo Alto Research Center
Ping Mei, Hewlett-Packard Laboratories

SESSION A1: NUCLEATION AND GROWTH
Chair: Robert W. Collins
Tuesday Morning, April 17, 2001
Metropolitan III (Argent)

8:30 AM *A1.1
ATOMISTIC SIMULATION AND IN SITU PROBING OF a-Si:H PLASMA DEPOSITION. Eray S. Aydil, Dimitrios Maroudas, Sumit Agarwal, Saravanapriyan Sriraman, Denise C. Marra and Shyam Ramalingam, Chemical Engineering Department, University of California Santa Barbara, Santa Barbara, CA; W.M.M. Kessels and M.C.M. Van de Sanden, Department of Applied Physics, Eindhoven University of Technology, THE NETHERLANDS.

Hydrogenated amorphous silicon (a-Si:H) deposited by plasma assisted methods is a cost effective alternative to crystalline silicon in photovoltaics and thin film transistors for flat panel displays. We have developed an in situ method based on attenuated total internal reflection Fourier transform infrared (ATR-FTIR) spectroscopy to determine the surface coverage of silicon hydrides on the deposition surface. Using this method, we determined the concentrations of mono-, di- and tri-hydrides on the surface as a function of deposition temperature and ion bombardment flux. Characterizing the evolution of the surface hydride composition as a function of temperature and ion flux allowed us to determine the major deposition precursor and possible key reactions that take place on the surface during deposition of a-Si:H. Lower hydrides on the surface are created by sequential decomposition of the adsorbed SiH_3 on the surface to SiH_2 and SiH through reactions that require presence of dangling bonds on the surface. Increased ion bombardment flux to the surface creates more dangling bonds and helps dissociate the higher hydrides on the surface. In conjunction with experiments, we have developed and used a hierarchy of atomistic simulation tools based on molecular-dynamics (MD), molecular-statics, and Monte Carlo methods to study the interactions between silane fragments and various silicon surfaces. Most recently, we have studied the growth of a-Si:H on H-terminated Si (001)-(2x1) surfaces through molecular dynamics simulations of repeated SiHx radical impingement. Amorphous silicon films were grown using SiH_3, SiH_2 and SiH radicals, separately, as precursors. Results of these studies were compared with experimental measurements to validate the simulations and to provide supporting evidence for radical-surface interaction mechanisms hypothesized based on experimental data. Experimental measurements of the surface silicon hydride coverage and atomistic simulations will be used synergistically to elucidate elementary processes occurring on the surface during a-Si:H deposition.

9:00 AM A1.2
EFFECT OF STRAINED Si-Si BONDS IN AMORPHOUS SILICON INCUBATION LAYER ON MICROCRYSTALLINE SILICON NUCLEATION. Hiroyuki Fujiwara, Michio Kondo, Akihisa Matsuda, Electrotechnical Laboratory, Thin Film Silicon Solar Cells Super Lab., Tsukuba, JAPAN.

We have applied real time spectroscopic ellipsometry (SE) and infrared attenuated internal total reflection spectroscopy (ATR) to investigate microcrystalline silicon (μc-Si:H) nucleation mechanism in plasma-enhanced chemical vapor deposition using hydrogen dilution of SiH_4 source gas. In our previous studies, we found a new infrared absorption peak at $\sim$1937 cm^{-1} in a two-monolayer thick sub-surface of hydrogenated amorphous silicon (a-Si:H) at the onset of μc-Si:H nucleation from a-Si:H phase [1]. The absorbance of this peak showed a clear relationship with the μc-Si:H nucleation at different hydrogen dilution ratios. We assigned this peak to SiH_n (n=1$\sim$2) complex and proposed that the μc-Si:H nucleation occurs by the formation of the SiH_n complex in a-Si:H sub-surface [1]. In this study, we characterized the formation process of the SiH_n complex in greater detail. As a result, we found that the H_2-plasma treatment of a-Si:H layer leads to creation of the SiH_n complex while no complexes are created during the same treatment of c-Si. These results suggest that the SiH_n complex is formed by the insertion of H into *strained* Si-Si bonds in a-Si:H phase since there is no strained Si-Si bonds in c-Si. With increasing a-Si:H deposition temperatures, the number of the SiH_n complexes created by the H_2-plasma increases, implying that the number of strained Si-Si bonds is higher in a-Si:H layers deposited at high temperatures, in agreement with other results for stress measurements [2]. These results indicate that not only the surface reactions but also the local strain in the a-Si:H phase play a major role in the μc-Si:H nucleation process. [1] H. Fujiwara et al., J. Non-Cryst. Solids 266-269 (2000) 38, and MRS proceeding 609 (2000): in press. [2] T. Sakamoto et al., J. Non-Cryst. Solids 266-269 (2000) 481.

9:15 AM A1.3
QUANTITATIVE MODELING OF NUCLEATION KINETICS EXPERIMENTS FOR POLY-Si GROWTH ON SiO_2 BY HOT-WIRE CHEMICAL VAPOR DEPOSITION. M. Swiatek, J.K. Holt and H.A. Atwater, Thomas J. Watson Laboratory of Applied Physics, California Institute of Technology, Pasadena, CA.

We apply a rate-equation pair binding model of nucleation kinetics developed by Venables[1] to the experimental data for nucleation of Si islands grown by hot-wire chemical vapor deposition (HWCVD) on SiO_2 substrates. Previously, we had demonstrated an increase in grain size of polycrystalline Si films with H_2 dilution from 40 nm using 100 mT of 1% SiH_4 in He to 85 nm with the addition of 20 mT H_2. (2) This increase in grain size is attributed to atomic H etching of amorphous Si and small crystalline nuclei, decreasing the nucleation density. As shown through AFM measurements, the nucleation density increases sublinearly with time at low coverage, implying a fast nucleation rate until a critical density is reached, after which grain growth begins. The nucleation density decreases with increasing H_2 dilution (H_2:SiH_4), which is an effect of the aforementioned etching mechanism, and with increasing temperature, due to enhanced diffusivity of Si on SiO_2. From these temperature-dependent measurements, we estimate the activation energy for surface diffusion of Si on SiO_2 to be 0.423 eV. Using this estimate, we attempt to model the nucleation density as a function of temperature and H_2 dilution. Experimental results for epitaxial growth of Si by HWCVD will also be discussed. [1]J.A. Venables, Physical Review B, 36:4153 (1987) [2]M. Swiatek et. al, MRS Proceedings 609, to be published.

9:30 AM A1.4
ON THE GROWTH MECHANISM OF HYDROGENATED AMORPHOUS SILICON. M.C.M. van de Sanden, W.M.M. Kessels, A.H.M. Smets, Eindhoven University of Technology, Dept of Applied Physics, Eindhoven, NETHERLANDS; D.C. Marra, E.S. Aydil, UC Santa Barbara, Dept. of Chemical Engineering, Santa Barbara, CA.

The kinetic growth model for hydrogenated amorphous silicon (a-Si:H) from SiH_3 radicals is reviewed on the basis of recently obtained experimental and computational data. New surface reactions are considered and their implication for the a-Si:H growth mechanism are discussed. A central approach is the analysis of the bulk hydrogen content as function of substrate temperature in relation to the surface hydrides on the a-Si:H growth surface. The importance of surface processes in the elimination of bulk hydrogen will be emphasized.

9:45 AM A1.5
THERMODYNAMIC MODEL OF WHY HYDROGEN DILUTION STABILISES MICROCRYSTALLINE SILICON DEPOSITION. John Robertson, Cambridge Univ, Cambridge, UNITED KINGDOM.

The plasma deposition of microcrystalline silicon from hydrogen diluted silane is a standard means to make microcrystalline Si for solar cells and thin film transistors. However, the role of hydrogen has been variously attributed to - partial chemical equilibrium, the preferential etching of the less stable a-Si:H; the higher surface mobility of the silyl growth species, chemical annealing, aiding nucleation by providing a more flexible host network, or reducing disorder by raising the hydrogen chemical potential. It is noticeable that there is no definition of how hydrogen actually provides the driving force to stabilise crystalline silicon over a-Si:H, as would be required in conventional description of the nucleation and growth of a second phase in a 2 component system. We do this here. The free energy of the Si,H system is analysed using the Si-Si, Si-H and H-H bond energies. Hydrogen is shown to stabilise uc-Si over a-Si:H by causing a double minimum in the free energy curve of a-Si:H

networks. Networks with locally higher H contents are found to have a larger driving force for uc-Si nucleation, and lead to a segregation into uc-Si and H-rich a-Si:H tissue phases. The model accounts for various features of uc-Si deposition, such as an increased nucleation rate at medium temperatures.

SESSION A2: NOVEL CONCEPTS
Chair: Martin Stutzmann
Tuesday Morning, April 17, 2001
Metropolitan III (Argent)

10:30 AM A2.1
PHOTOVOLTAICS ON WIRE. M. Rojahn, M. Rakhlin, M.B. Schubert, University of Stuttgart, Institute of Physical Electronics, GERMANY.

Optoelectronic devices have generally been deposited on plane flexible or solid surfaces. We present a new design of electronically active thin films which we form on wire-like structures. Based on such structures, novel fabric networks can be developed which may incorporate optoelectronically active sensors or photovoltaic cells. We modify conventional PECVD-, sputter- and evaporation set-ups in order to transfer our planar processes to arbitrarily shaped surfaces with curvature radii of the order of 0.1 μm ... 1 mm. Using our experience in depositing and patterning amorphous silicon at temperatures below 100°C on flexible plastic foils and other polymer substrates, our approach investigates the growth of hydrogenated amorphous silicon (a-Si:H) and transparent conductive oxides (TCO) on artificial fibers. We report on the performance of first a-Si:H based nip-solar cells fabricated on insulated metal wires, and on fiber optic cables. Non-uniform covering of our substrates with amorphous silicon and TCO layers leads to changing light absorption and electrical field distributions and complicate the optimization of the device. At present, we focus on achieving sufficient homogeneity in terms of layer thickness as well as composition. This leads us to correlate deposition parameters such as the distance of the wire from the RF plasma electrodes with thermal distributions around our substrate. Subsequently, we propose patterning steps of such deposited thin film layers which allow for the bonding of fabricated devices. Moreover, we show that similar photolithographic steps can be used to series-connect neighboring photodiodes on one wire. The I-V-characteristics of such cells on a wire is compared with a-Si:H based micro-photodiodes that are laterally series connected on a plane substrate. Improving our technology will ease the fabrication of novel thin film devices, thus widening the range of commercial applications.

10:45 AM A2.2
HOLE-INJECTING SEMICONDUCTING CONJUGATE POLYMER WINDOW LAYERS FOR AMORPHOUS SILICON-BASED SOLAR CELLS. A.R. Middya and E.A. Schiff, Department of Physics, Syracuse University, Syracuse, NY.

We have explored a hole-transporting polymer [3,4 polyethylene-dioxythiophene (PEDOT)] as an alternative to silicon-based p-type window layers for a-Si:H solar cells. The dark J-V characteristics of these devices exhibit good diode properties and this is the first report on fabrication of polymer/a-Si:H heterojunction. In principle, a semiconducting polymer can allow adjustment of the dark Fermi level (doping activation range: 10^{-13} to 10^{2} S/cm) and of the conduction bandedge (relative to that of a-Si:H) over a larger range than achievable with doped silicon-based thin films. Polymer window layers are thus potentially interesting both for the insight they give into the open-circuit voltage and also from a solar cells manufacturing point of view, due to its easy-processibility, scalability and low-cost. We fabricated nip solar cell structures on stainless steel substrates with p-layer deposited by painting or spin-casting the PEDOT onto the intrinsic a-Si:H layer. The n- and i-layers of the devices have been deposited by conventional RF PECVD. The performance of these devices is found to be sensitive to the native oxide layer on the a-Si:H. We studied the effect of treating the top surface of the structure with HF acid prior to depositing the PEDOT layer; V_{oc} increases from 600 mV to 650 mV due to etching (for 30 second) of the oxide layer by 0.5% HF solution, increases to more than 700 mV for 1-5% and then drops rapidly below 500 mV for HF concentration greater than 10%. On optimization of these devices, the best polymer-based a-Si:H solar cell illuminated (AM 1.5) though p-layer exhibits $V_{oc} \approx$ 710 mV and Jsc $\approx$ 1.5 mA/cm^2. We attribute the low value of J_{sc} to the relatively thick PEDOT layer used for these devices. The experiments on optimization of PEDOT layer thickness, improvement of adhesion of polymer on Si-layer, reduction of metal/polymer contact resistance and also investigation of other polymer window layers, are underway. We will discuss the physics of relatively unknown semiconducting polymer/a-Si:H interface. This research was supported through the Thin Film Photovoltaics Partnership of the National Renewable Energy Laboratory.

11:00 AM *A2.3
SUBRETINAL IMPLANTS AND OPTICAL SENSORS. M.B. Schubert, University of Stuttgart, Institute of Physical Electronics, Stuttgart, GERMANY.

Restoring some degree of visual perception for patients with retinal degenerations is one of the most ambitious goals in neurotechnology. Pursuing this goal, we have fabricated a variety of microphotodiode arrays (MPDAs) for direct functional replacement of the degenerated, natural photoreceptor cells by these technical contraptions. This paper reviews the challenges of neatly joining microelectronic devices with biological systems, the various efforts of the German 'Retina Implant' consortium, our results, but also some remaining obstacles which still have to be resolved. While biocompatibility was the major concern for the initial selection of materials, biochemical stability of the technical MPDAs turns out to be the most critical issue for real life operation. Therefore we spend a lot of effort on sealing the microelectrodes which capacitively couple the MPDAs' electrical output to the adjacent retina cells. Successful nerve cell stimulation, and hence visual perception, will need an additional power supply to the implant, and comprise a hybrid system of thin films and bulk microelectronics. In addition to the microphotodiodes for vision repair, amorphous silicon enables a wealth of other specialized optical sensor applications. A brief survey of various cooperations in this field touches upon Thin-Film-on-CMOS cameras, non-pixelized imagers, position sensors for high energy physics, light-addressable microelectrodes for signal transduction from biological systems, and some novel ideas.

11:30 AM A2.4
PRINTED TRICHLOROSILANE MONOLAYERS ON AMORPHOUS SILICON. Laura L. Smith, Gregory N. Parsons, North Carolina State University, Dept of Chemical Engineering, Raleigh, NC.

The interaction between the surfaces of electronic materials and organic compounds is an area of great scientific and technological interest. A wide range of applications, including biosensor devices, flexible displays, and electronic textiles, will benefit from a greater understanding of Si surface derivatization and functionalization. In this study, low-temperature (25°C) plasma-deposited hydrogenated amorphous Si thin films (750Å thick) were functionalized with patterned self-assembled monolayers (SAMs) of hexadecyl-trichlorosilane ($C_{16}H_{33}SiCl_3$, HDTS). The HDTS patterns, consisting of (a) 5μm lines and (b) 5-30μm circuit patterns, were formed using (a) microcontact printing (μCP) and (b) photolithographic lift-off respectively. The microcontact printing process used a cast polydimethylsiloxane (PDMS) stamp with 5μm lines at a 5μm pitch. Printing "inks", using n-hexane or dimethylformamide as the solvent, were prepared with HDTS/solvent concentrations from 15 to 70 mM. The "inked" PDMS stamp was then used to transfer the pattern to the UV/O_3-treated a-Si surface. The photolithography lift-off process involved conventional photopatterning of the a-Si surface using a mask containing varied features ranging from 5μm to 30μm in width. Following the vapor-deposition of HDTS monolayers on the patterned a-Si surfaces, the photoresist was lifted off with an acetone rinse. The resulting patterned SAMs were characterized using several AFM techniques including topographic imaging, phase-contrast imaging, and lateral force microscopy (LFM). The HDTS layers were also examined via X-ray photoelectron spectrometry (XPS) and low-voltage scanning electron microscopy (SEM). The microcontact printing experiments showed that the higher-concentration printing "inks" resulted in the clearest patterns and the greatest surface chemical contrast. The patterned functionalization of the a-Si surface was visibly demonstrated by the subsequent preferential deposition of bovine serum albumin (BSA) from aqueous solution onto the hydrophilic non-HDTS areas of the samples, while the HDTS-patterned areas resisted BSA deposition.

11:45 AM A2.5
NANOCRYSTALLINE SILICON SINGLE-ELECTRON TRANSISTORS. Y.T. Tan[a,c], T. Kamiya[a,b,c], Z.A.K. Durrani[a,c] and H. Ahmed[a,c]. [a]Microelectronics Research Center, Cavendish Laboratory, University of Cambridge, UNITED KINGDOM; [b]Materials and Structure Laboratory, Tokyo Institute of Technology, Midori-ku, Yokohama, JAPAN; [c]CREST, JST, Shibuya, Tokyo, JAPAN.

We report the observation of single-electron charging effects in nanowire single-electron transistors (SETs) fabricated in hydrogenated nanocrystalline silicon (nc-Si:H) thin films. Nc-Si:H films were prepared by 100 MHz-VHF PECVD at 300°C. The Raman analysis indicated that the crystalline volume fraction was ~70% for 30 nm-thick films. We fabricated side-gated nanowire SETs using 30 nm-thick nc-Si:H and characterized electronic transport in the SETs with respect to the physical dimensions of the conducting channel. In addition, we have investigated the effect of defect density on the electrical characteristics by modifying the film structure using thermal

argon annealing or oxidation. We observed single-electron charging effects up to 16 K in the as-deposited SETs using nanowires of 50 nm width and 1 mm length. SETs using 30 nm x 30 nm point-contacts also exhibited single-electron charging effects, which persisted up to 58 K. These results indicate that a narrower channel limits electron transport paths better and helps to achieve higher temperature operation. However, activation energy measurements indicated that the maximum tunnelling barrier height was ~40 meV, which is not enough for electron confinement at high temperatures. In addition, it was found that the transport mechanism changes from a thermally-assisted tunnelling process to percolation conduction at a transition temperature of ~60 K. We also observed single-electron charging effects in annealed/oxidized nc-Si:H nanowires. In the as-deposited nc-Si:H nanowires, the grain boundary consists of amorphous silicon, which forms the tunnelling barrier. If the nc-Si is annealed, dangling bonds increase due to hydrogen effusion from grain boundaries. These bonds trap electrons and form tunnelling barriers.

SESSION A3: HOT WIRE CVD
Chair: Ruud E.I. Schropp
Tuesday Afternoon, April 17, 2001
Metropolitan III (Argent)

1:30 PM A3.1
IDENTIFICATION OF RADICAL GROWTH PRECURSORS IN HOT WIRE CVD OF AMORPHOUS SILICON FILMS. H.L. Duan, Gillian A. Zaharias and Stacey F. Bent Department of Chemical Engineering, Stanford University, Stanford, CA.

A novel laser technique has been applied to probe radical growth precursors in hot wire chemical vapor deposition (HW-CVD) of a-Si:H. The technique, vacuum ultraviolet single photon ionization (SPI), utilizes the ninth harmonic of a Nd:YAG laser to induce soft ionization of silicon-containing species formed from the hot wire dissociation of silane. The 10.5 eV photon used here is in most cases not of sufficient energy to further fragment the ionized radical; thus mass spectra of key species can be obtained without complication by daughter ions. It is shown that Si, SiH_3, and Si_2H_x are the major species evolved upon activating the hot wire. Filament temperatures between 900°C and 2000°C have been studied. At the lower filament temperatures (up to 1300°C), consumption of silane is observed without significant formation of Si radicals, suggesting that filament alloying is occurring. Heating the filament to higher temperatures increases the flux of Si, SiH_3 and Si_2H_x; however, no new species are detected as a function of filament temperature. At the highest temperatures studied, the saturation of Si and the relative increase of SiH_3 radicals indicate incomplete decomposition of silane at high temperature. Furthermore, filament condition and chamber history are found to influence the radical species produced. In conclusion, we have applied for the first time single photon ionization for direct, in situ detection of silicon-containing radicals during HW-CVD of amorphous silicon, and we have provided evidence for temperature dependent radical profiles and filament aging effects.

1:45 PM A3.2
RADICAL SPECIES DISTRIBUTIONS IN HOT-WIRE CHEMICAL VAPOR DEPOSITION PROBED VIA THRESHOLD IONIZATION MASS SPECTROMETRY AND DIRECT SIMULATION MONTE CARLO TECHNIQUES. J.K. Holt, M. Swiatek, D.G. Goodwin, and H.A. Atwater, Thomas J. Watson Laboratories of Applied Physics, California Institute of Technology, Pasadena, CA.

Radical species are known to play an important role in the deposition of silicon films via hot-wire chemical vapor deposition (HWCVD). The nature of the reactions on the filament surface and the gas-phase chemistry are not well understood, but are know to be critical to film microstructure. In particular, the relative abundance of the radicals SiH_2 and SiH_3 is thought to determine the balance between rough, island surface growth versus epitaxial silicon growth[1]. A combination of threshold ionization mass spectrometry measurements and Direct Simulation Monte Carlo (DSMC) calculations can be used to determine the relative abundance of radicals (e.g., Si, SiH_2, SiH_3, and Si_2H_x) present during growth. Mass spectrometry results thus far indicate that SiH_2 is the dominant radical at the surface for conditions of 2-200mTorr pressure (1% SiH_4 in He), at wire temperatures between 1750-1900°C (power 200-300W), and at wire-to-substrate distances of 2.5cm. The dominance of SiH_2 is attributed to pyrolysis of SiH_4, indicating that careful attention must be paid to substrate thermal management during HWCVD growth to insure catalysis at the wire, rather than thermal CVD at the substrate. Also investigated via mass spectrometry was the effect of hydrogen dilution, and these results confirm the expectation that atomic hydrogen is produced at the wire and reveal that etching is significant enough to regenerate SiH_x species from silicon-coated areas of the reactor. Simulation results using DSMC have predicted a transition in the dominant growth species from the highly reactive Si (for conditions[2] leading to amorphous growth) to the less reactive SiH_3 (for conditions[2] leading to polycrystalline growth). Ab-initio calculations are being performed which will provide input to the reactor simulation. One reaction being considered specifically is that of atomic silicon with silane, which we believe produces Si_2H_2, a radical of potential importance to high quality amorphous silicon growth[3]. [1]M. Ichikawa, T. Tsushima, A. Yamada, and M. Konagai, Jpn. J. Appl. Phys. 39 (8), 4712, 2000. [2]R. Schropp, K. Feenstra, E. Molenbroek, H. Meiling, and J. Rath, Philosoph. Mag. B 76 (3), 309, 1997. [3]D. Goodwin, Electrochem. Soc. Proc. 98-23, 227, 1998.

2:00 PM A3.3
THE PROPERTIES OF a-Si:H FILMS AND DEVICES DEPOSITED BY HOT WIRE CVD AT ULTRA HIGH DEPOSITION RATES. A.H. Mahan, Y. Xu, J.D. Perkins, L.M. Gedvilas, R.S. Crandall, and B.P. Nelson, NREL, Golden, CO; D.L. Williamson, Colo. School of Mines, Golden, CO; W. Beyer, Forschungszentrum Julich, Julich, GERMANY; and J.D. Cohen, Univ. or Oregon, Eugene, OR.

The film properties of device quality a-Si:H, deposited at rates in excess of 100Å/s by the hot wire chemical vapor deposition (HWCVD) technique, have been examined by x-ray diffraction (XRD), Raman spectroscopy, H evolution, small-angle x-ray scattering (SAXS), and drive level capacitance profiling (DLCP). These high rates are achieved by using multiple filaments and deposition conditions different than those used to produce our standard 20Å/s material. Structurally, we find that the short range order (from Raman), the medium range order (from XRD), and the peak position of the H evolution peak are invariant with respect to deposition rate, and exhibit structure consistent with state-of-the-art, compact a-Si:H deposited at low deposition rates. The only exception to this behavior is the SAXS intensity, which increases by a factor of ~100 over that for our best, low CH films deposited at ~5Å/s. We discuss the invariance of the short and medium range order with deposition rate in terms of growth models available in the literature, and relate changes in the film electronic structure (Urbach edge) to the increase in the SAXS intensities. We also note the invariance of the saturated defect density with deposition rate from 5-130Å/s, measured by DLCP after light soaking (ND(B) ~2-4e16/cm^3), and discuss possible reasons why the increase in the microvoid density apparently does not play a role in the Staebler-Wronski Effect for this type of material. Based upon these encouraging (low) values of ND(B), we fabricate single junction n-i-p test structures on untextured stainless steel substrates using this material. Preliminary efficiency results (as-grown, light soaked), with the i-layer deposited at rates up to 80Å/s, compare quite favorably with those reported in the literature using other deposition techniques at lower deposition rates (1). (1). S.J. Jones, X. Deng, T. Liu, and M. Izu, MRS Symp. Proc. 507, 113 (1998).

2:15 PM A3.4
AFM CHARACTERIZATION OF HOT-WIRE-GROWN MICROCRYSTALLINE SILICON WITH LARGE GRAINS. J.J. Gutierrez and C.E. Inglefield, Department of Physics, Weber State University, Ogden, UT; M.C. DeLong, and P.C. Taylor, Department of Physics, University of Utah, Salt Lake City, UT; S. Morrison and A. Madan, MV Systems, Golden, CO.

Microcrystalline silicon is an important material in the growing fields of large-area opto-electronics and photovoltaics, with increasing emphasis being placed on obtaining large grain size. We have characterized with contact-mode Atomic Force Microscopy microcrystalline silicon thin films with coalesced grains larger than 0.1 μm. The samples were grown by a novel technique combining both a Hot Wire Chemical Vapor Deposition (HWCVD) process and a post-growth hot-wire annealing treatment. During HWCVD, SiF_4 was used along with SiH_4 and H_2 to grow the thin films. From sample to sample, the partial pressure of SiF_4 in the growth chamber was varied and a trend was observed: as the partial pressure was increased the grains became larger with a maximum size occurring at a partial pressure of 2.4%. After growth, some films were hot-wire annealed in the same chamber with only SiF_4 and H_4 present. As result of this annealing, grains formed aggregates as large as ~0.5 μm, another positive effect. With these studies we hope to improve upon this growth technology with emphasis being placed upon fabricating more efficient solar cells. In this presentation, the experimental technique will be explained and qualitative and quantitative results will be discussed.

2:30 PM A3.5
T-SITE TRAPPED MOLECULAR HYDROGEN IN HOT WIRE a-Si:H. J. Herberg, P.A. Fedders, D.J. Leopold, R.E. Norberg, Department of Physics, Washington University, St. Louis, MO; R.E.I. Schropp, Debye Institute, Utrecht University, TA Ultrecht, THE NETHERLANDS; H. Branz, National Renewable Energy Lab, Golden, CO.

Proton NMR and proton-^{29}Si double resonance NMR have been performed on hot wire a-Si:H films deposited from SiH_4. Results are compared with those from conventional plasma enhanced chemical vapor deposition a-Si:H and multiple quantum NMR experiments. Proton nutational angle studies and proton-^{29}Si spin-echo double resonance (SEDOR) signals at 80 and 300 K indicate that a significant proton resonance population arises from T-site-trapped molecular H_2. This fractional population however is about twenty percent, that is about half that reported[1,2] for conventional PECVD a-Si:H films. [1]R.E. Norberg, D.J. Leopold, P.A. Fedders, R. Borzi, P.H. Chan, J. Herberg, and N. Tomic, Materials Research Symposium Proceedings (2000) (to be published). [2] P.A. Fedders, D.J. Leopold, P.H. Chan, R. Borzi, and R.E. Norberg, Phys. Rev. Lett. **85** 401 (2000).

2:45 PM A3.6
p-TYPE WINDOW LAYERS FOR PIN SOLAR CELLS ENTIRELY FABRICATED BY HOT-WIRE CVD. Urban Weber, Markus Koob, Chandrachur Mukherjee, Dept of Physics, University of Kaiserslautern, Kaiserslautern, GERMANY; D Chandrashekhar, Rajiv O. Dusane, Dept of Metallurg Eng and Mat Science, IIT Bombay, INDIA; Bernd Schroeder, Dept of Physics, University of Kaiserslautern, Kaiserslautern, GERMANY.

Recently, pin solar cells were fabricated entirely by Hot-Wire (HW) or thermo-catalytic CVD with initial efficiencies up to 8.8% by our group. An a-SiC:H p-layer was used in these cells. However, using methane as a carbon precursor gas is problematic since extreme deposition conditions have to be used to meet the requirements needed for the window layer. The resulting porous and hydrogen-rich material may be one reason for irreversible degradation which takes place in the mentioned pin solar cells. In a comparative study, we investigate a-SiC:H p-layer deposition by HWCVD using three different carbon precursor gases, methane, ethane, and acetylene. Carbon incorporation results from gas phase reactions rather than direct dissociation on the hot filament both for methane and ethane, but ethane can be dissociated more easily leading to less extreme deposition conditions for ethane-based p-layers. All three types of materials show at least a conductivity of $\approx 10^{-5}$ $(\Omega\mathrm{cm})^{-1}$ and a band gap of $\approx$1.95 eV and meet the requirements on a window layer for solar cells. Higher conductivity and lower activation energy are obtained for ethane pointing towards a better network structure which is supported by the respective infrared signatures. Initial results show that a larger band gap (2.1 eV) can be obtained for the same conductivity ($\approx 10^{-5}$ $(\Omega\mathrm{cm})^{-1}$) with the use of acetylene. We compare these results with the utilization of microcrystalline silicon p-layers. For the deposition of these films, an adequate substrate preparation (a very thin seed layer) is found to be equally important as the deposition conditions for optimum performance in solar cells. All p-layer types are incorporated into pin solar cells. Methane- and ethane-based a-SiC:H-p-layers yield similar V_{oc} and FF ($\approx$850 mV and 66 to 71% respectively). Work on acetylene-p-layer-based solar cells is in progress. Microcrystalline p-layers improve V_{oc} and FF (up to 900 mV and 72%, respectively) and stability, however the higher absorption leads to lower short circuit current and prevents an increase of overall efficiency beyond 8%. Both p-a-SiC:H and p-μc-Si:H were also incorporated into tandem (pinpin) solar cells with initial efficiencies up to 7.0%.

SESSION A4: HIGH RATE DEPOSITION

Chair: Eray S. Aydil
Tuesday Afternoon, April 17, 2001
Metropolitan III (Argent)

3:30 PM A4.1
DIAGNOSTICS OF VHF PLASMA CVD FOR MICROCRYSTALLINE SILICON DEPOSITION. Toshiaki Sasaki, Takehito Wada, Takashi Yoshida, Fuji Electric Corporate Research and Development, Ltd., Yokosuka, JAPAN; Yukimi Ichikawa, Fuji Electric Co. Ltd., Matsumoto, JAPAN; Akihiro Kubota, Tomoya Moriki, Shosaku Matsumura, Musashi Institute of Technology, Tokyo, JAPAN.

We have experimentally studied plasma CVD for deposition of microcrystalline silicon (μc-Si) films to understand the effects of discharge frequency on the properties of μc-Si films. To measure precise plasma parameters of VHF (13-100MHz) plasma CVD, we developed two new probe techniques; (1) modified capacitance probe to measure the amplitude of plasma potential variation (Vsp-p) at discharge frequency, (2) compensation single probe by which variation of the plasma potential is compensated and precise current voltage characteristics are measured. We used SiH_4 diluted by H_2 (H_2/SiH_4=50) or H_2 discharge generated by a capacitively coupled plasma CVD apparatus with parallel-plate electrodes. A dark region so-called sheath followed by a bright region was observed near both electrodes. The thickness of the dark region decreases as frequency increases from 13.6MHz to 100MHz, and the bright region approaches the electrodes. In the bulk plasma region, Vsp-p and time averaged plasma potential (Vs) are almost constant and they sharply change in the dark region towards the electrodes. As frequency increases from 13.6MHz to 100MHz, Vsp-p decreases from 70V to 40V in the bulk plasma region, and Vs decreases from 35V to 20V. Thus, at 100MHz the energy of incident ions to the substrate is lower than that at 13.6MHz and it may help c-Si formation. In fact, the intensity ratio of c-Si peak at 520cm^{-1} and a-Si peak at 480cm^{-1} of μc-Si films measured by Raman scattering increased from 5 to 11 and the grain size of c-Si increased from 100nm to 500nm, respectively, as the frequency increases from 13.6MHz to 100MHz. At 100MHz, the electron density is 2x10^{9}cm^{-3} which is an order of magnitude lager than that at 13.6MHz, and the deposition rate of μc-Si is 16nm/min which is 8 times lager than that at 13.6MHz. The deposition mechanism of μc-Si is discussed at the presentation.

3:45 PM A4.2
MATERIAL PROPERTIES AND GROWTH PROCESS OF MICRO-CRYSTALLINE SILICON WITH GROWTH RATES IN EXCESS OF 1 NM/S. Edward A.G. Hamers, Arno H.M. Smets, Chiel Smit and M.C.M. van de Sanden, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS.

In the past an expanding thermal plasma source has been studied extensively to deposit device quality hydrogenated amorphous silicon at growth rates of 7 nm/s. The same plasma source is now used to deposit microcrystalline silicon at rates of up to 3 nm/s. The material is highly crystallised as is evidenced from X-Ray diffraction (XRD) and Raman measurements. The grain size is about 20 nm with a preferential {111} orientation. The photoconductivity is typically 2×10^{-5} S/cm, while the dark conductivity is 2×10^{-7} S/cm. The activation energy is around 600 meV. The defect density as measured with dual beam photoconductivity is around 5x10^{16} cm^{-3}. We will try to incorporate this material in a solar cell. The growth process is studied extensively. The gas depletion is typically 60%. SiH_x radicals have been measured in the gas phase. SiH_3 seems to be an abundant growth precursor just as in the case of a-Si:H deposition with the same method. In-situ ellipsometry is used to determine the complex refractive index and the roughness evolution. The roughness evolution is comparable to that of amorphous silicon. A typical roughness is 15 nm at a total thickness of 1 micron. Atomic Force Microscopy results yield comparable values. In order to get a better understanding of the influence of atomic hydrogen on the formation process of the crystalline material we studied the etch process by atomic hydrogen as function of temperature by ellipsometry. Although the etch rate decreases drastically with substrate temperature in the studied range of 150-450°C, the material deposited at these different temperatures has nevertheless the same growth rate and similar material properties. The insights into the growth process will be compared with results on hot wire or catalytic CVD and RF/VHF CVD. Special focus will be on the growth precursors in these different processes.

4:00 PM *A4.3
HIGH RATE GROWTH OF DEVICE GRADE SILICON THIN FILMS FOR SOLAR CELLS. Michio Kondo, Susumu Suzuki, Yoshiyuki Nasuno, Akihisa Matsuda, Electrotechnical Laboratory, Tsukuba, JAPAN.

High through-put processes such as high rate and large area deposition for cost reduction are key issues of photovoltaic devices. In particular, growth rate is of practically crucial importance for hydrogenated microcrystalline silicon (μc-Si:H) because of the low absorption coefficient for sun light. We have developed a plasma enhanced chemical vapor deposition (PECVD) technique for high-rate growth of μc-Si:H at low temperatures using hydrogen diluted monosilane source gas under high-pressure depletion conditions, and we demonstrated a growth rate up to 5 nm/s at 250°C which is enough for mass production of μc-Si solar cells [1]. However, it was also found that material qualities deteriorate, e.g. crystallinity decreases and defect density increases up to 1x10^{17}cm^{-3}, with increasing growth rate mainly due to ion damage from the plasma. In this work, we have found that deuterium dilution improves not only the crystallinity but also defect density as compared to hydrogen dilution and that deuterium to hydrogen ratio incorporated in the film has a good correlation with crystallinity. The advantages of the deuterium dilution are ascribed to lower ion bombardment due to slower ambipolar diffusion of deuterium ion from the plasma as well as higher stability of a surface Si-D bond due to lower vibration frequency. Further improvement of material quality has been achieved using a triode technique where a mesh electrode inserted between cathode and anode electrodes prevents from ion bombardment. In combination with a shower head cathode, the triode technique remarkably improves the crystallinity as well as defect density at a high growth rate. As a consequence, we have succeeded to obtain much better crystallinity and uniformity at about 6 nm/s with a defect density of 2x10^{16}cm^{-3}. We also discuss the limiting factors of

growth rate and material quality for μc-Si solar cells. [1] M. Kondo et al. J. Non-Cryst Solids, 266-269 (2000) 84.

4:30 PM A4.4
EVALUATION OF MICROCRYSTALLINE SILICON FILMS DEPOSITED BY ULTRAFAST THERMAL PLASMA CVD.
Yongkee Chae, Hiromasa Ohno, Keisuke Eguchi, Toyonobu Yoshida, Univ of Tokyo, Dept of Materials Engineering, Tokyo, JAPAN.

This research is the first attempt to apply thermal plasma chemical vapor deposition (TPCVD) for the ultrafast deposition of Si films for solar cells. A conventional deposition process of Si films such as plasma-enhanced chemical vapor deposition (PECVD) is capable of a deposition rate around 5 $\AA$/s at most, and it takes a relatively long time to deposit an intrinsic layer. In this paper we report a novel ultrafast deposition approach using dc-rf hybrid TPCVD. The extreme improvement of stability, controllability, and cleanliness of the process enabled the deposition of microcrystalline Si films at the ultrafast rate of over 1000 nm/s, which is about 2000 times faster than in conventional CVD. Moreover, a minimum defect density of $7.2x10^{16}$ was achieved by post-treatment of film in 2 Torr H_2/Ar plasma. Monte-Carlo simulation and step coverage analysis suggested that the precursor is an approximately 1 nm cluster with a sticking probability of about 0.6. The success of this research will lead to the development of commercially viable technology in a roll-to-roll system in the near future, and will fundamentally change the established concepts of Si deposition technology.

4:45 PM A4.5
PROPERTIES OF LARGE GRAIN-SIZE POLY-Si FILMS BY CATALYTIC CHEMICAL SPUTTERING.
Atsushi Masuda, Koji Kamesaki, Akira Izumi, Hideki Matsumura, Japan Advanced Institute of Science and Technology, Ishikawa, JAPAN.

Large grain-size polycrystalline silicon (poly-Si) films are obtained on glass substrates by newly developed catalytic chemical sputtering method at low temperatures around 400°C. Si films are also epitaxially grown on single-crystalline Si substrates. In the method Si films are deposited by the chemical transport of Si-related species generated by the reaction between solid Si target and catalytically generated H atoms. Efficient deposition is realized using the remarkable difference in the etching rate with Si-target temperatures. That is, Si-related species are efficiently generated on cooled Si target by atomic-H etching and deposited on substrates with suppressed etching phenomena by heating. Full-width at half maximum of TO Raman signals originating from crystalline phase for the obtained poly-Si films is narrower than that for excimer-laser annealed poly-Si. It was noticeable that the grain size exceeds 1.5μm for the films with a thickness of about 1μm and is much larger than that for poly-Si films deposited at low temperatures ever reported. Growth modes of poly-Si films especially in the initial stage are remarkably changed with a difference in the type of substrates. These phenomena are well explained in terms of initial nucleation and etching by atomic H. It was found that formation of seed layer enhances the growth of poly-Si films on glass substrates.

SESSION A5: POSTER SESSION
GROWTH OF SILICON AND SILICON-ALLOY THIN FILMS

Chair: Michio Kondo
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A5.1
ADVANCED SPECTROSCOPIC STUDY OF THE DENSITIES AND KINETICS OF SiH_x RADICALS DURING HIGH-RATE PLASMA DEPOSITION OF a-Si:H.
J.P.M. Hoefnagels, W.M.M. Kessels, A.A.E. Stevens, D.C. Schram, M.C.M. van de Sanden, Dept of Applied Physics, Center of Plasma Physics and Radiation Technology, Eindhoven University of Technology, NETHERLANDS.

At the Eindhoven University of Technology a remote Ar-H_2-SiH_4 plasma is used for high rate deposition of device quality hydrogenated amorphous silicon (a-Si:H). In order to optimize the deposition process and film properties, detailed insight in plasma processes and film growth is essential. Therefore, fundamental studies of SiH_3, SiH, and Si radicals have been performed by means of direct measurement using the highly sensitive cavity ring down absorption spectroscopy technique. The aim of these studies is twofold: to obtain densities and contributions to film growth of the SiH_x radicals and to study their kinetics, consisting of gas and surface reactions. It has clearly been demonstrated that the properties of a-Si:H strongly improve with increasing contribution of SiH_3 to film growth. Furthermore, for conditions where the "optimum" a-Si:H quality is obtained, a total ground state density up to 10^{19} m^{-3} has been observed for SiH_3, which can about fully explain the corresponding a-Si:H deposition rate. On the other hand, under these conditions total ground state densities of about 10^{16} m^{-3} and 10^{15} m^{-3} have been observed for SiH and Si, respectively. A completely new experiment for time-resolved density measurements has been setup in order to study the kinetics in a silane plasma and its interaction with the a-Si:H surface. For this, the density of SiH_x radicals is modulated in time by the application of a pulsed RF signal to the substrate holder in addition to the regularly operating expanding thermal plasma. With the use of a model, measurement of the exponential decay time of the density of the SiH-$_x$ radicals in the RF afterglow enables the determination of their gas and surface reaction probability. Preliminary measurements in the case of SiH suggest the importance of surface reactions. Moreover, surface reaction probabilities for the case of SiH_3 and SiH will be presented.

A5.2
DIAGNOSTICS OF PLASMA USED FOR DEPOSITING a-Si AND a-(Si,Ge) FILMS AND DEVICES IN AN ECR REACTOR.
Vikram L. Dalal, Matt DeFreese, Iowa State University, Dept. of Electrical and Computer Engr., Ames, IA.

In this paper,we report on the diagnosis of ECR induced plasmas used for depositing a-Si, a-(Si,Ge) and a-Ge films and devices. Both optical emission spectroscopy and Langmuir probes were used to diagnose what was happening in the plasma. For the first time ever, we detected the elusive GeH peak in optical emission spectroscopy. This peak, at 247 nm, is obscured by effects due to hydrogen,but by using a He dilution mixture, we could distinctly identify the peak. We also studied the influence of hydrogen dilution and bias on SiH, GeH and Ge peaks, and found that adding hydrogen fundamentally changes the electron temperature of the plasma and drastically reduces each of the three peaks. Thus, contrary to conventional wisdom, adding hydrogen reduces growth rate not because of etching alone, but also because the plasma chemistry is changing drastically. We also found that when one puts a bias on the substrate, both ion energies and flux densities change non-linearly with bias, again contrary to conventional wisdom. The relationships of these observations to film and device properties will be discussed.

A5.3
FUNDAMENTAL CONSIDERATIONS OF GROWTH CHEMISTRY OF AMORPHOUS AND MICROCRYSTALLINE Si AND Ge FILMS.
Vikram L. Dalal, Iowa State University, Dept. of Electrical and Computer Engineering, Ames, IA.

In this paper, we show that the fundamental consideration that governs how one can grow high quality amorphous and microcrystalline Si and Ge films and devices is how to eliminate excess H from the lattice and the surface. The conventional model, which states that H is eliminated by H bond breaking with Si at the surface, and interaction between liberated H from neighboring SiH_3 radicals, is simply wrong. The surface bond breaking reaction is not thermodynamically likely at the growth temperatures involved. Rather, H is primarily eliminated by interactions with H atoms and ions, and by bombardment with inert gases such as He or Ar, if such are present. H atoms eliminate H by both surface and subsurface reactions, and the inerts only at the surface. Experimental evidence from many groups supporting this model will be shown. The new model also explains why hot wire deposited devices, while very good intially, degrade even more rapidly than low rate glow discharge devices. Using these insights, one can design new growth processes to increase growth rates while maintaining device quality and stability, and these will be discussed.

A5.4
PHASE DIAGRAMS FOR THE OPTIMIZATION OF PLASMA-ENHANCED CVD Si:H: THE ROLES OF PLASMA POWER AND SUBSTRATE TEMPERATURE.
Andre S. Ferlauto, Randy J. Koval, Christopher R. Wronski, Robert W. Collins, Materials Research Laboratory and Center for Thin Films Devices, Pennsylvania State University, University Park, PA.

Phase diagrams for plasma-enhanced chemical vapor deposition (PECVD) of thin film silicon describe the regimes of thickness and hydrogen dilution ratio R=[H_2]/[SiH_4] (or another key deposition parameter) within which amorphous silicon [a-Si:H], mixed-phase silicon [(a μc)-Si:H], and coalesced single-phase microcrystalline silicon [μc-Si:H] films are fabricated for a given substrate material. Our studies have demonstrated clearly that the i-layer R value for optimum solar cell performance is the maximum that can be sustained while remaining within the amorphous film growth regime. As a result, the phase diagram concept has suggested a two-step (R=40/10) i-layer process for optimized p-i-n a-Si:H solar cells [1], and can also explain the variations in open-circuit voltage with d and R that identify the optimum i-layer for world-record efficiency n-i-p

solar cells [2]. In this paper, we report phase diagrams (versus d and R) for PECVD Si film growth on crystalline silicon wafer and amorphous silicon thin film substrates at different rf power levels and substrate temperatures. In particular, we describe the changes that occur in the phase diagrams from those reported earlier for low rf plasma power (0.08 W/cm^2) and low substrate temperature (T=200°C) [3]. We focus on an increase in the rf power by factor of 10 (leading to an increase in deposition rate from 0.5 to 4 Å/s at R=10), as well as an elevation of the substrate temperature (the latter leading to a shift in the phase boundary to lower R). Based on these results, approaches for rf PECVD of a-Si:H at higher rates are proposed for optimum i-layer performance in p-i-n and n-i-p solar cells. [1] J. Koh, Y. Lee, H. Fujiwara, C.R. Wronski, and R.W. Collins, Appl. Phys. Lett. 73, 1526 (1998). [2] J. Yang, A. Banerjee, K. Lord, and S. Guha, 28th IEEE Photovoltaic Specialists Conference, Sept. 15-22, 2000, Anchorage, Alaska. [3] J. Koh, A.S. Ferlauto, P.I. Rovira, C.R. Wronski, and R.W. Collins, Appl. Phys. Lett. 75, 2286 (1999).

A5.5
VHF LARGE AREA PLASMA PROCESSING AT MOVED SUBSTRATS. J. Kuske, U. Stephan, R. Terasa[a], H. Brechtel[a], A. Kottwitz[a], Forschungs- und Applikationslabor Plasmatechnik GmbH Dresden, F.R. GERMANY; [a]Semiconductor and Microsystems Technology Laboratory, Dresden University of Technology, F.R. GERMANY.

The production of amorphous and microcrystalline silicon, e.g. for solar cells, requires large area, high-deposition rate plasma reactors. Increasing the frequency from the conventional 13.56MHz up to VHF has demonstrated higher deposition and etch rates and lower particle generation, a reduced ion bombardement and lower breakdown, process and bias voltages. But otherwise the use of VHF for large area systems leads to some problems. The non-uniformity of deposition rate increases due to the generation of standing waves and evanescent waveguide modes at the electrode surface. One possibility to process large area substrates is the use of a one-dimensional extended, homogeneous plasma source in combination with a moved substrate. The requirements, which result from the deposition process and from the r.f.-engineering, corresponds with the developed plasma source, using deposition frequencies in the VHF-range (50 ... 100 MHz), almost perfectly. Using a source of 550mm length, experiments were done with 81.36MHz at RF power densities of 70...180mW/cm^2, silane/hydrogen pressures of 5...30Pa, and flow rates of 10...300sccm. The measured potential distribution error was ±2%. Optical emission spectroscopy delivers discharge intensity errors of ±3...10%. Deposition rates up to 20μm/h for amorphous silicon (60Å/s) and film thickness inhomogenities less than ±5% were achieved (with a area of the moved substrate of 30cm x 30cm). Experimental results of the film properties will be discussed in dependence on the rate of the substrate movement and the deposition parameters. Deposition limitations will be discussed among other things on the basis of complementary experiments, carried out on a small scale equipment (with excitation frequencies up to 165 MHz), and simulations of the growth process. Especially the deposition of microcrystalline silicon considering the etching of weak bonded silicon (in dependence on the substrate temperature) was investigated.

A5.6
CLUSTER-LESS PLASMA CVD REACTOR AND ITS APPLICATION TO a-Si:H FILM DEPOSITION. Masaharu Shiratani, Takeshi Sonoda, Kazunori Koga, Yukio Watanabe, Kyushu University, JAPAN.

In order to deposite high quality a-Si:H films at a high rate using SiH_4 RF discharges, we have developed a cluster-less plasma CVD reactor since cluster-size particles are believed to degrade film quality. The reactor was designed taking into account notable effects of pulse modulation of discharges, heating of the GND electrode, gas flow as well as H_2 dilution on suppression of cluster growth, all of which were revealed by using two novel in-situ methods for determination of size and density of cluster-size particles below 10 nm in size.[1,2] By using the cluster suppression effects, a-Si:H films of microstructure parameter R of 0.01 can be deposited at a rate of 0.2 nm/s, while the best a-Si:H films deposited without using such effects have R=0.1. We also study nucleation and subsequent growth of clusters by using the newly developed double-pulse-discharge method which realizes in-situ measurement of their size and density in a size range 0.5-4 nm.[3] Clusters begin to be composed of two size groups at about 10 ms after the discharge initiation; small clusters have an almost constant average size of 0.5 nm through the discharge period, while large clusters grow in a monodisperse way. A critical cluster size for the nucleation is found to be Si_nH_x (n is about 4).
[1]Y. Matsuoka, *et al.*, Jpn. J Appl. Phys., **38** (1999) 4556.
[2]M. Shiratani, *et al.*, Jpn. J Appl. Phys., **39** (2000) 287.
[3]K. Koga, *et al.*, Appl. Phys. Lett., **77** (2000) 196.

A5.7
ION-ASSISTED SPUTTER DEPOSITION OF MICRO-CRYSTALLINE SILICON FILMS WITH PULSED-DC PLASMA EXCITATION. P. Reinig, F. Fenske, B. Selle, W. Fuhs, Hahn-Meitner-Institut Berlin, Dep. Silicon-Photovoltaics, Berlin, GERMANY.

We have applied a novel Ion-Assisted Sputter Deposition (IASD) method to deposit microcrystalline silicon (μc-Si) thin films with high deposition rates. An unbalanced magnetron sputter source together with a pulsed-DC plasma excitation was used for realizing high ion fluxes to the growing film. We studied the influence of pulsed plasma excitation on the microstructure of the films using pulse frequencies in the range of 50-250 kHz. The structural properties of the films were determined both by Raman spectroscopy and a combination of Rutherford-backscattering (RBS) and FTIR measurements. For the characterization of the film crystallinity we propose a new method which compares the optical thickness n•d determined by FTIR measurements with the atomic area density N•d as given by RBS analysis. We found that the ratio R_C = n•d / N•d correlates well with Raman spectroscopical results obtained from a series of amorphous and μc-Si films deposited with IASD under a variety of conditions. By taking the void content of the films into account the ratio R_C can be used as a figure of merit for the film crystallinity. Films deposited in the temperature range from 25-400°C with pulsed-DC plasma excitation exhibit a higher degree of crystallinity in comparison to films obtained with conventional DC-sputtering. The void content of the films is less than 10%. This was concluded by comparing RBS area densities N•d and the film thickness measured by a profilometer. In pure Ar atmosphere nominally undoped μc-Si films can be grown with our IASD technique at temperatures T > 400°C with grain sizes up to 300 nm (SEM results). Addition of hydrogen reduces the growth temperature of microcrystalline Si films. First experiments with pulsed-DC H_2 /Ar plasma excitation resulted in μc-Si:H growth at temperatures as low as T = 210°C.

A5.8
THE PROPERTIES OF LOW HYDROGEN SILICON THIN FILMS DEPOSITED BY MESH-TYPE PECVD. Se-won Ryu, Do-hyun Kwon, Sung-gye Park, Seung-eui Nam, Hyoung-june Kim, Hongik Univ, Dept of Metallurgical Engineering & Materials Science, Seoul, KOREA.

Polycrystalline silicon thin film transistors have been studied extensively because of their applications for the high resolution active matrix liquid crystal displays (AMLCDs) on large area substrates. However, AMLCD can only be made using a low temperature process (<400°C) to avoid damage to the glass substrate. The need of low temperature substrates in the display applications makes it difficult to obtain high electrical characteristics. To overcome this problem, one of the most promising method to fabricate high performance poly-Si TFTs on a glass substrate is the excimer laser crystallization (ELC) technique. However, a-Si deposited by conventional plasma enhanced chemical vapor deposition (PECVD) contents 10∼50at% hydrogen. Therefore, ELC process results in hydrogen explosive eruption. In this study, triode PECVD system was suggested to minimize the hydrogen concentration. The main structural difference between the triode system and a conventional system is that a third electrode, a mesh, was attached to the substrate holding electrode. We investigated several conditions to compare with conventional PECVD. It was found that the hydrogen concentration decreased to 3at% and deposition rate also decreased to 42Å/min at 300°C. The main effect of mesh was to minimize the substrate damage by ion bombardment and to enhance the surface reaction to induce hydrogen desorption. It was also found that hydrogen concentration decreased to 2at% but deposition rate increased to 105Å/min as increasing applied bias. Applied DC bias enhanced sputtering process. Intense ion bombardment causes the weakly bonded hydrogen or hydrogen-containing species to leave the growing film and increased adatom mobility. Furthermore, poly-Si TFT fabricated showed good electrical properties comparatively. It is considered to contribute on promoting the ELC technology and improving of poly-Si TFTs' characteristics.

A5.9
BORON SURFACE SEGREGATION AND FILM GROWTH KINETICS DURING ULTRA-HIGH DOPED $Si_{1-x}Ge_x$(001):B GAS-SOURCE MOLECULAR BEAM EPITAXY. H. Kim, G. Glass, P. Desjardins, Y.L. Foo, J.A.N.T. Soares, J.E. Greene, Materials Science Department and the Frederick Seitz Materials Research Laboratory, University of Illinois, Urbana, IL.

B-doped $Si_{1-x}Ge_x$(001) layers, with concentrations C$-B$ between 2x10^{16} and 2x10^{21} cm^{-3}, were grown on Si(001)2x1 at T_s = 500-700°C by gas-source molecular beam epitaxy (GS-MBE) from Si_2H_6, Ge_2H_6, and B_2H_6. Secondary-ion mass spectrometry and Auger electron spectroscopy measurements demonstrate that B doping has no effect on the Ge incorporation probability. Steady-state

B and Ge surface coverages (θ_B and θ_{Ge}) were determined as a function of C_B using *in − situ* isotopically-tagged temperature programmed desorption. Results for $Si_{0.82}Ge_{0.18}$ layers grown at T_s = 500°C show that θ_{Ge} remains constant at 0.63 ML while the bulk B concentration increases linearly up to 2.4×10^{21} cm^{-3}, corresponding to saturation B coverage of 0.5 ML, with the incident precursor flux ratio $\xi = J_{B_2H_6}/(J_{Si_2H_6}\ J_{Ge_2H_6})$. B is incorporated into substitutional electrically-active sites over this entire concentration range. Room-temperature hole mobilities are equal to the best reported $Si_{0.82}Ge_{0.18}$:B bulk values. At higher B concentrations, C_B increases faster than x and there is a large decrease in the activated fraction of incorporated B. Electrically inactive B is incorporated substitutionally as sp^2 bonded B dimmers on single lattice sites. The B segregation enthalpy during $Si_{0.82}Ge_{0.18}(001)$ growth is -0.42 eV, compared to -0.53 and -0.64 eV during Si(001):B and Ge(001):B GS-MBE, respectively. Measured segregation ratios $r_B = \theta_B/x_B$, where x_B is the bulk B fraction, range from 15 to 500 with a temperature dependence which is consistent with equilibrium segregation. Film deposition rates $R_{SiGe}(C_B)$ decrease by up to a factor of two with increasing $C_B \geq 5\times10^{19}$ cm^{-3}. This is due primarily to a B-segregation-induced decrease in the dangling-bond density. The above results were used to develop a robust model for predicting the steady-state H coverage θ_H, θ_B, θ_{Ge}, and R_{SiGe} as a function of ξ and T_s.

A5.10

LOW TEMPERATURE Si_2H_6-H_2 SOURCED SELECTIVE SILICON EPITAXY WITHOUT CHLOLINE BY LPCVD. Yong-Hoon Son, Sung-Gye Park, Seoung-eui Nam, Hyoung-june Kim, HongIK Univ, Dept of Metallurgical Eng. & Materials Sci., Seoul, KOREA.

We propose the use of Si_2H_6/H_2 chemistry for selective silicon epitaxy by low-pressure chemical vapor deposition (LPCVD) in the temperature range 600∼710°C under an ultraclean environment. As a result of ultraclean processing, an incubation period of Si deposition only on SiO_2 was found, and low temperature epitaxy selective deposition on Si was achieved without addition of HCl. P-type (100) Si wafer patterned with 1000Å SiO_2 islands was used as substrate and the Si films were deposited under low pressure using Si_2H_6-H_2 gas mixture where the total gas flow rate and deposition pressure were 16.6sccm and 3.5mtorr, respectively. In this condition, we selectively obtained high-quality epitaxial Si layer of the 350∼1050Å thickness. In order to extend the incubation period, we kept high pressure H_2 environment without Si_2H_6 gas for few minutes after first incubation period and then we confirmed the existence of second incubation period.

A5.11

LOW-TEMPERATURE (630 deg. C) EPITAXY OF SILICON ON SEEDED GLASS BY ION-ASSISTED DEPOSITION. Armin G. Aberle, Nils-Peter Harder, Univ. of New South Wales, Centre for Photovoltaic Engineering, Sydney, AUSTRALIA; Stefan Oelting, ANTEC GmbH, Kelkheim, GERMANY.

The formation of device-grade polycrystalline Si (poly-Si) films on low-cost substrates at low temperature using simple and fast processes is of enormous interest for solar cells and large-area electronics. In this paper, we report the successful realisation of thick (5 microns), large-grained (5 microns), uniform poly-Si films on glass at a substrate temperature below 650 deg. C. This significant technological advance has been achieved by using ion-assisted deposition of silicon at 630 deg. C for thickening a thin poly-Si seeding layer made on the glass at 460 deg. C by aluminium-induced crystallisation (AIC) of amorphous silicon. Transmission electron micrographs reveal an epitaxial relation between about 50% of the grains of the IAD layer and the AIC seeding layer. Thus, the grain size of the IAD-grown poly-Si film is determined by the grain size of the underlying poly-Si seeding layer, a clear experimental proof of the "seeding layer concept" on glass. Poly-Si films grown by IAD on glass at a reduced temperature of 500 deg. C also contain grains that clearly reveal an epitaxial relation with the underlying grain in the seeding layer. These grains have a columnar structure and run across the entire film thickness. Our work shows that the combination of AIC and IAD is highly promising for the low-temperature fabrication of high-quality polycrystalline silicon films on glass.

SESSION A6: POSTER SESSION CRYSTALLIZATION

Chair: Norbert H. Nickel
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A6.1

A NEW AMORPHOUS Si CRYSTALLIZATION PROCESS FOR HIGH PERFORMANCE LOW TEMPERATURE POLY-Si TFT'S. Sang-Jin Park, Ah-Lon Song, Sung-Gye Park, Seung-Eui Nam, Hyoung-Jun Kim, HongIk University, Seoul, KOREA.

In recent years many studies on poly-Si TFT's have focused either on reducing the process time or on lowering the process temperature. We have crystallized using the transformation of amorphous silicon (a-Si) to a polycrystalline-Si (Poly-Si) phase by alternating magnetic flux. The crystallization rate is accelerated with increasing alternating magnetic flux. The annealing temperature was varied from 430°C upto 500°C and the annealing time was 1 hour. The annealed films were characterized using X-ray diffraction (XRD), Four Point Probe, Maxwell 2D simulator, Raman Spectroscopy, Atomic Force Microscopy (AFM), and Field Emission Scanning Electron Microscopy (FE-SEM). Both alternating magnetic flux crystallization and conventional Solid Phase Crystallization (SPC) were compared to enhance the crystallization of a-Si. We have found that the low temperature crystallization method at 430°C by alternating magnetic flux aided. Besides, this annealing has very short crystallization time, but then the conventional SPC specimen is crystallized after 10hour at 600°C. We also have been applied the Metal Induced Crystallization (MIC) and the Metal Induced Lateral Crystallization (MILC) by alternating magnetic flux aided. In this work, Ni-MIC under alternating magnetic flux was carried out low temperature at 300°C within 30 minute. MILC (Ni 30Å) velocity as the strength of alternating magnetic flux increased to 73μm/h. MILC (Ni 30Å) distance in conventional furnace was 8μm/7h.

A6.2

FORMATION OF POLYCRYSTALLINE SILICON FILMS USING ELECTRICAL-CURRENT-INDUCED JOULE HEATING. Nobuuyuki Andoh, Hiroyuki Takahashi and Toshiyuki Sameshima, Tokyo University of Agriculture and Technology, Faculty of Technology, Tokyo, JAPAN.

We report melt-regrowth properties of silicon films caused by electrical-current-induced joule heating. When silicon films formed on glass substrate were melted by irradiation with 5 ns-355 nm-pulsed laser during voltage application using metal electrodes, joule heating with a high intensity of 1.5×10^6 W/cm^2 caused by high electrical current occurred. The joule heating continued the melting of silicon to 75 μs at room temperature when the total electrical energy density 36 J/cm^2 was applied to the silicon films. We demonstrate crystalline grain growth in the lateral direction by spatial distribution of joule-heating intensity using tapered-shaped electrodes. High electrical current flowed in the narrow gap region and it caused high intensity of joule heating, while low current flowing in the wide gap region leaded to low intensity of joule heating. Temperature distribution is generated in the lateral direction. We present grain growth larger than 15 μm with the preferential crystalline orientation (110). We also report crystalline properties of the silicon films. The numerical analysis of the electrical conductivity with statistical thermodynamical conditions resulted in a low density of defect states of 3.5×10^{16} cm^{-3} localized at grain boundaries. The low defect density realized a low potential barrier height at 0.09 eV for 7×10^{17} cm^{-3} phosphorus doping case. Decay of photo-induced current caused by pulsed laser is also discussed in order to investigate photoresponse characteristics.

A6.3

ELECTRICAL PROPERTIES OF SOLID PHASE CRYSTALLIZED SILICON FILMS. Tadashi Watanabe, Hajime Watakabe and Toshiyuki Sameshima, Tokyo University of Agriculture and Technology, Faculty of Technology, Tokyo, JAPAN.

We report electrical properties of solid phase crystallized (SPC) silicon films analyzed with free carrier optical absorption. 50-nm thick amorphous silicon films formed on quartz substrates were crystallized by heat treatment at 600°C for 48 hr. Phosphorus and boron atoms with a density of 2×10^{20} cm^{-3} were then doped by ion implantation. Samples were annealed at 600°C for 24 hr for dopant activation. Analysis of the free carrier optical absorption in the infrared region resulted in the average carrier mobility of 40 cm^2/Vs for phosphorus doped films and 20 cm^2/Vs for boron doped films. These results mean that the SPC films have crystalline grains with excellent properties like single crystalline silicon because the free carrier optical absorption occurs very locally inside crystalline grains via excitation induced by the electrical field of incident photons followed by energy relaxation in the crystalline grains. On the other hand, the carrier density was estimated to be 3×10^{19} cm^{-3} for phosphorus doped films and 4×10^{19} cm^{-3} for boron doped films. Those values were much lower than that of the initial dopant concentration. Regions with inactivated dopant atoms seriously remained. The doped SPC films were subsequently melted and recrystallized by irradiation with 30-ns XeCl excimer laser at 500 mJ/cm^2. The electron carrier mobility did not change after laser recrystallization for phosphorus doped films, while the hole mobility slightly increased to 28 cm^2/Vs. On the other

hand, the carrier density was increased to 6×10^{19} cm^{-3} for phosphorus and boron doped films by the laser recrystallization. The dopant atoms were incorporated to substitutional lattice sites. The crystalline domains with a high carrier mobility was increased by the laser recrystallization. We will also report the carrier mobility and the carrier density obtained by Hall effect current measurements in order to understand electronic structure such as defect states of SPC films.

A6.4

SUPER POLY-Si AND TRANSISTOR FORMED BY NICKEL-INDUCED-LATERAL CRYSTALLIZATION. C.F. Cheng, M.C. Poon, T.C. Leung, G.K. Zhu, Hong Kong University of Science and Technology, Dept. of Electrical and Electronic Engineering, Sai Kung, HONG KONG.

Nickel-induced-lateral-crystallization (NILC) of amorphous Si (a-Si) has attracted much attention. The poly-silicon (poly-Si) films formed have very large grains (~10 to 100 mm) and the fabricated thin-film-transistors (TFT) are highly comparable (>40%) to silicon-on-insulator (SOI) TFTs. Such results have potentials in many applications such as low cost, large area and even low temperature novel devices and circuits. This work presents the new results in NILC poly-Si and TFT obtained from the optimization of nickel and a-Si parameters. 1000-6000Å of LPCVD a-Si was formed on 7000Å thermal oxide, followed by 4000Å of LTO. LTO was patterned and 50Å of Ni film with different length and width was deposited. NILC of a-Si film was then performed at 550-650°C. Some samples were further annealed at 800°C to enlarge the grains. Results show that the quality of poly-Si and TFT formed is comparable to SOI. The quality improves (by over 20%) when the poly-Si is formed adjacent to Ni film with short length. Moreover, the quality further improves (by over 30%) when the poly-Si is formed near the bottom of thick a-Si. The other poly-Si and TFT properties such as the control of grain location, size, uniformity, mobility, on-off characteristics, and quality due to different Ni and a-Si parameters will be further compared and discussed.

A6.5

A NOVEL BACK-REFLECTING UV-ASSISTED METAL INDUCED CRYSTALLIZATION OF SILICON ON GLASS. Leila Rezaee, S. Shamsoddin Mohajerzadeh, A. Khakifirooz, S. Haji and E. Soleimani, University of Tehran, Dept of Electrical and Computer Engineering, Thin-Films Lab., Tehran, IRAN.

We report a novel back-reflecting UV-assisted MIC technique to grow silicon on ordinary glass at temperatures below 400°C. The fabrication process starts by depositing a back-reflector layer of 2000Å Cr on ordinary glass followed by sputtering of 1000Å SiN and 1500Å Si. The crystallization seed is a 30Å thick layer of Ni, being deposited using E-beam evaporation. Samples with different thickness of Cr and Si have been prepared to study the effect of strain on the crystallinity. For the samples without back-reflector only the chromium deposition step was skipped. The annealing procedure is accomplished by heating the sample on a hot plate at temperatures between 350 and 400°C for a period of 3 to 8 hours. During this step, samples are exposed to UV light with radiation intensity of 10-25 mW/cm^2 measured at a wavelength of 360nm. SEM and XRD analyses were used to study the morphology and crystallinity of the samples. SEM micrographs show the presence of surface features with the size of 0.2 μm. XRD spectroscopy clearly indicates the crystallinity of the samples with back-reflector, annealed at 400°C. The $< 110 >$ orientation of the sample with back-reflector is about 5 times higher than $< 110 >$ peak of the sample without back-reflector. Also for the sample with back-reflector the $< 110 >$ peak is about 2 times higher than its $< 111 >$ peak. In the sample prepared without back-reflector the $< 111 >$ orientation is not discernible. Based on the results obtained , we speculate that the energetic UV photons impart energy to the crystallizing Si, reducing the annealing temperature. We believe the presence of the back-reflector leads to trapping of UV light in the optical cavity formed in this structure, significantly enhancing the crystallization. Fabrication of low temperature poly-Si solar cells and TFTs on glass substrates are being pursued using this technique.

A6.6

A NEW FIELD AIDED GERMANIUM INDUCED LATERAL CRYSTALLIZATION OF SILICON. Kianoush Naeli, S. Shamsoddin Mohajerzadeh, A. Khakifirooz, S. Haji and E. Asl-Soleimani, Univ of Tehran, Dept of Electrical and Computer Engineering, Thin-Films Lab., Tehran, IRAN.

Metal induced lateral crystallization is a promising technique in fabricating large area Si-based thin film electronic devices due to its lower processing temperature. Addition of an external electric field could enhance the crystallization, leading to lower annealing temperatures. The major drawback of this technique, however, is the penetration of seed metal into the crystallized region, adversely affecting the electrical performance of electronic devices. To remove this metal contamination, thermal lateral crystallization with a semiconductor seed like Ge, in temperatures about 600°C, has been reported . In this paper we report a new field aided Ge induced lateral crystallization in which crystallization occurs at a low temperature of 480°C enabling one to use inexpensive glass substrates. In this technique, 1500Å silicon layer was deposited on 7059 corning glass with E-beam evaporation followed by 2000Å SiO_2 deposition. Ge was deposited on Si through 5mm apart parallel windows in the oxide. Since lateral crystallization occurs in the space between Ge pads and to perform XRD analysis, a large distance between pads had to be chosen. By applying an electric field of 1000V/cm onto Ge pads for 4 hours and at a temperature of 480°C, crystallization progresses from cathode to anode. This experiment was repeated at 500-600°C annealing temperatures. After removing the oxide, the region between pads was cut out. XRD spectroscopy on this region shows Si peaks in $< 111 >$ and $< 110 >$ orientations. Also peaks corresponding to Ge and SiGe crystals are observed which could be due to the remaining Ge, not completely etched, or the penetration of Ge into crystallized Si. SEM micrographs show that the size of poly-Si grains reduces gradually from cathode towards anode. Also optical microscopy evidences some streaks between two electrodes. Further study of the samples with TEM and RBS is underway.

A6.7

DIRECTIONAL FIELD AIDED LATERAL CRYSTALLIZATION OF AMORPHOUS SILICON THIN FILMS. M.A.T. Izmajlowicz, A.J. Flewitt, W.I. Milne, Engineering Dept, Cambridge University, UNITED KINGDOM.

For application to active matrix liquid crystal displays (AMLCDs), a low temperature (< 600°C) process for the production of polycrystalline silicon is required to permit the use of inexpensive glass substrates. Current low temperature processes include excimar laser annealing (ELA) and solid phase crystallization (SPC). It is known that by adding small amounts of metals such as nickel the solid phase crystallization temperature can be reduced. The rate of this solid phase metal induced crystallization is increased in the presence of an electric field, and most of the work on field aided crystallisation (FAC) has reported crystal growth that is independent of the direction of the electric field. In this work directional crystallization of amorphous silicon thin films was observed during heat treatment in the presence of an electric field. A thin nickel layer was deposited on top of the amorphous silicon and patterned lithographically. As well as directly beneath the nickel patterns, crystal growth occurred around the edges of the patterns. Without the presence of an electric field this lateral crystallization proceeded uniformly in all directions, however, when an electric field of 500 V/cm was applied the lateral crystallization proceeded towards the negative terminal only. This is the first time that such an effect has been observed. This crystallization method will be used in the manufacture of low temperature polysilicon thin film transistors.

A6.8

THE EFFECTS OF Cu ON FIELD AIDED LATERAL CRYSTALLIZATION (FALC) OF AMORPHOUS SILICON (a-Si) FILMS. Jae-Bok Lee, Chul-Ho Kim, Se-Youl Kwon, Duck-Kyun Choi, Hanyang Univ, Dept of Ceramic Engineering, Seoul, KOREA.

A novel concept of field aided lateral crystallization (FALC) and the effects of Cu on FALC of amorphous silicon (a-Si) were investigated. Cu was found to induce the lateral crystallization toward a metal-free region as well as the crystallization of a-Si in contact with Cu. In particular, the lateral crystallization caused by Cu layer was noticeably accelerated at the edge near the negative electrode side in every pattern with an aid of electric field, while the lateral crystallization was retarded at the positive electrode side. These phenomena will be interpreted in terms of the dominant diffusing species in the reaction between Si and metal. The FALC velocity increased with the applied field intensity and the annealing temperature, but it decreased with the size of test pattern. The crystallization of a-Si was achieved at a temperature as low as 375° when the annealing time or the applied field intensity was increased. Therefore, we could demonstrate the possibility of low temperature (<500°) polycrystalline (poly-Si) formation using FALC technology.

A6.9

CW Ar-ION LASER CRYSTALLIZATION OF a-Si:H THIN FILMS. A. Sunda-Meya[a], D. Gracin[b], B. Vlahovic[a,e], J.M. Dutta[a], R.J. Nemanich[c] and V. Borjanovic[d]. [a]Department of Physics, North Carolina Central University, Durham, NC. [b]Materials Science Division, Rudjer Boskovic Institute, Zagreb, CROATIA. [c]Department of Physics, North Carolina State University, Raleigh, NC. [d]Electrical Engineering Faculty, University of Zagreb, Zagreb, CROATIA. [e]Jefferson Laboratory, Newport News, VA.

Thin a-Si:H films, thickness of 1 μm, with different hydrogen concentrations, prepared by hot wire deposition and magnetron

sputtering, were crystallized by a cw Ar ion laser of 514.5 nm wavelength, with power density between 0.8×10^6 W/cm^2 and 1.2×10^6 W/cm^2. The process was monitored in situ by Raman spectroscopy (ISA U-1000 spectrometer supplied by water-cooled photomultiplier). The transformation from the amorphous to crystalline phase was detected by the change in the peak position, from 480 cm^{-1} to 505-516 cm^{-1} and the change in the peak shape. The laser irradiation increases the initial crystalline peak intensity, peak frequency shifts towards higher wavenumbers and FWHM decreases. After some exposure time, the process saturates and there are no further changes. The grain size was estimated from Raman spectra, by using a semi-empirical formula related to the peak position while the average temperature of the irradiated volume was determined using the ratio of the Stokes and Anti-stokes intensities. Analyzing the area under the crystalline peak as a function of time, the activation energy of crystallization process was estimated. The dependency of crystals size and activation energy on the initial degree of ordering, hydrogen concentration and power density is discussed.

A6.10
ELECTRICAL PROPERTIES AND DEFECT STATES OF LASER CRYSTALLIZED POLYCRYSTALLINE SILICON FILMS.
Nobuyuki Andoh, Tadashi Watanabe and Toshiyuki Sameshima, Tokyo University of Agriculture and Technology, Faculty of Technology, Tokyo, JAPAN.

We report analysis of electrical properties of polycrystalline silicon (poly-Si) films. A two-dimensional numerical analysis program with the finite-element method (FEM) combined with statistical thermodynamical conditions was developed. We considered localized defects states at a deep energy level and tail states localized at grain boundaries. The 50-nm-thick poly-Si films doped with 7×10^{17} cm^{-3} phosphorus were formed by pulsed excimer laser crystallization at 400 mJ/cm^2. The analysis of temperature change in the electrical conductivity resulted in that the poly-Si films had high densities of the deep level state at the mid gap, 9×10^{17} cm^{-3}, and of the tail states, 4×10^{18} cm^{-3}, with a width of 0.4 eV. These high density of defect states localized electron carriers at grain boundaries and made the electrical conductivity very low at $\sim 10^{-5}$ S/cm. The potential barrier height was high at 0.38 eV at grain boundaries. On the other hand, the electrical conductivity was markedly increased by oxygen plasma treatment at 250°C for 40 min as well as heat treatment at 270°C with 1.3×10^6-Pa pressure H_2O vapor for 3 h. The oxygen plasma treatment effectively reduced the density of localized deep level defect states to 2×10^{16} cm^{-3}. The dangling bonds at grain boundaries were probably oxidized well during the oxygen plasma treatment and the defects became electrically inactive. On the other hand, the high pressure H_2O vapor annealing effectively reduced the density of tail states to 3×10^{17} cm^{-3}. The bonding network at grain boundaries were probably relaxed by the heat treatment. The potential barrier height was reduced to less than 0.05 eV by those post heating treatments. We propose the effective post heating condition for defect reduction for polycrystalline silicon films at low temperature.

A6.11
EXCIMER LASER RECRYSTALLIZATION OF SELECTIVELY FLOATING a-Si ACTIVE LAYER FOR LARGE-GRAINED POLY-Si FILM.
Cheon-Hong Kim, Juhn-Suk Yoo, In-Hyuk Song and Min-Koo Han, Seoul Nat'l Univ, School of Electical Engineering, Seoul, KOREA.

Excimer laser recrystallization of amorphous silicon (a-Si) film on glass substrate has attracted a considerable interest. Polycrystalline silicon (poly-Si) thin film transistors (TFTs) employing XeCl laser annealing may exhibit decent electrical properties, but the device characteristics such as mobility and threshold voltage are limited by the grain size. It has been already reported that excimer laser annealing of thin a-Si film on SiO_2 membrane structure enlarged the grain size. However, the membrane structure is not practical for TFT applications because underlying substrate should be etched out and the membrane would not be immune to a mechanical stress. We propose a new excimer laser annealing method in order to enlarge the grain size by employing selectively floating a-Si active layer structure. Although Si melt adherent to the substrate cools off rapidly, the vertical cooling rate in the floating active region is significantly reduced because the floating a-Si and the substrate are separated by air-gap. The considerable lateral temperature gradient is induced so that very large grains may be grown laterally from the edge to the center of floating a-Si region. A thin (50~150nm) Al sacrificial layer was deposited on oxidized Si substrate by electron-gun evaporation. After patterning of Al rectangular layer, a thin (50~150nm) buffer oxide and an 80nm-thick a-Si layer were deposited. The a-Si layer and the buffer oxide were patterned across the sacrificial Al pattern. The sacrificial Al layer under the a-Si active layer was completely removed by Al wet etchant. As a result, the a-Si layer, which has been located on the Al sacrificial pattern, is selectively floating. This bridge structure was irradiated with XeCl excimer laser in a vacuum chamber. The lateral grain size is larger than two microns with the laser energy density of 350mJ/cm^2. The large-grained poly-Si layer recrystallized employing selectively floating a-Si active layer structure can be used as a channel region of the practical TFT device. We will also report the mechanical stability of our structure.

SESSION A7: POSTER SESSION
HOT WIRE CVD
Chair: A. Harvin Mahan
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A7.1
Abstract Withdrawn.

A7.2
HOT WIRE DEPOSITION OF A μc-Si:N ALLOY.
A.C. Dillon, L. Gedvilas, J.T. Thiesen, D.L. Williamson[a], and A. H. Mahan National Renewable Energy Laboratory (NREL), Golden, CO; [a]Physics Dept., Colo. School of Mines, Golden, CO.

We report the first deposition by hot wire chemical vapor deposition (HWCVD) of a μc-Si:N alloy consisting of silicon crystallites embedded in an a-Si:N tissue. Films were deposited employing a tertiary gas system consisting of SiH_4, NH_3 and H_2. The deposition temperature, filament current and NH_3 and H_2 dilutions were systematically varied. X-ray diffraction (XRD) and Raman spectroscopy were used to probe the film structure (crystallite size, crystalline volume fraction) in the μc-Si:N films, and to examine medium range order (MRO) and short range order (SRO) in the fully amorphous samples (the μc-Si:N "tissue"). The nitrogen content in the films was estimated via transmission Fourier transform infrared (FTIR) analyses from the intensity of the Si-N stretch mode located at 850 cm^{-1}. For most of the micro-crystalline films, additional (unusual) absorption features at ~760 and 960 cm^{-1} were observed in the infrared spectra. These features may be associated with Si_3N species present at the grain boundaries of the silicon crystallites. In general as the nitrogen levels in the tissue increased, both the MRO and SRO decreased and micro-crystallinity in the samples was gradually lost. By increasing either the filament current or the film deposition temperature, micro-crystallinity was maintained for higher nitrogen contents. A mechanism for the decrease in film ordering with N incorporation, as well as the optimal conditions for obtaining μc-Si:N films, will be provided. Differences in film properties for films deposited with N_2 will also be presented. The μc-Si:N alloy films constitute a new class of material with unique properties that may make them very attractive to the micro-electronics and thin film electronics industries. They may also be applicable to next generation μc-PV devices.

A7.3
THE EFFECT OF MODERATE HYDROGEN DILUTION ON THE STABILITY AND STRUCTURE OF AMORPHOUS SILICON DEPOSITED BY HOT-WIRE CVD.
Urban Weber and Bernd Schroeder, Univ of Kaiserslautern, Kaiserslautern, GERMANY.

The effect of moderate hydrogen dilution (R = $[H_2]/[SiH_4]$ = 0 to 4) on the properties of a-Si:H is discussed for the Hot-Wire or Thermo-catalytic CVD. Dielectric properties were measured by spectroscopic ellipsometry and are related to the stability and the hydrogen bonding configuration for films deposited with varying hydrogen dilution at different substrate temperatures. The stability was determined by comparing defect densities and Urbach energies obtained by photoconductivity in the constant photocurrent mode (CPM) before and after pulsed-light soaking. At low substrate temperatures (160-200°C), which are relevant for the preparation of pin-type solar cells, moderate hydrogen dilution ($R = 0.33$) improves the quality of the material regarding mass density and oscillator bandwidth as obtained by spectroscopic ellipsometry as well as the stability. At higher substrate temperatures (300°C), stability and hydrogen bonding configurations are generally better, however even moderate hydrogen dilution already deteriorates these properties compared to undiluted material. These results are discussed with respect to the initial growth of the material as monitored by kinetic ellipsometric measurements. The incorporation of the material into pin-type solar cells at low substrate temperatures (160°C) is also discussed and a very good correlation of the ellipsometric results with the solar cell performance is observed. Here also, the optimum hydrogen dilution is found to be $R = 0.33$ for i-layer deposition yielding solar cell initial efficiency of up to 8.8% for a cell entirely fabricated by HWCVD.

A7.4
LARGE RED SHIFT OF PL PEAK ENERGY IN HIGH GROWTH RATE A-Si:H PREPARED BY HOT-WIRE CVD. Daxing Han, Guozhen Yue, Dept of Physics & Astronomy, Univ of North Carolina at Chapel Hill, Chapel Hill, NC; Yueqin Xu and Qi Wang, National Renewable Energy Laboratory, Golden, CO.

Device quality a-Si:H prepared by hot wire (HW) CVD has attracted a great deal of attention because of the high deposition rate and several interesting properties compared to plasma enhanced (PE) CVD materials. More recently, scientists in the National Renewable Energy Laboratory (NREL) have made device-quality a-Si:H films with high growth rate by HW-CVD. The growth rate can be as high as 50 to 150 Å/s compared to ~10 Å/s by standard HW-CVD and 1 Å/s by plasma-enhanced CVD. The preliminary studies of photo-response and defect density indicate that the same quality as the standard device-quality film has been made by the high growth rate. In this work, we report the microstructure and electronic states by measuring mass density, H1 NMR, Raman, and photoluminescence (PL). Comparing the growth rate ~50 Å/s to the $\leq$ 10 Å/s a-Si:H films, although the Raman and optical absorption results showed identical spectra, we observed new features in both PL and NMR. The new PL features are: a) the main peak energy is as low as ~1.1 eV compared to ~1.4 eV at 80 K; and b) the total intensity is more than one order of magnitude higher. Meanwhile, we found a very narrow Lorentzian component in NMR spectrum, i.e. 0.6-1.0 kHz compared to 3-5 kHz of the conventional narrow component, on the top of the conventional Gaussian and Lorentzian components. Possible explanations related to long-range microstructures are suggested. The work is supported by NREL subcontract XAK-8-17619-11 and thin film PV partnership. Yue is partially supported by NSF-Int-9604915. Han is partially supported by CGP Fund, NSF-Int-9802430. Xu and Wang are supported by DOE subcontract DE-AC36-99GO10337.

A7.5
HIGH QUALITY AMORPHOUS SILICON GERMANIUM ALLOY SOLAR CELLS MADE BY HOT WIRE CVD AT 10 Å/s. Qi Wang and Eugene Iwaniczko, National Renewable Energy Laboratory, Golden, CO; Jeffrey Yang, Kenneth Lord and Subhendu Guha, United Solar Systems Corp., Troy, MI.

High quality amorphous silicon germanium (a-SiGe) alloys are obtained using hot wire chemical vapor deposition (HWCVD) from a gas mixture of silane, germane, and hydrogen at a deposition rate of 10 Å/s. Solar cells in a ss/nip/ITO configuration are evaluated in which the n and i layers are deposited by HWCVD at the National Renewable Energy Laboratory, and the microcrystalline p layer by conventional RF PECVD in a separate reactor at United Solar Systems Corp. Hydrogen dilution and step-wise bandgap profiling have been studied and optimized. The intrinsic layer of the best cell has an optical bandgap of ~1.6 eV and incorporates multi-bandgap steps where the narrowest bandgap is near the p-i interface. J-V characteristics are measured under AM1.5 illumination with a $\lambda >$ 530 nm filter. The best initial power output obtained exceeds 4 mW/cm^2, which indicates a good quality mid-gap cell. Double-junction cells are made on textured Ag/ZnO back reflectors. The bottom cell uses the optimized a-SiGe alloy cell with HWCVD n and i layers, and the top cell uses an optimized a-Si alloy cell near the amorphous-to-microcrystalline transition deposited at ~1 Å/s. The best double-junction cell made to date exhibits an initial AM1.5 active-area efficiency of 11.5%. The stability of a-SiGe alloy single-junction and a-Si/a-SiGe alloy double-junction devices will be examined and the results presented.

A7.6
PROPERTIES OF NANOCRYSTALLINE N-TYPE SILICON FILMS PRODUCED BY HOT WIRE PLASMA ASSISTED TECHNIQUE. I. Ferreira, F. Braz Fernandes, P. Vilarinho[a], E. Fortunato and R. Martins, CENIMAT, Departamento de Ciencia dos Materiais da Faculdade de Ciencias e Tecnologia da Universidade Nova de Lisboa and CEMOP/UNINOVA, PORTUGAL. [a]Universidade de Aveiro.

We introduced the plasma assisting the hot wire process to produce amorphous and crystalline silicon thin films. The system that we use has the possibility to produce in the same reactor films by the plasma enhanced chemical vapor deposition, hot wire or both techniques. Thus, it is possible to take the advantage of each technique to obtain silicon base devices. The plasma assisting the hot wire technique has the advantage to produce compact films at high growth rate. In this work, we present the properties on n-type silicon films obtained by hot wire plasma assisted technique at different rf power and gas flow rate. The films were produced at a filament (Ta) temperature of 2000°C and the rf power was varied from 0W to 80W while using rf power of 50W we varied the gas flow rate from 15 to 100sccm. In this flow rate range, the films produced have a growth rate changing from 5Å/s to 250Å/s and electrical conductivity varying from 10^{-2} to 10 $(\Omega cm)^{-1}$. On the other hand, we observed that the electrical conductivity increase from 2 to 6 $(\Omega cm)^{-1}$ as rf power change from 0W to 80W. Nevertheless, the infrared analysis revealed that the films, which have the small post-oxidation effect are those produced at 50W, since the peak located at 1050-1150cm^{-1} have no significant increase when compared to the one of films obtained at 0W. The X-ray diffraction data show the (111) Si diffraction peak and the SEM micrographs reveal a granular surface morphology with grains size less than 60nm.

SESSION A8: POSTER SESSION
SILICON-BASED ALLOYS
Chair: Jeffrey C. Yang
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A8.1
A SYSTEMATICAL STUDY OF THE SiGe ALLOY AND ITS INTRINSIC DEFECTS. P. Venezuela, Universidade Metodista de São Paulo, SB Campo, SP, BRAZIL; G.M. Dalpian, Antonio J.R. da Silva and A. Fazzio Instituto de Física da USP, São Paulo, SP, BRAZIL.

We have done a systematical ab-initio study of the electronic and structural properties of the SiGe alloy. Our focus was the disordered phase of the alloy which is the thermodinamically favorable one at room temperature. In order to generate a truly disordered alloy we use a procedure that is similar to the Special Quasi-Random Structure model [1]. The alloy properties are then determined by an LDA-pseudopotential calculation in a 128-atom cell. We will discuss how composition variation affects the local structure of the alloy. The Si-Si, Si-Ge and Ge-Ge bond-length distributions present interesting behavior due to the competition between topological constraints and chemical preferences as has been recently found experimentally [2]. We have also determined the formation energies and local relaxations of vacancies at different configurations. We will show the relative importance of the first and farther neighbors to the vacancies properties. The formation energy is about 2 eV for the vacancy surrounded by four Ge atoms, and it increases with the number of Si atoms in the near neighborhood. The formation energies of charged vacancies as a function of the electronic chemical potentials will be shown too. Those are relevant for the determination of the effective Mott-Hubbard U parameter. [1] S.-H. Wei *et al*, Phys. Rev. B 42, 9622 (1990). [2] J.C. Aubry *et al*, Phys. Rev. B 59, 12872 (1999).

A8.2
UNIQUE NANOSTRUCTURE, DEFECT DISTRIBUTION AND KINETICS OF DEGRADATION OF a-SiGe:H ALLOYS DEPOSITED UNDER UNEXPLORED REGIME OF PARAMETER SPACE OF RF PECVD. A.R. Middya[a], Swati Ray[a], Sukti Hazra[a], J.K. Rath[a], and J.P. Kleider[b], [a]Energy Research Unit, IACS, Calcutta, INDIA; [b]LGEP, Universites Paris VI et XI, Gif-Sur-Yvette, FRANCE.

Recently a new form of amorphous silicon has been invented in the γ'-regime or close to powder regime of radio-frequency plasma-enhanced chemical vapor deposition (RF PECVD)[1,2] which are reproduced at Ecole Polytechnique in 1996 and these materials are popularly known as "polymorphous silicon" thin films. Here we report on a-SiGe:H alloys deposited under similar regime of deposition parameter space, which also exhibits unusual high photoconductivity ($\sigma_{ph} \approx 1.4 \times 10^{-4}$S/cm, $\mu\tau \approx 10^{-5}$ $cm^2/V.s$) and photosensitivity ($5\text{-}8 \times 10^4$) for materials having 1.5 eV optical gap (E_C-$E_F \approx$ 0.65 -0.70 eV). Raman spectroscopy and X-ray diffraction (XRD) confirm amorphous phase of these materials. However small-angle-X-ray-scattering (SAXS) study shows integrated SAXS intensity ($\propto$ nanovoids) and anisotropy of SAXS (indication of aspect ratio of voids) of these a-SiGe:H alloys are much lower throughout the alloy region when compared with the best a-SiGe:H alloys reported in literature, indicating its unique nanostructure. Defect analysis of same series of samples by Electron Spin Resonance (ESR) reveals a "fine structure" of ESR spectra, i.e. the superposed signal can not be deconvoluted into modified Si- and Ge- dangling bonds as routinely done for conventional alloy samples rather additional resonances are needed to deconvolute the spectra.[3] The analysis of LESR-ESR spectra of intrinsic films (1.58 eV) of γ'-regime and ESR spectra of P- and B-doping of the similar samples indicate large density of e-h in the tail states and delocalization of holes. This delocalization of holes and the evolution of g-value with X_{Ge} indicate a more homogeneous chemical ordering (reduction of Si-Si and Ge-Ge clustering?) in the nanostructure of the a-SiGe:H alloys of γ'-regime , which is consistent with the SAXS observations. Concomitant with their improved nanostructure, density-of-state above E_F, stuided by Modulated Photocurrent experiment (MPC) is found to be one to two orders of magnitude lower than standard a-SiGe:H alloys (X_{Ge}Ge $\leq$0.2). The valence band tail remain below 55 meV even for 1.4 eV alloy films. The kinetics of light-induced degradation (100 mW/cm^2/50°C) of

photo- and dark conductivity of these a-SiGe:H films show two-step degradation and change of defect density does not obey $t^{0.33}$ power law. Besides the deconvoluted ESR spectra shows only Si-db increases upon light soaking while Ge-db remains constant and the total defect density (ESR, PDS, CPM) can not be correlated with change in electronic properties due to light soaking. We could attribute many of light-induced degrdation behavior of these alloy films to it's specific nanostructure and defect distribution and at the same time some of them remain puzzel. We also developed He-diluted a-SiGe:H alloys in the similar zone of deposition parameters which exhibits even superior electronic properties and stability than H-diluted materials indicating key role of nanostructure of alloy films and room for the improvement of electronic properties and stability. We will discuss future directions and potentials of these new type of a-SiGe:H alloys of γ'-regime for their applications in solar cells. 1. A.R. Middya et. al. MRS. Symp. Proc. 467 (1997) p. 615. 2. S. Hazra et. al. Appl. Phys. Letts. 76 (2000) p. 2340. 3. C. Malten et. al. Proc. MRS. Symp. 337 (1995) p. 559.

A8.3
STRESS INDUCED LATERAL CONCENTRATION PROFILES IN SiGe LAYERS GROWN ON Si(001) NON PLANAR SUBSTRATE. Anat Eshed, University of Texas at Arlington, Dept of Physics, Arlington, TX; Klaus Dettmer, Technical University, Institute of Semiconductor Physics and Optics, Braunchweig, GERMANY.

The growth of "self assembled" defect free quantum islands of SiGe/Si has been the subject of increasing investigation due to the potential for future novel applications. Despite extensive studies on surface condition of Ge covered Si(001), there are significant gaps in the understanding of the initial stages of the formation of the islands. Fundamental among those gaps is the lack of measurements and modeling of the composition gradient at the surface and subsurface regions as the coverage of the Ge changes. In this paper we report analysis of the mechanical stress field and concentration profiles of Ge the in SiGe layers grown on a two facet, mesa shaped Si(001) substrate. The Si(001) substrate was patterned using conventional lithography processes to form mesas with two crystal planes: the original (001) and the etched (111) planes. A SiGe layer, containing 70% Si, 50 nm thick strained layer was grown, on top of the substrate using Molecular Beam Epitaxy (MBE). Micro Raman experiments, using a 0.4 micron diameter laser beam, were used to measure the changes in composition across the layer. The layer thickness found at the center of both crystal planes matches well with the expected growth rates. The Ge concentration was found to vary laterally, with lower concentration of Ge found at the vicinity of the edges of the (001) planes relative to the center of those planes. We introduce a diffusion model for the growth process, in which the structural mechanical stress has been taken into account to explain our findings. The calculation using our model matched well with our experimental results. Our model may be a starting point in understanding the complexity of the diffusion processes in "self assembled" islands growth.

A8.4
ELECTRICAL AND OPTICAL PROPERTIES OF HIGH QUALITY LOW BANDGAP AMORPHOUS (Ge, Si) ALLOYS. S.R. Sheng, R. Braunstein, Department of Physics and Astronomy, University of California, Los Angeles, CA; V.L. Dalal, Department of Electrical and Computer Engineering, Iowa State University, Ames, IA.

High quality low bandgap a-(Ge, Si):H alloys across the entire range of Ge concentration (0%-100%) were prepared using low pressure, reactive ECR plasma deposition with high H dilution and ppm B-doping. Incorporating these high quality materials into devices leads to much lower gap a-(Ge, Si) solar cells (down to ~1 eV in a-Ge:H) with acceptable performance. The charge transport and optical properties of the materials as a function of alloy composition have been investigated by employing the microwave photomixing technique and optical absorption spectroscopy. From the measurements of electric field dependence of the drift mobility, we have found strong evidence for the existence of long-range potential fluctuations in a-(Ge, Si):H alloys, and determined the depth and range of the potential fluctuations, and subsequently the charged defect density, as a function of alloy composition. The Urbach energy obtained from the sub-gap absorption data was used to study the disorder in the alloy network structure. It was found that at SiH_4/ (SiH_4 GeH_4) ~30%, the photoresponse begins to decrease rapidly with increasing Si content due to the decreases in the mobility and lifetime, and meanwhile, both the charged defect density and the Urbach energy increase significantly. The latter indicates an increase in the compositional disorder. It is the potential fluctuations whose effect can be also enhanced by incorporating Si to the alloy system that result in the deterioration of the opto-electronic properties of a-(Ge, Si):H alloys, similar to the case of the incorporation of Ge at the Si end. This enhanced effect accompanies with an increase in the depth, and a decrease in the range of potential fluctuations, leading to a decrease in the mobility, and consequently in the photoconductivity. The increased charged scattering centers and compositional disorder upon adding Si or Ge to the alloys observed play an important role in the potential fluctuations.

A8.5
HYDROGEN CONCENTRATION ANALYSIS IN PECVD AND RTCVD SILICON NITRIDE THIN FILMS AND ITS IMPACT TO THE DEVICE PERFORMANCE. C.Y. Wang, E.H. Lim, H. Liu, T.C. Ang, V.Y. Vassiliev, J.L. Sudijono, R&D, Chartered Semiconductor Manufacturing Ltd., SINGAPORE.

Silicon nitride is frequently used as the etch-stop layer (ESL) for borderless contact that is the technique normally employed for sub-quarter IC devices at the PMD level. In our study it is found that this ESL nitride has a large impact on the device performance especially the threshold voltage. From SIMS analysis, it is found that different nitride gives different H concentration in the Gate oxide area. The higher H concentration in the nitride film, the higher H in the Gate Oxide area and the lower the threshold voltage. It is therefore proposed that this H may be has the same impact as B to the threshold voltage. It is also found using Ti silicide instead of Co silicide can help to stop the H from diffusing into Gate Oxide/channel area. Therefore less threshold voltage drift is found for the device employed Ti silicide. Study to control the H concentration in the nitride film is also carried out. In this paper, RBS, HFS and FTIR are studied to analyze the composition change of the Plasma enhanced Chemical Vapor deposition (PECVD), Rapid thermal chemical vapor deposition (RTCVD) silicon nitride films when changing the process parameters. Gas flow ratio, RF power and temperature are found to be the key factors that affect the composition and the H concentration inside the film. It is found that the nearer the SiN composition to stoichiometric Si_3N_4, the lower the H concentration in SiN film because theres no excess silicon or nitrogen to be bonded with H. However, no matter how we tune the gas flow ratio and power the lowest H concentration in the SiN film is limited by the temperature. The higher the process temperature the lower the hydrogen concentration can be obtained in the SiN film and the nearer the composition to stoichiometric Si_3N_4.

A8.6
HIGH-RATE DEPOSITION OF SILICON NITRIDE FILMS FOR PHOTOVOLTAIC APPLICATIONS: PLASMA CHEMISTRY AND FILM PROPERTIES. W.M.M. Kessels, F.J.H. van Assche, D.C. Schram and M.C.M. van de Sanden, Dept of Applied Physics, Center for Plasma Physics and Radiation Technology, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS.

A new technique has been developed for the deposition of silicon nitride (SiN_xH_y) thin films at deposition rates up to ~200 $\AA$/s by injecting SiH_4 into an expanding Ar-N_2-H_2 plasma. This so-called expanding thermal plasma technique is relevant for high-throughput deposition of SiN_xH_y anti-reflection coatings on (multi)-crystalline Si solar cells whereby the SiN_xH_y films can simultaneously lead to a reduction of the surface and bulk recombination velocity. Silicon nitride films with different Si/N ratios and hydrogen concentrations have been deposited on different types of multi- and mono-crystalline Si solar cells and it is shown that the optical properties can be fully tuned to obtain optimized anti-reflection working. Bulk passivation of multi-crystalline Si cells has been suggested by an enhanced red response of the coated cells, although preliminary results on surface passivation have not yet revealed sufficient reduction of the surface recombination velocity on mono-crystalline Si cells. The plasma and gas phase chemistry have been studied by several advanced diagnostics such as ion and threshold ionization mass spectrometry and cavity ring down spectroscopy revealing that optimum quality material is obtained for neutral dominated plasma chemistry. Direct radical measurements in the depositing plasma reveal a dominant creation of SiH_3 radicals by H from the plasma source suggesting the creation of a Si top layer, which is subsequently nitrated by N radicals from the plasma source. Real-time and in situ attenuated total reflection infrared spectroscopy studies are performed to extend the insight into the deposition mechanism of SiN_xH_y films.

A8.7
THERMAL ANNEALING STUDY OF VARIABLE BAND-GAP a-SiN:H ALLOY FILMS. Emilio Faro, N. Banerji, J. Serra, S. Chiussi, B. León, Dpto. Física Aplicada, Universidad de Vigo, SPAIN.

A study of the effect of thermal annealing on the bond structure, optical properties, morphology and composition of variable band gap a-$Si_{1-x}N_x$:H alloy films deposited by ArF LCVD has been studied. These films were generated through two different photochemical pathways resulting from the use of either SiH_4/NH_3 or Si_2H_6/NH_3 as precursor gases. Thermal annealing study of these films which span a wide compositional ($0.11 < x < 0.59$) and band-gap (1.9–5.2eV) range has led to the analysis of the stability of different bond configurations.

We report here hydrogen bond stability and rearrangement of the near-neighbour environment of SiN bonds analysed through FTIR, refractive index and band-gap variations measured by ellipsometry and UV spectroscopy, compositional variation determined through EDS and surface morphological changes observed through AFM. Results indicate that in the SiH_4/NH_3 deposited nitrogen-rich SiN films, SiH bonds are less thermally stable than SiH_2. and in their deconvoluted SiN band, a new peak at 1020 cm^{-1} evolves with temperature. Also, while the total bonded hydrogen decreases, the extent of SiN bond increases through a reaction mechanism involving: SiH NH $\rightarrow$ SiN H_2. In the Si_2H_6/NH_3 deposited silicon-rich film, whose initial spectra shows Si–H_n stretching and Si–H wagging bands, a rapid loss of SiH bonds occurs at $T \leq 650°$C and an SiN peak at 760 cm^{-1} attributed to isolated Si–N bonds is observed. The study of the correlation of the band-gap variation, film structure and composition with the annealing temperature has thrown useful insight on the evolution of the two film types with temperature. Based on the bond configurational interpretations of the Random bonding model proposed by Bustarret, we discuss the differences in the film modifications in the two film types.

A8.8
Ge ISLAND EVOLUTION DURING GROWTH, IN-SITU ANNEAL AND Si CAPPING IN AN INDUSTRIAL CVD REACTOR.
Roger Loo, Philippe Meunier-Beillard, Danielle Vanhaeren, Hugo Bender, Matty Caymax, Wilfried Vandervorst, IMEC, Leuven, BELGIUM; Didier Dentel, Michael Goryll, Lili Vescan, Research Centre Jülich, ISI, Jülich, GERMANY.

One possible solution to improve the radiative light emission in Si based materials is three-dimensional Stranski-Krastanov growth. We will discuss the growth kinetics as observed for Ge growth in a standard production oriented Chemical Vapor Deposition system. The island morphology and density can be controlled by varying the growth conditions or by applying a thermal budget after the island growth. Island densities up to $2.3 \times 10^{10} cm^{-2}$ have been obtained for depositions at 650°C. Increase of the deposition time leads to a change over from monomodal to bimodal island distribution. This appears on a critical island diameter, which decreases with decreasing temperature. Applying a thermal budget after the island growth initiates Ge surface diffusion and Si diffusion from the substrate through the islands. The results are an enhancement of the island diameter and height, but a reduced density. Furthermore, depending on the island distribution after Ge deposition, a transition from pyramid to dome or visa versa is observed during the in-situ anneal. A Si cap layer is needed for photoluminescence measurements as well as for some device structures. However, Si capping at 700°C, leads to a nearly total dissolution of small islands and a truncation of larger dome-shaped islands. This can be prevented by reducing the deposition temperature and by changing the Si gas source. Clear island luminescence is obtained in the spectral range from 1.35μm (920meV) to 1.50μm (828meV). At 20K, we found up to 70 times higher values for the integrated No-Phonon and the transversal-optical (TO) luminescence from the islands, compared to the integrated intensity from the Si TO-peak. Nevertheless, the PL intensity can be further enhanced by a thermal treatment in H_2 plasma. Clear island luminescence up to 200K has been observed after such thermal treatment, which shows the potential of this material system for optoelectronic device applications.

SESSION A9: POSTER SESSION STRUCTURAL PROPERTIES OF HETEROGENEOUS SILICON FILMS

Chair: Richard S. Crandall
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A9.1
THIN-FILM PROTON NMR TECHNIQUE AND ANISOTROPIC MICROSTRUCTURE IN a-Si:H.
Jonathan Baugh, Daxing Han, Alfred Kleinhammes, Yue Wu, Dept of Physics and Astronomy, Univ of North Carolina, NC.

Proton nuclear magnetic resonance (NMR) performed on a single thin-film of a-Si:H on quartz substrate eliminates the thin-film susceptibility broadening present in powdered samples that are typically studied. With this enhanced resolution, we have detected new narrow spectral features in some device-quality HWCVD and H-diluted PECVD a-Si:H films that are not present in conventional PECVD films. The orientation-dependent spectral shifts of these features differ from the intrinsic shift due to the bulk magnetic susceptibility of the thin-film. This indicates that such features are associated with microstructural anisotropies. Use of NMR techniques to further clarify the nature of such microstructures will be discussed.

A9.2
MICROSTRUCTURE CHARACTERIZATION OF HYDROGENATED AMORPHOUS SILICON FILMS BY RARE GAS EFFUSION STUDIES.
Wolfhard Beyer, Institut für Photovoltaik, Forschungszentrum Jülich GmbH, Jülich, GERMANY.

Previously it was demonstrated that effusion of implanted neon and argon is a useful technique for structural characterization of a-Si:C and a-Si:O alloys [1,2]. Since rare gas atoms do not react with silicon, their effusion behavior can give information on the microstructure of the material, in particular on presence and dimensions of network openings or interconnected void channels. Here, we report on rare gas effusion from a-Si:H films, implanted with Ne or He. For undoped and boron-doped (1%B) a-Si:H samples of various substrate temperatures T_S ($50<T_S<550°$C) Ne is found to effuse at rather high temperatures only, i.e. at or above the crystallization temperature T_C. In contrast, He effuses in one or two effusion stages predominantly at temperatures below T_C. The lower temperature effusion peak shifts with rising substrate temperature gradually from near 200°C to near 500°C. The second effusion stage is not observed for samples of highest and lowest hydrogen concentration. It is peaked near 700°C and is significantly more pronounced for boron-doped than for undoped material. Assuming that the first stage is related to doorway diffusion in as-deposited material [2], the results indicate gradually decreasing doorway dimensions with rising substrate temperature and indicate somewhat larger doorway dimensions for B-doped than for undoped a-Si:H. Apparently, the doorway dimensions of our a-Si:H, even when void-rich according to hydrogen effusion, are not large enough to allow diffusion of Ne below T_C. The second effusion stage of He effusion occurs subsequent to the major hydrogen release and is presumably related to precipitation of He in voids in the course of network reconstruction. The influence of annealing on the two He effusion stages is studied.
1. W. Beyer, J. Non-Cryst. Solids 266-269 (2000) 845.
2. W. Beyer, S.S. Camargo Jr. and R. Saleh, MRS Symp. Proc. 609 (2000)

A9.3
MULTI-LAYERED NANOCAVITIES IN SILICON WITH HELIUM IMPLANTATION.
Sanjay Rangan, S. Ashok, The Pennsylvania State University, University Park, PA; G. Chen, D. Theodore, Motorola Inc., Mesa, AZ.

Nanocavities in Si formed by He implantation and thermal anneal have been examined in recent years for applications such as gettering in Si technology and localized lifetime control in power devices. Our study focuses on generating multiple nanocavity layers, the optical and electrical properties of the void layers and influence of plasma hydrogen treatment. Such multi-layered cavity regions represent a genre of heterogeneous Si films and are of pontential use in optical, electronic and optoelectronic applications. The generation of these layered cavity regions is found to depend critically on the implant/anneal sequences employed. For instance, a sequence of three implants with decreasing energy (160 keV, 130 keV and 110 keV) followed by a single 800°C - 1 hour anneal results in the formation of a single void layer. But the same sequence interspersed with 800°C - 1 hour anneal after each implant gives rise to three distinct void layers, with the void density decreasing progressively from the top layer. The void layers and their evolution have been evaluated using scanning and transmission electron microcopy. Under isothermal anneal, the cavity shape changes from a distinct hexagonal geometry to a rounded spheroidal shape as the anneal time is increased. Photoluminescence spectra at 77 K reveal a broad peak at 0.8 eV for all the He-implanted and annealed samples, attributable to vacancy clusters. Current-voltage and capacitance- voltage measurements show the expected influence of the disordered cavity regions and deep level transient spectroscopy (DLTS) gives a minority carrier (electron in p-type Si) peak at 0.6 eV. Our results will also include the dependence on He dose, changes in electrical and optical properties under plasma hydrogenation, and the influence of Si self-implantation intended to alter the He- divacancy precursor reaction that ultimately impacts the He bubble (during implant) and void formations (following anneal).

A9.4
NEW MODELS OF PARACRYSTALLINE SILICON WITH DEFECT-FREE BANDGAP.
S.M. Nakhmanson, G.T. Barkema, N. Mousseau, P.M. Voyles, J.R. Abelson and D.A. Drabold.

Recent fluctuation electron microscopy (FEM) experiments have shown signatures of medium range order (MRO) in as-deposited amorphous semiconductor thin films [1]. We propose a new procedure for the preparation of physically realistic models of paracrystalline silicon, which contains randomly oriented c-Si grains embedded in a disordered matrix. Based on the modified bond-switching method of Wooten, Winer and Weaire [2,3], our technique allows us to create interfaces between crystalline and amorphous phases of Si with no or

just a few coordination defects. We have constructed three models of different size - 400, 1000 and 4000 atoms, respectively. All models have about 10% atomic density of crystalline phase; the two smaller ones contain a single crystalline grain and the 4000-atom model, 4 randomly oriented grains of roughly 100 atoms each. Our models show good geometrical and vibrational properties (compared to good models of pure a-Si) as well as the presence of MRO in their structure which is in agreement with the FEM experiments. Due to extremely low defect concentrations our models also display excellent optical properties, correctly reproducing the electronic bandgap for amorphous silicon. [1] M.M.J. Treacy and J.M. Gibson, Acta Cryst. A 52, 212 (1996); M.M.J. Treacy, J.M. Gibson and P.J. Keblinski, J. Non-Cryst. Solids 231, 99 (1998). [2] F. Wooten, K. Winer, D. Weaire, Phys. Rev. Lett. 54, 1392 (1985). [3] G.T. Barkema and N. Mousseau, Phys. Rev. B 62, 4985 (2000).

A9.5

STABILITY AND NANOSTRUCTURE OF HETEROGENEOUS AMORPHOUS SILICON THIN FILMS DEVELOPED UNDER HIGH CHAMBER PRESSURE (500 to 1800 mTorr) REGIME OF RF PECVD. A.R. Middya[a,b], Sukti Hazra[b], Swati Ray[b], S. Hamma[a], D.L. Williamson[c], and C. Longeaud[d]; [a]Ecole Polytechnique, Palaiseau, FRANCE; [b]IACS, Calcutta, INDIA; [c]Colorado School of Mines, Colorado, CO; [d]Universites Paris VI et XI, Paris, FRANCE.

Inspite of extensive research over two decades, the Staebler-Wronski effect in amorphous silicon remains the major drawback of a-Si solar cell technology. In 1994, we reported a new type of amorphous silicon thin films developed in the high chamber pressure regime ($P_r \approx 500$ to 1800 mT) of RF PECVD (called "γ'-regime"), which exhibit very high initial and stabilized mobility-lifetime products [$(\mu\tau)_{annld} \sim 10^{-4}$ cm^2/V.s, $\sigma_{ph}/\sigma_d \sim 5\text{x}10^5$, $(\mu\tau)_{sat} \sim 10^{-6}$ cm^2/V.s][1] and new features of defect distribution (analyzed by Modulated Photocurrent experiment)[2,3]. The kinetics of light induced degradation is found to be very fast and the saturation occurs (under 100 mW/cm^2/50°C) within 10 to 20 hours. Faster saturation (10^3 s vs. 10^5 s for standard sample) and low saturated defect density [N_S (CPM) $< 7.2\text{x}10^{16}$ cm^{-3}] have also been observed for volume absorbed intense light (340 mW/cm^2, $\lambda \approx 640$ nm, T $\approx$ 80°C). In this report the improved stability of these materials has been correlated to their unique nanostructure. Transmission electron microscopy (TEM) reveals its heterogeneous structure: clustered Si atoms/crystalline Si particles are randomly distributed in amorphous matrix and TED reveals "fine structure" in the diffraction ring masked by halo diffuse scattering. Consistent with this observation, the simulation of the experimental curve of the variation of dielectric constant with photon energy of these materials, obtained by UV-VIS ellipsometry, exhibits presence of small crystalline fractions ($f_c < 30\%$) which otherwise could not be detected unambiguously. The FWHM of first scattering peak of XRD of these samples are narrow, 5.4±0.1 degree (2θ) on Al-foil (independent of P_r) indicating ordering of Si-Si atoms beyond SRO. The in-depth microstructural analysis by small-angle x-ray scattering (SAXS), flotation density methods and FTIR, reveals a compact network structure ($C_H \sim$ 6-8at%, density $\approx 2.23\pm0.01$ g/cm^3, microvoid fractions below 0.01 vol%) along with large-scale features (<20nm) related to a weak columnar-like microstructure and a dominant SiH infrared vibrational peak at 2010 cm^{-1}, indicating most of the H atoms bonded to Si atoms on the surface of small crystallites which is consistent with the observations from TED and UV-VIS ellipsometry. We shall discuss a model based on selective recombination of excess photogenerated carriers in the crystalline phase or at the grain boundary instead of in the amorphous phase as a possible cause of suppression of light induced degradation in these heterogeneous materials. This type of materials was reproduced at Ecole Polytechnique in 1996 in a different reactor having different geometry and it is popular known as "polymorphous silicon" thin films[4]. 1. S. Ray. et. al. Proc. of the Ist World PVSC (1994) p. 581. 2. A.R. Middya et. al. Pro. MRS. Symp. 467 (1997) p. 615. 3. S. Hazra, et. al. Appl. Phys. Letts 76 (2000) p. 2340. 4. Pere Roca i Cabarrocas Proc. MRS Symp. 509 (1998) p. 855.

A9.6

NANOSTRUCTURED SILICON FILMS PRODUCED BY PECVD. Rodrigo Martins, Hugo Iguas, Vitor Silva, Isabel Ferreira, Ana Cabrita and Elvira Fortunato.

The aim of this paper is to determine the plasma process conditions that lead to the production of nanostructured silicon films constituted by aggregates of nanoparticles, grown by plasma enhanced chemical vapour deposition techniques. To do so, special emphasis will be put on the role of plasma impedance and of the second radio frequency harmonic on the determination of the process conditions that lead to the production of high quality electronic grade films within the so-called gamma regime, where powders are allowed to exist. Therefore, the powder management is one important issue to be addressed in this paper, together with the complex plasma chemistry (that involves the hydrogen dilution and ion bombardment used) and the incubation phase of the nanoparticles, aiming to control the characteristics of the grown nanostructured films. As a general rule we noticed that high quality films (low density of states and high mt products) are obtained under small ion bombardment and a high atomic hydrogen density of the growth surface, at high deposition pressure conditions, to allow the proper surface passivation and surface activation. As a general trend we noticed that the growth rates achieved using discharges under 13.56 MHZ are quite low, being able to be improved by about one decade by changing the frequency to 27 MHZ.

A9.7

EFFECTS OF HYDROGEN DILUTION ON HYDROGENATED AMORPHOUS SILICON FILMS AND SOLAR CELLS STUDIED BY RAMAN AND PHOTOLUMINESCENCE SPECTROSCOPY. Guozhen Yue and Daxing Han, Department of Physics & Astronomy, University of North Carolina at Chapel Hill, Chapel Hill, NC; Jeffrey Yang, Kenneth Lord, Baojie Yan and Subhendu Guha, United Solar Systems Corp., Troy, MI.

Hydrogenated amorphous silicon films and solar cells were prepared by plasma-enhanced chemical vapor deposition from a gas mixture of disilane and hydrogen. The samples were grown using no-, low-, standard-, and high-hydrogen dilution ratios. By increasing the hydrogen dilution ratio, the intrinsic (i) layer structure first showed an improvement of ordering and then a transition from amorphous to microcrystalline silicon. We use Raman, optical transmission, photoluminescence (PL) spectroscopy, and solar cell performance to examine the optical and electronic properties of the i layer. The main observations are: (a) the Raman spectrum shows a typical amorphous silicon mode for the no-, low-, and standard-diluted films, and an additional crystalline silicon peak for the high-dilution film; (b) the optical gap determined from the Tauc plot was 1.82 ± 0.02 eV for all the films except the high-dilution one; (c) below the onset of microcrystallinity, a blueshift of the 1.4 eV PL peak energy along with a decrease of the bandwidth occur as the structural order is improved; (d) above the onset of microcrystallinity, the PL efficiency decreases by a factor of 4-5 and the PL peak energy is redshifted toward 1.2 eV as the microcrystalline silicon volume fraction is increased; and (e) the solar cell open-circuit voltage (Voc) shows first an increase and then a decrease in value, consistent with the shift of the PL peak energy. Based on the above observations, it is noted that PL can reveal information additional to Raman and optical transmission. We conclude that PL and Voc are sensitive tools for characterizing film and solar cell structures, respectively, near the amorphous-to-microcrystalline transition.

A9.8

MORPHOLOGY, PHONON CONFINEMENT AND PROPERTIES OF a-Si:H FILMS. V. Ligatchev, Nanyang Technoligical University, SINGAPORE.

It is usually assumed that optical and electrical properties of amorphous semiconductors are determined by the short-range-order (SRO) parameters of atomic structure. In this report, the SRO parameters behavior is considered as governed by morphology geometrical parameters (MGP) alteration. For the particular case of columnar morphology, volume of the each column is assumed to be a thermal and 'frozen-in' phonons confinement volume. The assumption is essentially based on the experimental results on the columnar materials growth and texture investigations [1] as well as on non-equilibrium phonon lifetime studies in a-Si:H [2]. Approximately 10 ns lifetime is deduced for high-frequency phonons [2] and the phonons confinement sizes of order of 1 μm are expected. Generalized Skettrup model has been developed for a quantitative description of the MGP influence on the density of electron states distribution N(E). Common N(E) relation for the power, exponential and 'defects' regions of the dependence is derived both for adiabatic (optical) and non-adiabatic (thermal) electron excitation processes. Simulated (by the N(E) convolution) spectral dependence of optical absorption coefficient contains Tauc, Urbach and 'defects' parts. The E_G (optical gap) and E_U (Urbach tail slope energy) values are typical for the 'device quality' a-Si:H films at the averaged MGP values of order of 1 μm. Nearly linear E_G vs. E_U dependence is obtained at the MGP and temperature variation. Correlation between a defects concentration and Fermi level position also can be quantitatively simulated under assumption of the averaged MGP alterations, which are originated by the films deposition condition changes. Good agreement of experimental and the simulation results have been achieved for a-Si:H films, prepared both by RF (13. 56 MHz) sputtering and by silane decomposition. [1] Knights J.C. In: Physics of hydrogenated amorphous silicon. Springer, 1984. [2] Scholten A.J., Dijkhuis J.I., Phys. Rev. B., 53, 3837 (1996).

SESSION A10: POSTER SESSION
DOPANTS AND IMPURITIES
Chair: Paul Stradins
Tuesday Evening, April 17, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A10.1
WHERE OXYGEN DONORS LIVE IN MICROCRYSTALLINE SILICON. Toshihiro Kamei, Stanford Univ, Dept of Electrical Engineering, Stanford, CA; Takehito Wada, and Akihisa Matsida, Electrotechnical Laboratory, Tsukuba, JAPAN.

By just adding CO_2 gas to source gas mixtures of SiH_4 and H_2, oxygen concentration [O] in plasma deposited μc-Si:H can be controlled over a very wide range from 10^{16} to 10^{21} cm^{-3}. Both carbon and nitrogen concentrations are low enough that the obtained results are explained in terms of effects of oxygen impurities. While crystal quality does not deteriorate below $1X10^{20}$ cm^{-3} of [O], carrier density increase rapidly from 10^{13} to 10^{16} cm^{-3} above [O] of $1X10^{18}$ cm^{-3}. The superlinear dependence of electron carrier density on [O] from $1X10^{18}$ to $1X10^{20}$ cm^{-3} implies that oxygen aggregates act as donors. If oxygen donors were formed inside crystallites, potential barrier at grain boundary would change due to the formation of ionized donor states, as in the case of CVD grown polycrystalline Si films. This is, however, not the case in μc-Si:H. The potential barriers of μc-Si:H, estimated from temperature dependence of mobility (200K-400K), are 52-58 meV, almost independent of [O] in the range between $1X10^{16}$ and $4X10^{20}$ cm^{-3}. This result suggests that oxygen donors are formed in amorphous domain and/or at grain boundaries.

A10.2
CARBON LATTICE SITE DISTRIBUTIONS IN EPITAXIAL $Si_{1-y}C_y$ GROWN ON Si(001) BY MOLECULAR BEAM EPITAXY: AN X-RAY DIFFRACTION, *AB INITIO* CALCULATION, AND PHOTOLUMINESCENCE STUDY. S.Y. Park, J.A.N.T. Soares, D. Gall, Y.-W. Kim, H. Kim, and J.E. Greene, Univ of Illinois, Materials Science Dept, the Frederick Seitz Materials Research Laboratory, Urbana, IL; P. Desjardins, Groupe de recherche en physique et technologie des couches minces, dépt de génie des matériaux, école polytechnique de Montréal, Montréal, CANADA; S.G. Bishop, Univ of Illinois, Dept of Electrical and Computer Engineering, Computer and Systems Research Laboratory, Urbana, IL.

Epitaxial metastable $Si_{1-y}C_y$/Si(001) alloy layers with $y \leq 0.026$ were grown on Si(001) by solid-source molecular beam epitaxy at temperatures Ts between 380 and 680°C to study C lattice site distributions. All layers, irrespective of T_s and y, are completely coherent with their substrates as determined by high-resolution x-ray diffraction (HR-XRD) reciprocal lattice maps. Ab initio density-functional calculations show that substitutional C (C_s), with a formation energy per C atom of U = 1.39 eV, is the most stable C configuration in Si while U of the bistable substitutional-interstitial C pair (C_sC_i) in its A and B configuration is only 0.5 eV higher. The A configuration yields virtually no strain while the B configuration creates approximately half of the tensile strain associated with C_s. Using the calculated strain coefficients, the measured layer strain obtained from HR-XRD, and the total C fraction measured by secondary ion mass spectroscopy, we determine C lattice site distributions as a function of T_s and y. Growth at $T_s < 580$°C, irrespective of y, results in fully-substitutional C incorporation in perfect single-crystal layers as judged by cross-sectional transmission electron microscopy (XTEM). The significant decrease in tensile strain with increasing $T_s < 580$°C is attributed to partial C incorporation as CsCi pairs. This is supported by the presence, in these samples, of a low-temperature photoluminescence peak at 0.97 eV. In-situ reflection high energy electron diffraction and ex-situ XTEM analyses show that gradual surface roughening occurs during growth at such temperatures and that these layers exhibit planar defects regularly distributed along (001) planes with a periodicity of 130 ± 10 Å and interconnected by {113} segments.

A10.3
THE PRECISE CONTROL OF A SHALLOW P^+ /N JUNCTION DEPTH BY LASER DOPING AND ANNEALING OF PREAMORPHIZED Si ON N-TYPE Si(100). Myung Geun Han, Seonghoon Lee, Kwangju Institute of Science and Technology, Dept of MS&E, Kwangju, KOREA.

We have investigated the effect of the thickness of preamorphized Si on n-type Si(100) on a shallow p^+ /n junction depth formed by laser doping and annealing so called GILD(Gas Immersion Laser Doping) process. We produced various thicknesses of amorphous layers of Si on n-type Si (100) wafer with a resistivity of 3∼5 Ω cm by the plasma immersion ion implantation method. Mixtures of 2% SiH_4 in 98% H_2 was used as a reactant gas to generate amorphous layer of Si on n-type Si(100). We measured the thickness of amorphous layers of Si using x-ray reflectivity method and HTEM technique. We irradiated a 248nm KrF excimer laser beam on each samples of different thickness of amorphous Si on n-type Si(100) under a total pressure of 10 torr of 3% B_2H_6 in 97% N_2 ambient in order to form a precisely controlled shallow p^+ /n junction depth. After GILD process, using HRTEM method, we observed that the preamorphized Si on n-type Si(100) was transformed into crystalline Si through an epitaxial growth. We used Secondary Ion Mass Spectrometry (SIMS) to measure dopant (Boron) depth profiles. SIMS depth profile data clearly showed that the junction depth increased with the increase in the thickness of preamorphized Si on n-type Si(100) at the same laser fluence. We measured the sheet resistance of a doped area by a four-point probe method. It was 110 Ω/□. In the GILD process, the junction depth is controlled primarily by the laser fluence. Usually laser fluence of even a stable excimer laser fluctuates pulse to pulse. Here we present a new method to control a shallow junction depth precisely by an adjustment of the thickness of preamorphized Si on n-type Si(100) which undergoes an epitaxial growth during laser doping and annealing process and by a precise control of laser fluence together.

A10.4
RELATION BETWEEN ERBIUM PHOTOLUMINESCENCE AND DANGLING-BOND DEFECTS IN a-Si:H. Minoru Kumeda, Hiroshi Itoh, Norio Shitakata, Tatsuo Shimizu, Kanazawa Univ., Dept of Electrical and Electronic System Engineering, Kanazawa, JAPAN.

Er-doped a-Si:H have drawn a wide attention recently for the 1540 nm luminescence for the application in the optical fiber communication. The mechanism of the emission is not so clear, although a model of the energy transfer from the excited electrons in the conduction band to Er ions via dangling bonds has been proposed[1]. We studied the relation between the photoluminescence (PL) at 1540 nm at room temperature and the density of Si dangling bonds in a-Si:H films. The films were prepared by rf magnetron sputtering using Er tips and the Si target. The sample films were annealed for 30 min at temperatures up to 600 degrees centigrade, and PL, ESR and IR measurements were made. The density of ESR spins due to Si dangling bonds first decreases and then increases against the increase in the annealing temperature. The first decrease originates from a structural relaxation while the increase at a higher temperature originates from hydrogen evolution. The intensity of the PL originating from Er increases with the first decrease in the ESR spin density. However, the PL intensity further increases with the increase in the spin density due to Si dangling bonds originating from the hydrogen evolution. These results suggest the existence of two types of Si dangling bonds for the contribution to the Er emission. The first type of Si dangling bonds whose density decreases by a structural relaxation is a killer for the Er PL. Most of the photoexcited carriers recombine nonradiatively at this type of dangling bonds. Si dangling bonds created by hydrogen evolution appears to sensitize the Er PL. [1] I. Yassievich, M. Bresler and O. Gusev, J. Non-Cryst. Solids 226 (1998) 192.

A10.5
MECHANISM OF ERBIUM ELECTROLUMINESCENCE IN AMORPHOUS HYDROGENATED SILICON. Mikhail S. Bresler, Oleg B. Gusev, Evgenii I. Terukov, Konstantin D. Tsendin, Irina N. Yassievich, A.F. Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; Walther Fuhs, Hahn-Meitner Institut, Abteilung Photovoltaik, Berlin, GERMANY.

We have studied electroluminescence in the amorphous silicon-based erbium-doped structures at reverse bias in the temperature range 77-300 K. The intensity of electroluminescence at the wavelength of 1.54 μm corresponding to a radiative transition $^4I_{13/2} \rightarrow {}^4I_{15/2}$ in the internal 4f-shell of the Er^3 ion is low at 77 K but sharply increases starting from 220 K and exhibits a maximum near the room temperature. Theoretical analysis and comparison with the experiment have shown that the excitation of erbium ions occurs by an Auger process which involves the capture of conduction electrons by neutral dangling bonds (D^0) defects located close to erbium ions. Measurements of the resistance of the electroluminescent structure as a function of temperature performed in parallel with the measurements of the electroluminescence intensity demonstrated a correlation in behavior of these two quantities: a pronounced decrease of the resistance occurs at the same temperature where the luminescence intensity starts to rise. This result indicates a rise in concentration of free carriers in a high electric field applied to the structure which can be explained by a thermally activated tunnel emission of electrons from deep centers (erbium-oxygen complexes acting as donors and negatively charged dangling-bond defects (D^- defects)) to the conduction band of the amorphous matrix. It is this process that keeps the stationary current through the structure in the situation when free electrons are captured from the conduction band by D^0 defects. This work was partially supported by the INTAS 99-1872 project and the grants of the Russian Foundation of Basic Research.

A10.6
STIMULATED EMISSION OF ERBIUM IONS IN AMORPHOUS SILICON MATRIX AT ROOM TEMPERATURE. Mikhail S. Bresler, Oleg B. Gusev, Evgenii I. Terukov, Irina N. Yassievich, A.F. Ioffe Physico-Technical Institute, St. Petersburg, RUSSIA; Boris V. Kamenev, Pavel K. Kashkarov, Elizaveta A. Konstantinova, Viktor Yu. Timoshenko, Physical Department, M.V. Lomonosov Moscow State University, Moscow, RUSSIA.

Stimulated emission of erbium ions in amorphous silicon matrix was first observed under optical pumping at room temperature. An erbium-doped amorphous hydrogenated silicon layer of $\sim 1\ \mu$m thickness was magnetron sputtered on a quartz substrate. The concentration of erbium was 2.5×10^{20} cm^{-3}. The pumping was done by a nitrogen or copper vapor laser with an excitation beam focused to a 0.5 mm diameter spot on the surface of the sample. Due to differences in refraction indices of silicon and substrate and vacuum, the erbium-doped amorphous silicon layer formed a natural waveguide structure favouring the onset of stimulated emission. The photoluminescence intensity as a function of the excitation power demonstrated a linear rise, then a tendency to saturation below 50 kW/cm^2, and a superlinear increase above a threshold of $\sim$ 100-200 kW/cm^2. Simultaneously a drop of the decay time of erbium luminescence was observed from 8 μs in the linear and saturation regime to 3 μs above the threshold. A simple homogeneous model of lasing in the structures with saturation of the pumping rate characteristic of erbium ions in semiconductor matrices is developed. A comparison of the experimental data with the theoretical model permitted estimation of the radiative lifetime of erbium ions in the excited state $\sim$ 100 μs, a value, significantly lower than this lifetime in other solid state matrices ($\sim$ 1-10 ms). This work was partially supported by the INTAS 99-1872 project and the grants of the Russian Foundation of Basic Research.

SESSION A11: AMORPHOUS SILICON SOLAR CELLS

Chair: Vikram L. Dalal
Wednesday Morning, April 18, 2001
Metropolitan III (Argent)

8:30 AM *A11.1
TOWARDS STABILIZED 10% EFFICIENCY OF LARGE-AREA (> 5000 CM^2) a-Si/a-SiGe TANDEM SOLAR CELLS USING HIGH-RATE DEPOSITION. Shingo Okamoto, Akira Terakawa, Eiji Maruyama, Wataru Shinohara and Seiichi Kiyama, Sanyo Electric Co., Ltd., New Materials Research Center, Osaka, JAPAN.

High-rate deposition of photovoltaic layers of a-Si/a-SiGe tandem solar cells has been investigated using rf (13.56MHz) plasma-CVD method while keeping the substrate temperature below 200°C. A high photoconductivity of 10^{-5} S/cm and photo sensitivity of 10^6 of hydrogenated a-Si films maintain up to the deposition rate (Rd) of 15Å/s by optimizing hydrogen dilution and other deposition conditions. It is of great importance to utilize the effect of hydrogen dilution which can reduce the incorporation of excess hydrogen in the films. Compared at Rd = 5Å/s, the optical gap (Eopt) can be reduced by 0.08 eV (from 1.67 eV to 1.59 eV, determined from the cube root of $\alpha h\nu$ plots) by using the optimized hydrogen dilution. This Eopt narrowing leads a decrease in photovoltaic layer thickness required for obtaining a certain current level, which contributes to suppressing the light induced degradation of a-Si solar cells. The results suggest that the optimized hydrogen dilution in a high Rd region is effective in improving the stabilized efficiency from the viewpoints of both material quality and device design. As for hydrogenated a-SiGe films, we have also succeeded in increasing Rd to about 3Å/s with little degradation in the film quality. The world's highest stabilized efficiency of 9.3% has been achieved for a large-area (5150cm^2) a-Si/a-SiGe tandem submodule whose top and bottom photovoltaic layers were deposited at about 3Å/s using the optimized hydrogen dilution. A smart back reflector, with a high light-scattering effect, and other approaches to enhance the optical confinement effect, are also proposed for further improvement of cell performance. This work was supported in part by NEDO (New Energy and Industrial Technology Development Organization) as a part of the New Sunshine Program under MITI.

9:00 AM A11.2
HIGHER EFFICIENCY OF N-I-P SOLAR CELLS BY HOT WIRE CVD AT MODERATE TEMPERATURES. M.K. van Veen, R.E.I. Schropp, Utrecht University, Debye Institute, Physics of Devices, Utrecht, THE NETHERLANDS.

In the production of amorphous silicon based solar cells, it is of crucial importance that the manufacturing costs will be reduced. One way to achieve this is to enhance the deposition rate by using the Hot Wire CVD technique. Previously, we developed n-i-p cells, with the i-layer deposited at 430°C, with an efficiency of 5.5% using special temperature resistant n-layers and re-hydrogenation procedures after i-layer deposition. We are currently investigating methods to use the same low substrate temperatures as in PECVD, while maintaining a high material quality and a high deposition rate, so that cheap materials can also be used as a substrate in HWCVD. Therefore, we studied the role of the wire temperature, the substrate temperature, the hydrogen dilution during deposition, and the silane gas flow rate on the film parameters. As the substrate temperature is lowered, the hydrogen concentration in the layers is increased. However, the electrical properties of the HWCVD amorphous silicon layers remain of device quality. Layers deposited at 250°C have been applied in an efficient n-i-p solar cell, in which the doped, microcrystalline, layers have been deposited by PECVD. The growth rate of the intrinsic layer was about 10 Å/s. The deposition parameters were kept constant during i-layer deposition. No optical enhancements, like texturing or backreflectors, were used. The cell has a fill factor of 0.72 and an open-circuit voltage of 0.89 V. On a stainless-steel substrate, an initial efficiency of 7% was recorded.

9:15 AM A11.3
AMORPHOUS SILICON AND SILICON GERMANIUM ALLOY SOLAR CELLS DEPOSITED BY VHF AT HIGH RATES. Jeffrey Yang, Baojie Yan and Subhendu Guha, United Solar Systems Corp., Troy, MI.

We have recently reported that high-quality amorphous silicon (a-Si) alloy solar cells can be obtained by using a modified very high frequency (MVHF) technique at a deposition rate of 8 Å/s. The cells show good initial and stabilized efficiencies suitable for the top cell of a multijunction structure. In this study, we report our results on a-SiGe alloy solar cells using MVHF at 6 Å/s. Usually, higher deposition rates lead to poorer material quality especially for the a-SiGe alloys. Furthermore, the bandgap profiling design that has been very effective in enhancing a-SiGe alloy cell performance is more difficult to implement for high rates due to relatively short deposition time. We have improved our deposition process and successfully incorporated a desired bandgap profiling. This resulted in a significant increase in the cell performance over the flat gap design. In addition, we have incorporated appropriate buffer layers between the intrinsic layer and the doped layers. The structure prevented back diffusion of carriers from the doped layers into the intrinsic layer, thus improving the cell characteristics. An a-SiGe alloy solar cell incorporating both the bandgap profiling and buffer layers was deposited onto a stainless steel substrate. The intrinsic layer has an optical bandgap of 1.6 eV and was deposited at 6 Å/s. The I-V characteristic was measured under AM1.5 illumination with a $\lambda >$ 530 nm filter. The power output was found to exceed 4 mW/cm^2 , a value typically used to qualify a good mid-gap cell. Use of the optimized a-SiGe alloy cell in a multijunction structure leads to an initial AM1.5 active-area efficiency of greater than 11%. Details of this work along with the stability data will be presented.

9:30 AM *A11.4
TECHNOLOGY CHALLENGES IN THE MANUFACTURING OF a-Si:H TANDEM SOLAR CELLS. David E. Carlson, BP Solar, Toano, VA.

BP Solar started commercial production of amorphous silicon tandem solar cells in Toano, Virginia in 1997. The scale-up process has involved overcoming technical challenges in several areas. It was necessary to develop high speed, multiple beam laser scribing systems that could pattern photovoltaic modules over an area of 0.8 square meters with close dimensional tolerances. In the past year, the deposition rate of amorphous silicon was doubled and the deposition system was modified to meet capacity requirements. The utilization of feedstock gases was increased by 20% in order to reduce material costs. In addition, dimensional tolerances of the deposition system geometry were determined and controlled in order to assure uniform depositions of the amorphous silicon alloys. Sources of debris that could cause shunts and shorts in the devices were identified and minimized. Effects of contaminants (such as pump oils and residual dopants) on device performance were quantified. Current research efforts are focused on further increases in the amorphous silicon deposition rate, improvements in device performance and the development of in-situ diagnostic tools to monitor and control the manufacturing process.

SESSION A12: METASTABILITY I

Chair: Rana Biswas
Wednesday Morning, April 18, 2001
Metropolitan III (Argent)

10:30 AM A12.1
PHOTOCARRIER CAPTURE PROPERTIES OF LIGHT-INDUCED

DEFECTS IN a-Si:H. Paul Stradins, Satoshi Shimizu, Michio Kondo, and Akihisa Matsuda, Electrotechnical Laboratory, Tsukuba, JAPAN.

The non-unique relation between the photoconductive properties and the light-induced defect (LID) concentration suggests that LIDs have different photocarrier capture coefficients when created under different conditions [1]. In this work, the photocarrier capture coefficients are studied systematically as functions of the deposition techniques, light exposure conditions, and sample history. A large variety of samples were investigated such as PECVD RF, VHF, hydrogen diluted, thermal plasma, as well as hot wire, and deuteriated amorphous silicon. The dependences of the inverse electron mobility-lifetime product $(\mu\tau)^{-1}$ on the LID concentration N were obtained by photoconductivity, ESR, and subgap absorption measurements. These photodegradation properties were measured both during the light exposure and subsequent thermal anneal. It is found that the degradation of photoconductive properties is governed by the creation of LIDs with different effective capture coefficients as shown by $(\mu\tau)^{-1}$ vs. N dependences. Various a-Si:H films deposited at 250°C and exposed at room temperature exhibit very similar capture coefficients of LIDs. However, the capture coefficients get strongly reduced by either increasing the light exposure temperature or partial annealing of the exposed samples, or by replacing H with deuterium (a-Si:D). We suggest that the capture coefficients are governed by the microstructure around the LIDs. Existence of H atom in the close vicinity of LID may strongly enhance the photocarrier capture because of the efficient release of the recombination energy into energetic Si-H vibrations. Replacing H to D therefore is expected to weaken the photocarrier capture. The LIDs are likely created together with a metastable structural change in the surrounding microstructure. Modifications in this microstructure at higher T may explain the lowering of capture coefficients of LIDs created at or heated to these temperatures. The effects of deposition temperature, hydrogen dilution, and hole capture properties are also discussed. 1. P. Stradins, M. Kondo, A. Matsuda, IEEE 28th PVSC (2000).

10:45 AM A12.2
NEW EXPERIMENTS ON THE RELATIONSHIP BETWEEN LIGHT-INDUCED DEFECTS AND PHOTOCONDUCTIVITY DEGRADATION. Stephan Heck, Howard M. Branz, National Renewable Energy Laboratory, Golden, CO.

Because light-induced photoconductivity degradation anneals out at much lower T than the light-induced increase in deep defect density, Han and Fritzsche [JNCS, 59 & 60, p397 (1983)] suggested that two kinds of defects are created during illumination of hydrogenated amorphous silicon. In this view, one kind of defect degrades the photoconductivity and the other increases defect sub-bandgap optical absorption. However, the degradation model of Stutzmann et al.[PRB, 32, p23 (1985)] assumes that photoconductivity is inversely proportional to the dangling-bond defect density. Like Han and Fritsche, we observe two kinds of defects that are easily distinguished by their annealing activation energies, but remarkably, we find that their densities remain in strict *linear proportionality* during creation, i.e., the two kinds of defects are not completely independent. In our measurements of photoconductivity and defect absorption (constant photocurrent method) during 25°C light soaking and during a series of isochronal anneals between $25 < T < 190$°C, we find that the absorption measured with $E \leq 1.1$ eV, first increases during annealing, then exhibits the usual absorption decrease found for deeper defects. The maximum in this absorption at $E \leq 1.1$eV occurs simultaneously with a transition from fast to slow recovery of photoconductivity. We also measure isothermal annealing activation energies for photoconductivity, defect absorption at $E \leq 1.1$ eV, and absorption in the deeper dangling bond levels (E = 1.25, 1.3, 1.4 eV). The absorption for $E \leq 1.1$ eV shows *two* distinct annealing activation energies: the signal rises with about 0.85 eV and falls with about 1.15 eV. The 0.85 eV activation energy roughly equals the activation energy for the dominant, fast, recovery of photoconductivity. The 1.15 eV activation energy roughly equals the single activation energy for annealing of the light-induced dangling bond absorption.

11:00 AM A12.3
CONTRIBUTIONS OF D^0 AND NON-D^0 GAP STATES TO THE KINETICS OF LIGHT INDUCED DEGRADATION OF AMORPHOUS SILICON UNDER 1 SUN ILLUMINATION. J. Pearce, X. Niu, R. Koval, R.W. Collins, C.R. Wronski, Center For Thin Film Devices, Pennsylvania State University, University Park, PA; G. Ganguly, D. Carlson, BP Solar, Toano, VA.

The contributions of defects other than D^0 (1,2) to the 1 sun kinetics of light induced changes to the degraded steady state (DSS) in hydrogenated amorphous silicon (a-Si:H) materials have for the first time been quantified. To overcome the often observed discrepancies in the correlations between photoconductivity and the commonly used subgap absorption for photons of 1.2eV, $\alpha(1.2)$, a detailed study of the electron mobility-lifetime and subgap absorption using dual beam photoconductivity, for degradations at temperatures between 25 to 100°C was used. The results obtained for different thin film materials on the changes in mobility-lifetime product and the concomitant changes in both the magnitudes and shapes of $\alpha(E)$ were used to identify and quantify the contributions to the degradation kinetics of the non-D^0 defects. Both fast and slow degradation processes are clearly observable in the a-Si:H films studied and can be represented by two time constants. Correlations obtained between the fast process and the light induced non-D^0 states are presented and the ramifications of their temperature dependence on the mechanisms for the Staebler-Wronski effect are discussed.
(1) Han, D. and Fritzsche, H., *J. Non-Cryst. Solids*, **59-60**, 397 (1983). (2) R. Koval, et al, *MRS 2000 Spring Meeting*, April 24-28, 2000, San Francisco, California.

11:15 AM A12.4
LIGHT-INDUCED CREATION OF DEFECTS AND LIFETIME DISTRIBUTION OF PHOTOLUMINESCENCE IN a-Si:H BASED FILMS. Chisato Ogihara, Hitoshi Takemura, Yamaguchi Univ, Dept of Applied Science, Ube, JAPAN; Kazuo Morigaki, Hiroshima Institute of Technology, Dept of Electrical and Digital-System Engineering, Hiroshima, JAPAN.

We have studied the lifetime distributions of photoluminescence (PL) at 10K after the pulsed excitation for a-Si:H based films. Effects of light-induced creation of defects on the lifetime distributions have also been studied. The a-Si:H, a-$Si_{1-x}N_x$:H and a-Si:H/a-$Si_{1-x}N_x$:H multilayers were deposited from the mixture of SiH_4, H_2 and NH_3 in a capacitively coupled glow-discharge reactor. We also prepared band-edge modulated (BM) a-$Si_{1-x}N_x$:H films in which x is modulated sinusoidally to confine electrons and holes in sinusoidal potential wells. The PL decay after interband or sub-bandgap pulsed excitation from a YAG-OPO laser system was measured. The measurements were repeated after prolonged exposure of the pulsed light from the laser. The lifetime distributions in microsecond and nanosecond regions were obtained from Fourier transform of the PL decay. The defect densities were estimated from electron spin resonance (ESR) measurements. The lifetime distributions have a distinct component at about 10 ns together with a longer lifetime component seen in microsecond region. They are attributed to the emission from singlet excitons and localized electron-hole pairs respectively. In the case of the multilayers, the nanosecond component becomes dominant with decreasing well layer thickness showing that the confinement of electrons and holes stabilizes the excitons. Similar results have been obtained for the BM films. The PL decreases in intensity after the exposure of visible light. The decreasing of the nanosecond component is slower than that of microsecond component. The decreasing of the PL intensity and increasing of the defect density have also been observed in the case of exposure of sub-bandgap light although the absorption coefficient is much smaller than that of visible light. We discuss about the process of light induced creation of defects and photo-excited states in a-Si:H based films with the experimental results.

11:30 AM A12.5
LIGHT-INDUCED ANNEALING OF DEEP DEFECTS IN LOW Ge FRACTION a-Si,Ge:H ALLOYS: FURTHER INSIGHTS INTO THE FUNDAMENTALS OF LIGHT-INDUCED DEGRADATION. J. David Cohen, Jennifer T. Heath, and Kimon C. Palinginis, University of Oregon, Eugene, OR; Jeffrey C. Yang and Subhendu Guha, United Solar Systems Corp., Troy, MI.

We have used the modulated photocurrent (MPC) method to study deep defect creation and annealing kinetics in low Ge fraction a-Si,Ge:H alloys (Ge fractions below 10at.%). These intrinsic alloy samples were deposited by the glow discharge method onto p^+ crystalline Si substrates at United Solar from mixtures of disilane, germane, and hydrogen. We reported previously that our MPC measurements reveal two distinct bands of deep defects in each of these samples which we identified as neutral Si and neutral Ge dangling bonds. We also demonstrated that, upon heating in the dark from a strongly light degraded state, these two defects were reduced in a manner that indicated a direct competition between the annealing of the Si and Ge dangling bonds. This therefore implied a global reconfiguration mechanism. We have now carried out studies to compare purely thermal annealing with light-induced annealing in these a-Si,Ge:H alloys. This has led to several important additional insights into the degradation process. Most notably, we have found that the relative anneal rate for the two types of defects differs from the case of purely thermal annealing. This therefore tends to rule out models in which the rate limiting step in the annealing process comes from the release of the mediating entity (hydrogen? strain?) from a remote site. That is, if light simply accelerated this release, the relative rate of reduction for the two types of defects would be the same as for thermal annealing, contrary to observation. Specific microscopic models consistent with our experimental results will be presented.

11:45 AM A12.6

CHANGES IN HYDROGENATED AMORPHOUS SILICON UPON EXTENSIVE LIGHT-SOAKING AT ELEVATED TEMPERATURE.

Nobuhiro Hata, Electrotechnical Lab., Tsukuba, JAPAN; Charles M. Fortmann, Dept of Applied Mathematics, State Univ of New York at Stony Brook, Stony Brook NY; Akihisa Matsuda, Electrotechnical Laboratory, Tsukuba, JAPAN.

We find that extensive light-soaking (LS) of a-Si:H at elevated temperatures changes the time constants of light-induced metastable defect creation and annealing. The plasma-deposited a-Si:H film thicknesses and Tauc bands gap were about 1.3 microns and 1.76 eV, respectively. For the extensive LS at an elevated temperature of 250°C, 5 mJ cm^{-2} light pulses of 650 nm wavelength were used. The steady-state defect density is temperature dependent, and the value reached by the extensive LS at 250°C is about 1E+16 cm^{-3}, which was measured by constant photocurrent method. Further LS at 30°C with the light pulses resulted in the defect density exceeding 1E+17 cm^{-3}. Light-induced annealing (LIA) at 100°C was performed with a continuous red light having an intensity of 2 W cm^{-2}. The fully light-soaked samples were also subjected to isochronal annealings for two hours each at successively increasing temperatures from 100 to 200°C. They were then light-soaked with a pulsed laser at 30°C or with AM 1.5 white light with 100 mW cm^{-2} intensity at 50°C, to determine defect density dependence on light-soaking time. The time constants for LIA of metastable defects and for creation of metastable defects by LS both with pulse and continuous lights were compared for the samples before and after light-soaked at 250°C. The time constants decreased in the films that had been subject to the high temperature LS. Even larger changes resulted from higher temperature (T> 250°C) LS. We discuss these results, together with the earlier results [1] on light-induced changes in pseudo dielectric functions upon extensive LS, in terms of a model in which temperature and LS cause a change in structure.

[1] N. Hata and C.M. Fortmann, MRS Proc. 609, to be published (2000).

SESSION A13: HYDROGEN AND METASTABILITY

Chair: Christopher R. Wronski
Wednesday Afternoon, April 18, 2001
Metropolitan III (Argent)

1:30 PM *A13.1

DIFFUSION AND SOLUBILITY OF HYDROGEN IN AMORPHOUS AND MICROCRYSTALLINE Si:H FILMS.

Wolfhard Beyer, Institut für Photovoltaik, Forschungszentrum Jülich GmbH, Jülich, GERMANY.

Hydrogen diffusion and hydrogen incorporation in amorphous and microcrystalline silicon have been a matter of intensive research for many years. Diffusion was found to depend on various parameters like temperature, time, hydrogen concentration, doping, illumination, microstructure and others, and to differ for H in-diffusion (e.g. from a H plasma) and for interdiffusion between layers of Si:H. Several phenomena in Si:H have been related to hydrogen solubility. Data, models and concepts will be discussed aiming to elucidate the present state of knowledge. The widely different microstructure of the materials, depending on growth conditions and hydrogen concentration, results in both atomic and molecular H as the most mobile species. In particular, in amorphous silicon with hydrogen concentrations exceeding 15-20 at.% and in many microcrystalline Si:H samples hydrogen diffusion is predominantly carried by hydrogen molecules. For diffusion of atomic hydrogen, the results favor a band model of H diffusion to simple trapping models where the trap depth equals the diffusion energy. The experimentally observed wide variation of diffusion prefactor and diffusion energy is attributed in the band model of H diffusion to temperature shifts of the hydrogen chemical potential relative to the hydrogen transport path energy rather than to different diffusion processes or trap depths. The nature of the influence of doping and the Fermi level on hydrogen diffusion is not fully clarified. Hydrogen solubility has been found to limit hydrogen in-diffusion from a hydrogen-rich source layer but not from a hydrogen plasma. Another type of hydrogen solubility has been proposed to govern the presence of hydrogen-related microstructure. However, quite different solubility values were reported.

2:00 PM *A13.2

FORMS OF HYDROGEN AND HYDROGEN DIFFUSION IN REALISTIC a-Si:H.

P.A. Fedders, Department of Physics, Washington University, St. Louis, MO.

Over the years there have been many supercells of a-Si:H presented and used to investigate the energetics of various configurations of hydrogen in the supercells. However, none of them are adequate for studying all of the important forms of H in a single cell of a-Si:H. First of all, almost all supercells have way too many defects. In this paper we present a set of supercells of about 140 atoms and thebasic supercell contains no geometrical or spectral defects and thus has a substantial clean gap without excessive band tailing caused by strain defects. Next, experiments clearly show that there are at least three types of hydrogen present in a-Si:H in substantial amounts. This includes isolated bonded H, clustered bonded H, and molecular H. Further bond centered (BC)H is important because of its possible relevance to H migration. The distinction between isolated and clustered H is usually ignored theoretically although this work shows that they have very different energetics. We argue that an understanding of all four types of hydrogen is necessary in order to form an understanding of important phenomena such as light induced defects and the migration of hydrogen. For example, consider the following apparent paradox. Experiments clearly show that dangling bonds are rarely, if ever, accompanied by nearby hydrogen. Yet in a clustered region of hydrogen if an H atom leaves its dangling bond, one will have a dangling bond near a number of H atoms! We find that this paradox can be resolved by both a weakly and a strongly bonded form of clustered H that our supercells possess. This work provides a further understanding of H migration by eliminating some possibilities and giving credance to others. Also the possible conversion among different forms of H in a-Si:H is considered.

2:30 PM *A13.3

HYDROGEN EQUILIBRATION AND METASTABILITY IN AMORPHOUS SILICON.

Howard M. Branz and S.B. Zhang, National Renewable Energy Laboratory, Golden, CO.

Hydrogen motion is a key feature of light- and quenching-induced metastability in hydrogenated amorphous silicon (a-Si:H). Hydrogen pairing with negative effective correlation energy (U) accounts for a variety of experiments in a-Si:H.[Zafar and Schiff, PRL, **66**, 1493, 1991; Branz, PRB, **59**, 5498, 1999] (1) Equilibration of a paired H configuration with isolated SiH bonds gives rise to a Si dangling-bond (DB) density that is thermally activated above about 200°C; at higher T, paired H evolves with little DB creation. (2) In the H collision model of light-induced metastability, mobile H emitted from SiH bonds traps in pairs, consistent with the observed anti-correlation of H and DBs. Remarkably, these two negative-U paired H configurations must be distinct in order to account for the different behaviors of H in equilibration/evolution and in metastability experiments. A realistic model will relate these H pairing configurations to the known H microstructure of a-Si:H.
Here, we propose a microscopic model unifying H equilibration and metastability. Using *ab initio* pseudopotential calculations, we find that fully-H-terminated, small m-vacancies (m missing Si) bind *additional* H pairs in two distinct negative-U configurations: (1) Ejection of a neighboring monovacancy binds two H with about 1.4 eV per H for m $\geq$ 2. (2) Formation of an internal Si-Si dimer [(001) surface-like] binds two H on backbond neighbors with about 0.8 eV per H for any m. Binding of single H atoms in these sites is also studied. We propose that these two pairing configurations are the equilibration/evolution site (1.4 eV) and the metastability site (0.8 eV) of the Zafar-Schiff and Branz phenomenological models.

SESSION A14: METASTABILITY II

Chair: J. David Cohen
Wednesday Afternoon, April 18, 2001
Metropolitan III (Argent)

3:30 PM A14.1

SILICON NETWORK REBONDING MODEL FOR META-STABILITY IN AMORPHOUS SILICON.

Rana Biswas,Y. Ye, Bicai Pan, Iowa State University, Dept. of Physics, Microelectronics Research Center and Ames Lab, Ames, IA.

We propose a new silicon network rebonding model to describe light-induced metastability in hydrogenated amorphous silicon. The first step in the process is the breaking of weak silicon bonds generating a dangling bond and floating bond pair. The mobile floating bond diffuses away leaving behind an isolated dangling bond in agreement with ESR measurements. Tight-binding molecular dynamics simulations show clear evidence for each of these processes. Floating bonds are an intermediate transient species that do not remain in the light-soaked steady state. Floating bonds annihilate in pairs generating strained silicon bonds. In addition, floating bonds react with SiH bonds to generate diffusing H. Further interactions of the mobile H with the Si network and the annealing of metastable defects will be described with molecular dynamics calculations. The analogies and differences with the H-collision model of Branz will be discussed. This new model involving long-range motion accounts consistently for major experimental features of the Staebler-Wronski effect. The breaking of weak silicon bonds can account for the anti-correlation between the location of dangling bonds and hydrogen, seen in hyperfine experiments. Activation energies and energy barriers

for silicon bond-breaking are in agreement with experiment. This process has a $t^{1/3}$ kinetics for the growth of defects. Results from rate equations will describe the kinetics and steady state.

3:45 PM A14.2
INVESTIGATION OF LIGHT-INDUCED DEFECT DEPTH PROFILE IN HYDROGENATED AMORPHOUS SILICON FILMS. Satoshi Shimizu, Paul Stradins, Michio Kondo, Akihisa Matsuda, Electrotechnical Laboratory, Tsukuba, JAPAN.

It has been suggested that the depth profile of light-induced defects (LID) is determined by non-uniform mechanical and/or electrical properties [1] or inhomogeneous photocarrier generation and recombination in hydrogenated amorphous silicon (a-Si:H) [2]. We have developed a novel layer-by-layer wet etching technique which does not introduce extra surface defects as well as surface roughness for investigating the depth profile of LID in a-Si:H directly. The Si dangling bond defect concentration after each etching step was measured by ESR. In case of long wavelength red light exposure on the a-Si:H, LIDs are created almost uniformly up to 3 microns in the depth of the film. This suggests that the LID creation efficiency has little variation throughout the films. For strongly non-uniformly absorbed green light, the measured defect distribution profile N(x) as a function of depth x, is spatially wider than photocarrier generation rate G(x). We consider two possible origins for this dependence of N(x) with respect to G(x). Firstly, the number of defects generally depends sublinearly on photocarrier generation rate [1] because of bimolecular recombination. This approximately agrees with our measured dependence $N(x) \propto G^{0.55}(x)$. Secondly, the profile N(x) may get additionally widened by ambipolar diffusion of photocarriers in the depth of the film. The effects of tail-to-tail recombination and photocarrier diffusion on the local LID creation are investigated by comparing the exposure temperature dependence on N(x) with that of photocarrier diffusion length. Numerical simulations are also performed in order to model the depth profile of carrier recombination. 1. M. Stutzmann, W.B. Jackson and C.C. Tsai, Phys. Rev. Lett. B 32 (1985) 23. 2. J.H. Zhou, M. Kumeda and T. Shimizu, Appl. Phys. Lett. 66 (1995) 742.

4:00 PM A14.3
ILLUMINATION- AND ANNEALING-INDUCED CHANGES IN INFRARED AND RAMAN SPECTRA OF a-Si:H. L.-F. Arsenault, S. Lebib, E. Sacher and A. Yelon, Ecole Polytechnique, Department of Engineering Physics and Materials Engineering, Montreal, CANADA.

We have investigated the changes produced by light-soaking in both the IR and Raman responses of the Si-H stretching peaks near 2000 cm^{-1}. Our observations of the IR response are in qualitative agreement with those of Kong and co-workers [1]. That is, short-term light-soaking produces an increase in the intensity of the signal and a simultaneous shift to lower frequency. Exposure for times on the order of 100 h leads to non-monotonic changes. In contrast, short-term light-soaking decreases the total intensity of the Raman signal in the 2000-2100 cm^{-1} range (normalized to the phonon peak at approximately 530 cm^{-1}). In both cases, these modifications are reversed by annealing at 200°C. We suggest that these changes may be attributed to changes in the environment of the Si-H bonds, which result in a transfer of intensity between IR and Raman matrix elements. Details of the evolution of the components of the Raman spectrum between 1970 and 2150 cm^{-1}, under illumination, are presented and compared with IR changes in the same range. [1] Y. Zhao, D. Zhang, G. Kong, G. Pan and X. Liao, Phys. Rev. Lett. 74, 558 (1995); S. Sheng, G. Kong and X. Liao, Solid State Commun. 116, 519 (2000).

4:15 PM A14.4
IS INTERSTITIAL HYDROGEN PLAYING A ROLE IN THE STAEBLER-WRONSKI EFFECT? C. Longeaud, D. Roy, Laboratoire de Gènie Electrique de Paris, Gif sur Yvette, FRANCE.

We studied transport properties of many different series of a-Si:H samples prepared in radio-frequency powered deposition system. Samples were obtained from decomposition of pure silane or of mixtures of silane with argon, helium or hydrogen. The deposition pressures were ranging from 5 mTorr to 2.2 Torr, the RF power from 5 to 100 mW/cm^2 and two deposition temperatures were used 150°C and 250°C The samples were deposited onto glass and fitted with two coplanar parallel ohmic electrodes. We measured the dark and photo-conductivity, the density of states above the Fermi level by means of the modulated photocurrent technique and the minority carriers diffusion length L_d by means of the steady state photocarrier grating technique. All these measurements were performed in the as-deposited, light-soaked and annealed states. For all the samples the behaviour under light-soaking is the same: 2 mn of light-soaking are enough to increase the deep states density and after full saturation both the deep states and the conduction band tail exhibit a large increase. The result of the annealing process is sample dependent, the density of states being restored as in the as-deposited state for some samples or almost insensitive to the annealing process in some cases. Even some samples showed an increase of the deep defect density upon annealing at 460 K. To explain all these results, and particularly the increase of the deep defect density upon annealing, following some recent results on the properties of H in a-Si:H, we propose a mechanism of light-soaking/annealing in which interstitial hydrogen molecules could be involved. This mechanism could also explain the possibility of light-soaking at very low temperature where long range diffusion of H is absent and takes into account the fact that dangling bonds are not correlated with H atoms.

4:30 PM A14.5
THE STAEBLER-WRONSKI EFFECT AND 1/F NOISE IN AMORPHOUS SILICON. T. James Belich, J. Kakalios, School of Physics and Astronomy, The University of Minnesota, Minneapolis, MN.

Recent models of the microscopic origin of light induced conductivity degradation (the Staebler-Wronski effect) in hydrogenated amorphous silicon (a-Si:H) suggest that extended illumination can alter the long range disorder (LRD) present in the film due to potential fluctuations and compositional microstructure. We report experimental measurements of the light soaking dependence of both the Q-function (a comparison of the conductivity and thermopower activation energies) and the spectral wandering of 1/f noise (a measure of the non-Gaussian statistical character of the fluctuations) in n-type doped a-Si:H. There is a significant decrease in the spectral wandering of the non-Gaussian 1/f noise following light soaking of a device quality film, consistent with an increase in LRD. However, we find no corresponding change in the Q-function following illumination. For films deposited at lower temperatures (which thus contain more hydrogen microstructure) we also observe a shift in the spectral wandering after illumination, which is accompanied by a small change in the Q-function. By comparing the temperature dependence of the 1/f noise for films grown at varying substrate temperatures we find that the light-induced changes in the LRD appear to depend on the annealed state resistance value of the a-Si:H film. This research is supported by NREL/AAD-9-1866-13 and the University of Minnesota.

4:45 PM A14.6
DEFECT CREATION BY ELECTRON BEAM IRRADIATION IN AMORPHOUS SILICON NITRIDE FILMS COMPARED WITH THAT BY LIGHT SOAKING. Tatsuo Shimizu, Yuji Kawashima, Minoru Kumeda, Kanazawa Univ, Dept of Electrical and Electronic System Engineering, Kanazawa, JAPAN.

Creation mechanism of metastable dangling-bond defects in a-Si:H-related materials is an important issue for clarifying the origin of the Staebler-Wronski effect. It is well known that the intensity of the ESR signal due to Si dangling bonds increases by light soaking. The increased ESR signal has the same shape, linewidth and g-value as those before the light soaking. It is interesting to compare the defect creation mechanism by light soaking with that by electron-beam irradiation. We found the change in the ESR signal by electron-beam irradiation in a-Si-N:H films. The acceleration voltage of the electron beam was 20 kV. For the film with x (atomic ratio N/(N Si)) = 0.06, the ESR spin density increases by the electron-beam irradiation without changes in the g-value. However, for the film with x = 0.47, the ESR spin density increases with accompanying the decrease in the g-value from 2.0042 to 2.0034. The linewidth almost unchanged in spite of the decrease in the g-value. The decrease in the g-value is thought to be caused by an increase in the fraction of Si dangling bonds with increasing number of the backbonding N neighbors. Judging from the comparison of the observed g-value with the theoretically simulated one in the sample with x = 0.47 before irradiation, Si dangling bonds appears to locate preferentially at Si-rich regions, i.e., they have a smaller number of backbonding N atoms than expected from the random attachment. The bandgap-light irradiation gives rise to Si dangling bonds with a similar environment as before the irradiation, while in the case of the electron beam irradiation excited electrons have larger energy than in the case of the bandgap-light irradiation. Hence Si dangling bonds are created randomly without the preference of Si-rich region.

SESSION A15: MICROCRYSTALLINE SILICON SOLAR CELLS
Chair: David E. Carlson
Thursday Morning, April 19, 2001
Metropolitan III (Argent)

8:30 AM A15.1
ASSESSMENT OF THE USE OF MICROCRYSTALLINE SILICON MATERIALS GROWN AT RATE OF 15 Å/S AS I-LAYER MATERIAL FOR SINGLE AND MULTI-JUNCTION SOLAR

CELLS. S.J. Jones, R. Crucet, R. Capangpangan, M. Izu and S.R. Ovshinsky, Energy Conversion Devices, Inc., Troy, MI; A. Banerjee, United Solar Systems Corp., Troy, MI.

A microwave-based technique has been used to prepare microcrystalline Si materials at rates of 15-20 Å/s with the best films made using rates near 16 Å/s. In this manuscript, the use of these materials as i-layers for single and multi-junction devices will be assessed. Since the high deposition rates allow for fabrication of the required thicker microcrystalline Si i-layers in a similar amount of time to those used for high quality a-SiGe:H i-layers (rates of 1-3 Å/s), the materials can be tested as a low cost replacement for a-SiGe:H bottom cell i-layers in a-Si:H/a-SiGe:H and a-Si:H/a-SiGe:H/a-SiGe:H multi-junction cells. Single-junction nip, a-Si:H/microcrystalline Si and a-Si:H/a-SiGe:H/microcrystalline Si devices have been fabricated. For these devices, the doped and amorphous layers were made using standard PECVD practices and separate deposition equipment from that used to fabricate the microcrystalline Si materials. Presently for the single-junction devices, stable 7% efficiencies have been achieved while pre-light soaked 9.8 and 11.2% efficiencies have been achieved for the tandem and triple-junction devices, respectively. The efficiencies for the single-junction devices degrade by only 0-2% after long term (1000 hrs.) of light soaking demonstrating a high degree of stability. To increase these efficiencies, work is presently being done to alter the film microstructure through alteration of the deposition conditions. The manuscript will discuss which cell parameters (open circuit voltage, fill factor, short circuit current) limit the efficiency and how determination of the limiting parameters depends on the cell structure (single, tandem, triple-junction) used. Also the ability to achieve improvements in the cell efficiencies and the best potential use for these materials in a device structure will be assessed.

8:45 AM A15.2
STRUCTURAL PROPERTIES OF MICROCRYSTALLINE Si SOLAR CELLS. Martina Luysberg, Carsten Scholten, Lothar Houben, Institut of Solid State Research, Research Center Jülich, GERMANY; Oliver Vetterl, Reinhard Carius, Friedhelm Finger, Institute of Photovoltaics, Research Center Jülich, Jülich, GERMANY.

The structural properties of high efficiency microcrystalline nip solar cells grown by plasma enhanced chemical vapour deposition are investigated by transmission electron microscopy and Raman spectroscopy. First, n-type contact layers are deposited on textured ZnO substrates choosing highly crystalline growth conditions, in order to achieve high conductivity. Secondly, intrinsic absorber layers are grown with different SiH_4 dilutions in H_2 onto the n-μc-Si. Thirdly a p-type μc-Si layer is grown followed by the deposition of the ZnO front contact. In all cases investigated columnar structures of the microcrystalline silicon layers are observed. The columns consisting of highly twinned crystallites always extend perpendicular to the textured TCO substrate's surface resulting in a fan-like arrangement at the cusps. The nucleation of the n-layer on the ZnO substrate shows a high density of randomly orientated crystallites forming a porous layer, which is in agreement with our previous observations for the growth of highly crystalline Si films e.g. on glass substrates. Thus, the nucleation of μc-Si on TCO is similar to that on glass substrates. The nucleation of the intrinsic μc-Si:H on top of the n-layer follows a local epitaxy. This is concluded from two observations: (i) In case of highly crystalline i-layers, the interface to the n-layer cannot be detected by TEM, revealing a perfect epitaxy of individual crystallites with respect to the nuclei of the n-layer. (ii) Towards amorphous growth conditions, crystalline columns extending throughout the whole layer are embedded in an amorphous matrix also containing small crystallites. This is in contradiction to the growth on glass substrates, where small crystallites embedded in an amorphous matrix are formed through heterogeneous nucleation. Therefore, the structural properties of the intrinsic μc-Si:H are determined by the presence of the crystalline nuclei within the n-layer.

9:00 AM A15.3
IMPROVED INTERFACE BETWEEN FRONT TCO AND MICROCRYSTALLINE SILICON P-I-N SOLAR CELLS. Evelyne Vallat-Sauvain, Sylvie Faÿ, Ulrich Kroll, Johannes Meier, Julien Bailat, Arvind Shah, University of Neuchatel, Institute of Microtechnology, Neuchatel, SWITZERLAND.

In thin-film silicon solar cells with the superstrate configuration (e.g. glass, conductive oxyde, p-i-n) it is essential, for the realisation of high-efficiency devices, to obtain a good electrical contact between the front conductive oxyde (TCO) and the p-type silicon. An improved interface between the TCO and the p-layer will avoid for unintentionnal barrier or series resistance apparition, which decrease sensitively the fill factor of the p-i-n device. In this paper, a study of the interface between zinc oxyde (ZnO) and microcrystalline silicon (μc-Si:H) p-layers will be presented. Zinc oxyde was deposited on glass by Low Pressure Chemical Vapor Deposition (LPCVD). Scanning Electron Microscopy (SEM) observations of these layers reveal that the surface topography consists of regular pyramids. X-Rays studies of this TCO show that a preferential growth with the c-axis parallel to the substrate ((110) crystallographic texture) takes place. Boron-doped microcrystalline hydrogenated silicon (p-μc-Si:H) layers were grown by Very High Frequency (VHF) Glow Discharge at 70 MHz. Transmission Electron Microscopy (TEM) studies of the interface between the ZnO layer and the p-microcrystalline silicon show a surprising good matching between the ZnO (102) planes and the silicon (220) planes. This observation is in agreement with the tabulated values for the interplanar distance $d_{Si(220)}$=0.19201 nm and $d_{ZnO(102)}$=0.1911 nm; This results in a lattice mismatch Δd/d of only 0.48%. Such a good lattice matching suggests that the growth of p-μc-Si:H on ZnO is epitaxial, providing, hence, an excellent electrical contact; this is confirmed by IV curves and Spectral Response measurements on the corresponding μc-Si:H solar cells.

9:15 AM A15.4
TAILORING THE STRUCTURE OF LOW-TEMPERATURE-DEPOSITED MICROCRYSTALLINE SILICON FILMS BY BIASING THE SUBSTRATE. Mario Birkholz, Burkhardt Selle, Walther Fuhs, Hahn-Meitner-Institut, Silizium-Photovoltaik, Berlin, GERMANY; D.L. Williamson, Department of Physics, Colorado School of Mines, Golden, CO.

Thin polycrystalline silicon films as prepared with a low thermal budget at low temperatures are structurally characterized by small grains exhibiting grain sizes on the order of magnitude of 10 nm. Applications in photovoltaics and microelectronics, however, necessitate larger grain sizes to enable reasonable mobility of electronic charge carriers. We present the results of structural investigations (Raman and FTIR spectroscopy, RBS, XRD, SAXS) of thin silicon films that were prepared at 325°C and 0.93 Pa from silane-hydrogen mixtures by electron-cyclotron resonance chemical-vapor deposition (ECR CVD). The effect of biasing the substrates during the deposition has been investigated in the range of positive dc susceptor biases V_S from 0 to 45 V. For stainless steel substrates with an artificially enlarged surface roughness (smart substrates) an increase of the crystallinity could be observed with Raman spectroscopy that was associated with a reduction of the FWHM of the c-Si LO/TO peak down to 6.3 cm^{-1}. This value is close to that of a Si wafer measured under the same conditions of 3 cm^{-1} and is the smallest value ever obtained in our deposition experiments. Films prepared under a susceptor bias of 15 V exhibited a texture inversion of preferential (110) to (111) oriented grains, which was accompanied by an increase in grain size from 18 to 42 nm. Small-angle X-ray scattering (SAXS) revealed the films as deposited on Al foil to exhibit significant free volume fractions (microvoids) and slight increases in the fraction with increasing V_S. The ability of tailoring the structure of thin Si films by applying a susceptor bias is discussed in terms of controlling the ion flux to the surface of the growing film. This can efficiently be achieved in an ECR system, where the average mean free path of gas particles exceeds the thickness of the plasma sheath.

9:30 AM *A15.5
MICROCRYSTALLINE SILICON THIN-FILM SOLAR CELLS PREPARED AT LOW TEMPERATURE USING RF-PECVD. Yoshiyuki Nasuno, Michio Kondo, Akihisa Matsuda, Thin Film Silicon Solar Cells Super Lab., Electrotechnical Laboratory, Ibaraki, JAPAN.

Low temperature processing for high performance solar cells based on hydrogenated microcrystalline silicon (μc-Si:H) has been developed using a conventional RF plasma enhanced chemical vapor deposition (PECVD) technique at an excitation frequency of 13.56 MHz. Among pin type solar cells, it is found that deposition temperature of i-layer lower than 180°C is effective particularly for improving open circuit voltage (Voc). Carrier density of undoped μc-Si arising from oxygen-related donors abruptly decreases for deposition temperatures lower than 180°C and the improvement of Voc is ascribed to a decrease of shunt leakage current arising from the oxygen-related donors. This implies that oxygen-related donors can be passivated at low deposition temperatures probably owing to hydrogen. As a consequence, conversion efficiency of 8.9% (Voc = 0.51V, Jsc = 25mA/cm^2, FF = 0.70) has been obtained on Asahi-U substrate in spite of an oxygen concentration of 2×10^{19} cm^{-3} in combination with optimization of underlying p- layer. Effect of deposition temperature of i-layer upon other solar cell parameter, short circuit current (Jsc) and fill factor (FF) is also discussed. And a texture of transparent conductive oxide (TCO) substrate has been optimized for μc-Si:H solar cells by using Ga-doped ZnO. The texture of the ZnO substrates was formed by the wet etching process using 0.5% HCl water solution at various etching time. Surface morphology of substrates was measured by atomic force microscopy (AFM). We defined average angle of surface textures as tanθ. The relationship between μc-Si solar cell performance and tanθ was studied. As a result, the highest efficiency of 9.4% (Voc = 0.526V, Jsc = 25.3mA/cm^2, FF = 0.710) in our study was obtained using an

optimized substrate texture ($\tan\theta = 0.08$). This efficiency is better than that of the cell prepared by VHF-PECVD, indicating that RF-PECVD is still promising for fabricating good performance μc-Si solar cells.

10:00 AM A15.6
THIN FILM poly-Si/a-Si MULTIBANDGAP TANDEM SOLAR CELLS WITH BOTH A LAYERS DEPOSITED BY HOT WIRE CVD. R.E.I. Schropp, C.H.M. van der Werf, M.K. van Veen, P.A.T.T. van Veenendaal, Z. Hartman, and J.K. Rath, Utrecht University, Debye Institute, Physics of Devices, Utrecht, THE NETHERLANDS.

The first poly-Si/a-Si multibandgap tandem solar cells have been made in which the two intrinsic absorber layers are deposited by Hot Wire CVD. Previously, we developed n-i-p type single junction cells on plain stainless steel using plasma deposited doped layers and hot-wire deposited intrinsic layers, where the i-layer is either amorphous or polycrystalline. The efficiency for a thin polycrystalline cell currently is 4.4%, while the efficiency for an amorphous cell recently has been improved to 7.2%. For the first time we have now combined these two technologies into one multibandgap tandem stack. In this tandem configuration, all doped layers, including the tunnel-recombination junction, were made of doped microcrystalline layers by plasma deposition. Both intrinsic layers were made by decomposing the primary source gas, silane, at hot filaments. For the two layers we used individually optimized parameters, such as gas pressure, filament temperature, substrate temperature, and hydrogen dilution ratio. The solar cell does not comprise an enhanced back reflector, but it does feature a natural mechanism for light trapping, since the poly-Si absorber is textured and all subsequent layers are deposited conformally. The total thickness is less than 2 μm. The deposition rate for i-layer deposition was higher than 10 Angstrom/s. The temperature was lower than 500 degrees C at all times. The efficiency that has been obtained with the first tandem cells was 8%.

SESSION A16: TRANSPORT IN μC-Si

Chair: Shingo Okamoto
Thursday Morning, April 19, 2001
Metropolitan III (Argent)

10:30 AM *A16.1
MICROSCOPIC ASPECTS OF CHARGE TRANSPORT IN HYDROGENATED MICROCRYSTALLINE SILICON. Antonín Fejfar, Jan Kocka, Institute of Physics, Academy of Sciences of the Czech Republic, Prague, CZECH REPUBLIC.

Charge transport in hydrogenated microcrystalline silicon (μc-Si:H) is determined by structure on several size scales: i) local atomic arrangement (¡1 nm), ii) crystalline grains and their boundaries (1-10 nm), iii) grain aggregates or columns (0.1-1 μm) and finally iv) features comparable to layer thickness (0.1-10 μm): incubation layer, transition to fully microcrystalline growth and further evolution of structure [1]. Standard techniques for characterization of microstructure (Raman spectroscopy, X-ray diffraction and IR absorption) and transport (dark conductivity, constant photocurrent method, SSPG) assume homogeneous material and average out structural effects. We have used AFM with conductive tip to resolve differences of local conductivities down to the nm sizes, i.e., the size of single grains (ii) [2]. Large grain aggregates or columns (iii) with preferential growth direction may lead to transport anisotropy and we developed methods to measure dark conductivity and ambipolar diffusion length parallel and perpendicular to the substrate to prove it [3]. As the structure evolves on still larger scale (iv), i.e., even after the transition to fully crystalline growth is completed, we observed changes of dark conductivity values as well the corresponding activation energies and prefactors. Other transport parameters, e.g. the diffusion length, also change with thickness. The importance of the thickness dependence will be illustrated by comparing results measured on thickness series of samples with different silane in hydrogen dilutions. Finally, we show how it enters as an important parameter into a growth model and corresponding effective medium model of the transport which predicts the observed thickness dependencies. [1] J. Kočka, A. Fejfar, V. Vorlíček, H. Stuchlíková, J. Stuchlík: MRS Proc. 557 (1999) 483. [2] B. Rezek, J. Stuchlík, A. Fejfar, J. Kočka: Appl. Phys. Lett. 74 (1999) 1475-1477. [3] J. Kočka et al: Polyse 2000, Saint Malo, France, to appear in 'Solid State Phenomena' series, Scitech Publ.

11:00 AM A16.2
CARRIER TRANSPORT IN ULTRA-THIN NANO/POLYCRYSTALLINE SILICON FILMS. T. Kamiya[a,b,d], Y.T. Tan[b,d], Y. Furuta[c,d], H. Mizuta[c,d], Z.A.K. Durrani and[b,d] H. Ahmed[b,d], [a]Materials and Structure Laboratory, Tokyo Institute of Technology, Midori-ku, Yokohama, JAPAN; [b]Microelectronics Research Center, Cavendish Laboratory, University of Cambridge, UNITED KINGDOM; [c]Hitachi-Cambridge Laboratory, Cambridge, UNITED KINGDOM; [d]CREST, JST, Shibuya, Tokyo, JAPAN.

We report on carrier transport in ultra-thin nano/polycrystalline (nc-/poly-Si) silicon films and nanowires. Nc-Si:H films were prepared by 100 MHz-VHF PECVD using a SiF_4, H_2 and SiH_4 gas mixture at 300°C and in situ doping with PH_3. 50 nm-thick poly-Si films were prepared by solid-phase-crystallization at 850°C for 30 min after ion-implanting the film with phosphorus atoms. The nanowire structure was defined by electron-beam lithography. In nc-Si:H films, Hall mobility increased from 0.1 cm^2/Vs to 1.8 cm^2/Vs as film thickness was increased from 10 nm to 50 nm. At larger thickness the mobility saturated, suggesting that an electron percolation path was formed through crystalline grains when the film thickness was greater than 50 nm. The crystalline volume fraction was ~70% for a 50 nm-thick film. These results suggested that crystalline grains were isolated by amorphous tissues in films of thickness less than 50 nm. 50 nm x 1000 nm nanowires were fabricated in 30 nm-thick nc-Si:H films. We observed Coulomb blockade effects at $<$16 K. Activation energy of conductivity increased with increasing temperature and decreasing width. The high temperature behavior is consistent with the percolation conduction model, i.e., the Fermi level in the amorphous tissues may have statistical fluctuations which result in a variety of conduction band offsets. In nanowire fabricated in as-deposited poly-Si, we did not observe Coulomb blockade effects. However, some nanowires exhibited non-linear I-V characteristics which may be explained by a thermionic emission model at the grain boundaries. The activation energy of conductivity depended on nanowire width and differed even if the nanowire dimensions were the same. These results indicate that grain boundary structures are different between nc-Si:H films and poly-Si films and that there is a direct proof of the variation in grain boundary potential barrier from our experiments.

11:15 AM A16.3
IMPROVEMENT IN ELECTRICAL PROPERTIES OF POLYCRYSTALLINE SILICON FILMS BY THE H_2O VAPOR ANNEALING METHOD. Toshiyuki Sameshima, Katsumi Asada, Yoshiyuki Tsunoda, Yoshiyasu Kaneko, Tokyo University of Agriculture and Technology, Faculty of Technology, Tokyo, JAPAN.

We discuss improvements of electrical properties of polycrystalline silicon (poly-Si) films and SiO_2/Si interfaces by high pressure H_2O vapor annealing. 50-nm thick poly-Si films were fabricated by irradiation with 30-ns-pulsed XeCl excimer laser at 400 mJ/cm^2 at room temperature. ESR measurements revealed that the poly-Si films had a high dangling bond density of $1.5x10^{18}$ cm^{-3}. Heat treatment at 310°C with $1.3x10^6$ Pa H_2O vapor markedly reduced the dangling bond density to $1x10^{17}$ cm^{-3}. The numerical analysis of the electrical conductivity using the finite-element method (FEM) combined with statistical thermodynamical conditions resulted in that heat treatment with high pressure H_2O vapor effectively made the defect states inactive Moreover the analysis revealed that the density of tail states were markedly reduced from $4x10^{18}$ cm^{-3} to $3x10^{17}$ cm^{-3} by the heat treatment. The density of SiO_2/Si interface trap stets was also effectively reduced from $1x10^{12}$ to $2x10^{10}$ $cm^{-2}eV^{-1}$ by the heat treatment for Al-gate MOS capacitors. The surface recombination velocity was reduced from 400 to 10 cm/s. We discuss improvement of characteristics of poly-Si thin film transistors (TFTs) fabricated with laser crystallization. The TFTs were heated at 270°C with $1.3x10^6$ Pa H_2O vapor. The threshold voltage were markedly reduced from 4.1 to 1.2 V because of the density of defect states at the SiO_2/Si interface and in poly-Si films were effectively reduced. The leakage current was also reduced to $5x10^{-15}$ A/μm. It means that the junction of drain/source were formed well due to defect reduction by the H_2O vapor annealing. The combination of high pressure H_2O vapor annealing with hydrogen or florin plasma treatment is also presented as the method of defect reduction of poly-Si film below 200°C.

11:30 AM A16.4
EVOLUTION OF THE MOBILITY GAP WITH THICKNESS IN HYDROGEN-DILUTED INTRINSIC Si:H MATERIALS IN THE PHASE TRANSITION REGION AND ITS EFFECT ON SOLAR CELL CHARACTERISTICS. R.J. Koval, J.M. Pearce, A.S. Ferlauto, R.W. Collins and C.R. Wronski, The Pennsylvania State University, Center for Thin Film Devices, University Park, PA.

Research has been carried out to probe the phase transitions between amorphous and microcrystalline silicon as a function of thickness using spectroscopic ellipsometry (SE) and atomic force microscopy (AFM) [1, 2]. In the study reported here, the insights obtained into the growth mechanisms and the evolution of microstructure in the intrinsic films from previous studies have been supplemented by the characterization of the electrical properties of the corresponding solar cells. To assess the effects of such phase transitions, cell structures without any phase transition regions and ones with phase transition at different depths in the i-layer from the p-contact have been

investigated. Experimental results are presented that clearly demonstrate the role of changes in mobility gap of the materials as their microstructure evolves with thickness, providing further support for the importance of the hydrogen dilution ratio R ($R=[H_2]/[SiH_4]$) on the transitions between the amorphous and microcrystalline phases. Room temperature light and dark J-V characteristics at different temperatures were measured on a variety of p(a-SiC:H)-i(Si:H)-n(mc-Si:H) solar cell structures with i-layers having different thicknesses and R values. Using the AMPS transport simulation code, both the light and dark J-V characteristics can be self-consistently modeled with an abrupt change in the mobility gap at the thicknesses determined from SE and AFM. It is also shown how the mobility gaps of both the amorphous and microcrystalline intrinsic-layer materials can be obtained from dark J-V measurements.

[1] J. Koh, Y. Lee, H. Fujiwara, C.R. Wronski, R.W. Collins, Appl. Phys. Lett. 73, 1526 (1998).
[2] A.S. Ferlauto, P.I. Rovira, R.J. Koval, C.R. Wronski, and R.W. Collins, Mater. Res. Soc. Symp. Proc. 609 (in press, 2000).

11:45 AM A16.5
FEMTOSECOND CARRIER DYNAMICS IN NANOCRYSTALLINE SILICON FILMS: THE EFFECT OF THE DEGREE OF CRYSTALLINITY. K.E. Myers[a], Q. Wang[b] and S.L. Dexheimer[a]. [a]Department of Physics and Materials Science Program, Washington State University, Pullman, WA. [b]National Renewable Energy Laboratory, Golden, CO.

We present studies of the ultrafast dynamics of photoexcited carriers in HWCVD nanocrystalline silicon thin films to address the underlying physics of carrier trapping and recombination processes. The degree of crystallinity is controlled by varying the H-dilution during deposition, yielding materials that span the transition from the amorphous to the nanocrystalline state, with increasingly larger grain size and crystalline fraction at higher dilution values. Time-resolved measurements of the carrier dynamics were carried out using a femtosecond pump-probe method, in which a short pump pulse excites carriers in the sample and a time-delayed probe pulse measures the resulting change in the optical properties as a function of the pump-probe delay time. The thin film samples were excited with pulses 35 fs in duration centered at 1.55 eV, which corresponds to a transition energy in the region of enhanced optical absorption in nanocrystalline silicon. Probe pulses of variable wavelength were produced using a femtosecond white-light continuum. Photoexcitation of carriers resulted in an induced absorbance signal that shows a nonexponential time dependence strongly dependent on excitation density. For pump-probe delay times greater than $\sim$1 ps, the response is well characterized by bimolecular recombination, with a recombination constant of similar magnitude to that observed on picosecond time scales in a-Si:H and related materials, together with an additional, slowly relaxing component. However, at short times, the response of nanocrystalline silicon differs dramatically from that of the amorphous materials, showing a rapid relaxation component with an amplitude that correlates strongly with H-dilution. The measurements indicate the presence of rapid carrier interactions in the nanocrystalline grain and grain-boundary regions that are distinct from those associated with band tail states in a-Si:H.
This work is supported by NREL and by NSF.

SESSION A17: THIN FILM TRANSISTORS
Chair: James B. Boyce
Thursday Afternoon, April 19, 2001
Metropolitan III (Argent)

1:30 PM *A17.1
TECHNOLOGICAL DEVELOPMENT OF LOW TEMPERATURE POLY-Si TFT-LCD. Katuhiro Kawai, Akihiko Imaya, Sharp Corporation, Liquid Crystal Laboratories, Tenri, JAPAN.

The display market has been changing with the emerging of the new application, Mobile display terminal. The display is trying to be more compact and more versatile by integrating the functions. The Low Temperature Poly Silicon TFT is one of the most expected device to realize the integrated circuits on the display panels. In this presentation, the technology of Low Temperature Poly Silicon TFT-LCD is summarized and the future directions of the technology, equipment, and applications are discussed.

2:00 PM A17.2
P-CHANNEL POLYCRYSTALLINE SILICON THIN FILM TRANSISTORS ON STEEL FOIL SUBSTRATES. Ming Wu and Sigurd Wagner, Princeton University, Department of Electrical Engineering, Princeton, NJ.

Steel foil is an attractive alternative to plastic substrate for large-area electronic backplanes. Amorphous and polycrystalline silicon transistors have been made on steel foil as thin as 3 μm. Despite the large difference in thermal expansion coefficients α between stainless steel ($\alpha = 18{\cdot}10^{-6}/°C$) and transistor materials ($\alpha \approx 3{\cdot}10^{-6}/°C$), silicon on steel can be cycled between room temperature and 950°C without incurring electrical or mechanical damage. We have been focusing at TFT-on-steel fabrication at high temperature with the goal of adopting integrated circuit processes, analogous to the fabrication of polysilicon TFTs on quartz glass. Here we report the successful fabrication of p-channel TFTs. 200 μm stainless steel foil was coated on both sides with $\sim$0.5 μm SiO_2 for passivation and electrical insulation. 160 nm a-Si:H was deposited by plasma enhanced chemical vapor deposition (PECVD) at a substrate temperature of 150°C, and then furnace crystallized at temperatures/times of 750°C/2min or 950°C/20sec. The TFTs were made with a self-aligned process reaching a maximum temperature of 700°C. 150 nm gate SiO2 was deposited by PECVD at 350°C, and 200 nm n^+ a-Si:H by PECVD at 270°C and then patterned by reactive ion etching to form the eventual gate. The SiO_2 layer was wet etched to open the source and drain, which were boron-ion implanted at 35 keV and a dose of $2{\cdot}10^{15}$ cm^{-2}. The implant damage was annealed out and the gate silicon crystallized by a 30-min furnace anneal at 700°C, which was the maximum device process temperature. Then a 200 nm SiO_2 passivation layer was deposited by PECVD at 250°C, and source/drain and gate contact windows were opened by wet etch of the SiO_2. 200 nm Al was thermally evaporated and patterned to form the source/drain and gate electrodes. Finally, the TFTs were annealed in forming gas at 250°C. The TFTs made from 950°C and 750°C polysilicon have hole field effect mobilities of 22 $cm^2V^{-1}s^{-1}$ and 14 $cm^2V^{-1}s^{-1}$ in the linear regime. The drain current ON/OFF ratio and the OFF current at 10 V drain-source voltage are $\sim 10^6$ and 4×10^{-10}A in both cases. These results suggest that the polysilicon films were not contaminated from the metal substrate. The successful fabrication of p-channel polysilicon TFTs is an important step toward a high temperature CMOS technology on steel foil. This work is supported by the DARPA MLP program.

2:15 PM A17.3
TOWARDS AN ALL HOT WIRE TFT: SILICON NITRIDE AND AMORPHOUS SILICON DEPOSITED BY HOT WIRE CHEMICAL VAPOR DEPOSITION. B. Stannowski, M.K. van Veen and R.E.I. Schropp, Utrecht University, Debye Institute, Physics of Devices, TA Utrecht, THE NETHERLANDS.

We developed silicon nitride layers with good electronic quality by the Hot Wire Chemical Vapor Deposition (HWCVD) technique. Stochiometric layers (Si_3N_4) with a hydrogen content as low as 9.2 at.-% were deposited at a substrate temperature of 340 degrees C. Previously, Thin Film Transistors (TFTs) incorporating hot wire deposited amorphous silicon have been shown to exhibit state-of-the-art performance and a superior stability upon gate-bias stress. Thus far, the gate dielectric used in such TFTs was glow-discharge silicon nitride or thermally grown silicon oxide. Presently, hot wire deposited silicon nitrides have been incorporated as the gate dielectric in bottom gate transistors with a hot wire deposited amorphous silicon layer on top. The silicon was deposited at a temperature of only 250 degrees C and at a deposition rate of 1 nm/s. Preliminary TFTs exhibit a field effect mobility of around 0.3 cm^2/Vs. This shows that the critical interface in TFTs, namely that of the insulator/semiconductor channel region, can be produced in an all hot wire process. In the paper we present the electrical and structural properties of hot wire deposited silicon nitride as well as characteristics of TFTs incorporating this material.

2:30 PM A17.4
JET-PRINTED FABRICATION OF a-Si:H THIN FILM TRANSISTORS AND ARRAYS. W.S. Wong, S.E. Ready, R. Matusiak, S.D. White, R. Lau and R.A. Street, Xerox Parc, Palo Alto, CA.

Direct write technologies for materials processing presents opportunities to enhance conventional large-area electronic device manufacturing. For example, directly printing or writing of mask features onto a substrate or thin film, eliminating the need for standard photolithography, can reduce the complexity and cost for amorphous silicon large-area displays and image sensors. However, applications to matrix-addressed arrays require minimum feature sizes no greater than 20-30 μm and similar layer-to-layer registration, which has so far proved difficult to achieve. The spatial control of jet-printing makes it an ideal technology for implementing the direct writing of etch masks. We have demonstrated etched feature sizes below 25 μm in films of a-Si:H, a-Si_3N_4 and metals, using a combination of small drop volume and a wax medium that allows control over substrate wetting. Layer registration accuracy of better than 20 μmm was also achieved over print areas of about 5x5 cm^2. Based on this methodology, we have fabricated a-Si:H thin-film transistors (TFTs) processed using printed wax masks in place of conventional lithography. Bottom-gate TFTs with source-drain

contacts overlapping the channel were created using a four-mask process. The TFTs have I-V characteristics comparable to photolithographically patterned devices, with mobility of 0.6-0.9 cm^2/Vs, threshold voltage of 2-3 V, and on/off ratios exceeding 10^7, for devices with channel lengths below 50 μm. We will discuss the critical parameters affecting feature size and printed wax-mask resolution. Having established a small feature size printed-TFT process, we will discuss the design and implementation of active-matrix pixels.

2:45 PM A17.5
TFTS WITH 50 NM THICK DEPOSITED NANOCRYSTALLINE SILICON CHANNEL LAYER, 10 $CM^2V^{-1}s^{-1}$ ELECTRON MOBILITY AND 10^8 ON/OFF RATIO. Robert Min, Sigurd Wagner, Princeton Univ, Dept of Electrical Engineering, Princeton, NJ.

Directly deposited nanocrystalline silicon (nc-Si:H) can sustain n and pchannel thin film transistor (TFT) operation. Because nc-Si:H is grown similar to hydrogenated amorphous silicon but is capable of CMOS operation, it is a desirable candidate for monolithic, fully integrated electronic backplanes. To date, high performance nc-Si:H TFTs have been made from relatively thick ($\sim$300 nm) nc-Si:H films, which require impractically long growth times and cause high TFT OFF currents. Here we report an n channel TFT made from a 50-nm thick nc-Si:H layer and an OFF current of $\sim 10^{-14}$ A/μm. The TFT is made in a top gate configuration. 50 nm of nc-Si:H was deposited directly on Corning 1737 glass by plasma enhanced chemical vapor deposition (PECVD) from a mixture of SiH_4, SiF_4 and H_2. The growth temperature was 350°C and the growth time 15 minutes. Without breaking vacuum an 80 nm n layer was deposited next from SiH_4, H_2 and PH_3. The doped layer was patterned by reactive ion etching (RIE) to define the channel with length / width = 180 μm/ 45 μm and form the source and drain layers. Then the TFT islands were defined by RIE. A 250 nm SiO_2 gate dielectric layer was deposited at 250°C by PECVD. The source / drain contact holes were wet etched into the SiO_2, and Al was thermally evaporated and patterned to form source, drain and gate electrodes. The TFT ON and OFF currents are $\sim 7\times10^{-5}$ A and 10^{-12} A respectively. The electron field effect mobility of 10 $cm^2V^{-1}s^{-1}$ suggests well developed crystallinity at the top of the thin nc-Si:H layer. This result agrees with experimental observations, such as the evolutionary phase diagram of Collins et al., which show that PECVD films grown on amorphous substrates can be made crystalline over a small film thickness. Even though the process technology for the present top gate transistor needs improvement, the relatively short deposition time combined with low OFF current and high electron mobility constitute important steps toward fully integrated silicon backplanes with low power consumption. This research is supported by the DARPA HDS program and the New Jersey Commission on Science and Technology.

SESSION A18: SENSORS

Chair: Antonin Fejfar
Thursday Afternoon, April 19, 2001
Metropolitan III (Argent)

3:30 PM A18.1
TWO-DIMENSIONAL AMORPHOUS SILICON COLOR SENSOR ARRAY. F. Lemmi, M. Mulato, J. Ho, R. Lau, J.P. Lu and R.A. Street, Xerox Palo Alto Research Center, Palo Alto, CA.

This paper reports on the first full realization and characterization of a two-dimensional array of amorphous silicon (a-Si:H) color sensors, addressed by integrated amorphous silicon-based thin-film transistors (TFTs). The array includes 512 x 512 pixels with 75-μm pitch, or about 340 dpi. Each pixel features a color sensor realized by a p-i-n-i-p stack of doped and undoped a-Si:H layers, and a TFT. The color sensors are made of two anti-serial p-i-n diodes, which selectively sense the illumination according to the polarity of the applied bias voltage. The sensor layers are grown on top of the TFTs to improve the array fill factor. The p-i-n-i-p sensor stack is mesa-isolated into single sensors to reduce cross-talk. Images are acquired using two bias voltages and yield the red and blue/green components of the original with a good color separation. An image is reconstructed using the information from the two images acquired. Aside a color bias, which is expected for a two-color reconstruction, the imaging system proves to be working very well. In particular, the array shows very low leakage currents, which enable a very large dynamic range and sensitivity. In the response of the array to a light pulse, the bottom thick diode ensures a fast drop in the signal after the flash, while the top thin diode exhibits some residual image lag.

3:45 PM A18.2
DESIGN AND MODELING OF OPTICAL SENSORS IN MULTI-CHANNEL TECHNOLOGY. Dietmar Knipp, Helmut Stiebig, Research Center Juelich, Institute of Photovoltaics, Juelich, GERMANY; Patrick Herzog, Aachen University of Technology, Technical Electronics Department, Aachen, GERMANY.

Multi-channel sensors realized by vertically integrated diodes have been developed. Due to the wavelength dependent absorption of amorphous silicon alloys and the design of the multi-layer stack the spectral sensitivity in the individual diodes can be adjusted. For a three-channel sensor mainly blue light is absorbed in the top diode and green light in the second diode, whereas red light mainly determines the photocurrent of the third diode. Nevertheless, the color recognition of multi-channel sensors is limited by a mismatch between the spectral sensitivity of the sensor and the human eye. The realization of an absorption layer with a low product of the layer thickness and the absorption coefficient limit the blue sensitivity of the top diode. Particularly, on one hand there is a lack of absorption materials with high optical band gap (>2.3eV) and good electrical properties. On the other hand, the thickness of the diodes can only be reduced to a certain extent, since the dynamic reduces by decreasing the layer thickness due to a decrease of the photocurrent and an increase of the dark current caused by micro shunts. As a consequence the spectral sensitivity of the top diode is widened and a further decrease of the color error of the sensor is restricted. These limitations can be reduced by a smart utilization of interference effects within the multi layer stack, which occur as a consequence of reflections of light especially at the interface of amorphous silicon and the transparent contact layers. The paper will present optical calculations of the spectral sensitivities of each diode as a function of the design of the multi-layer stack and the applied absorption materials and the simulations will be compared with data of realized multi-channel sensors.

4:00 PM A18.3
PERFORMANCES PRESENTED BY A 32 LINEAR ARRAY POSITION SENSITIVE DETECTOR BASED ON PIN a-Si:H STRUCTURES. Rodrigo Martins, João Figueiredo, Fernando Soares, Donatello Brida, Vitor Silva, Ana Cabrita, Andreia Lopes, Elvira Fortunato.

In this paper we will present the details of the fabrication process and of the performances exhibited by a position sensitive detector constituted by an integrated array of 32 one-dimensional amorphous silicon thin film position sensitive detectors, with a total active area size below $1cm^2$. The main emphasis will be put on the device linearity, its spatial resolution and response time, that makes it one of the most interested analogue sensor detector to be used in unmanned optical inspection control system, where a continuous detection process is required. This characteristic makes these devices more adequate for this type of operation, even when compared with the actual CCD matrix detector systems, open so a new field of a wide range of applications of amorphous silicon based devices.

4:15 PM A18.4
MECHANISMS OF CROSS-TALK IN LARGE AREA a-Si:H CONTINUOUS IMAGE SENSORS. M. Mulato, J.P. Lu, S.E. Ready, K. Van Schuylenbergh, J. Ho, R. Lau, J.B. Boyce and R.A. Street, Xerox Palo Alto Research Center, Palo Alto, CA.

High sensitivity and resolution (pixel pitch smaller than 100 μm) large area two-dimensional imagers, used for X-ray medical applications such as mammography and also CMOS sensors, can only be satisfactorily manufactured through the use of the high fill factor design. The increased performance is achieved by depositing a continuous a-Si:H layer over the whole surface area of the array. A buried material with low dielectric constant insulates the sensors from the TFT addressing electronics. This structure brings the possibility of extra parasitic capacitance in the addressing data lines and lateral conduction between pixels. Optimization of the array is a complex materials problem involving the dielectric, the interface to the a-Si:H sensor and the array operation. We have explored different dielectric materials to simultaneously minimize the capacitance and interfacial conduction. This involves new insulator materials such as polymer-based resins that can be made thicker than the standard silicon oxynitride. We have studied the interfacial conduction in detail both by experiments and simulations, and have identified three mechanisms for this process. There is an asymmetric image spreading caused by a parasitic TFT that is mainly dominated by the imager operation conditions, i.e. the presence of the gate address lines and their addressing sequence. We show that the undesired asymmetric image spreading can be controlled. There also is an interfacial conduction that depends on the details of the processing of the insulator and a-Si:H film. Finally, there is a field-dependent electron injection mechanism at the edge of the sensor that arises when the pixel approaches saturation. Images from 512x512 sensor arrays illustrating these effects will be shown.

4:30 PM A18.5
TAILORED LASER SCANNED PHOTODIODES (LSP) FOR IMAGE RECOGNITION. M. Vieira, M. Fernandes, P. Louro, R.

Schwarz, Electronics and Communications Dept., ISEL, Lisboa, PORTUGAL; M. Schubert, Institut fur Physikalische Elektronik, Universitat Stuttgart, Stuttgart, GERMANY.

A tailored ZnO:Al/a-pin Si_xC_{1-x}:H/Al configuration for the laser scanned photodiode (LSP) imaging detector is proposed. The LSP utilises self- field-induced depletion layers as detector and a laser beam for readout. The LSP consists of a single sensing p-i-n Si_xC_{1-x}:H photodiode; a front transparent and a back metal gates to tailor and collect the photogenerated charges, and a low-power modulated laser scanner for the sequential readout. The effect of the sensing element structure (layers composition and thickness), cell configuration (homostructure or heterostructure), and light source flux (intensity and wavelength) are investigated and correlated with the sensor output characteristics. Data reveal that the sensitivity, the responsivity, the spatial resolution and the noise are limited by the cell configuration while the linearity depends mainly on the i-layer thickness, on the light source flux and on the wavelength used to map the image onto the sensor. In the tailored configuration the higher optical gap and the lower conductivity of the doped a- Si_xC_{1-x}:H (2.2 eV, 2×10^{-12} Ω^{-1} cm^{-1}), when compared either with the intrinsic a-Si:H layer (1.8 eV, 7×10^{-11} Ω^{-1} cm^{-1}) or with the doped layers in the homostructure (1.8 eV, 1.8×10^{-5} Ω^{-1} cm^{-1}) are responsible by an induced inversion layer at the illuminated interfaces which blocks the carrier collection. Those insulator-like layers act as MIS gates that prevent excess signal charge from blooming to the nearby dark regions which could lead to image smearing. The optical-to-electrical transfer characteristics show high quantum efficiency, broad spectral response, low dark current and reciprocity between light intensity and image signal intensity only limited by the i-layer thickness and doped layer composition. By using tailored heterostructures an increase on the image signal optimised to the blue response is achieved with a responsivity of 0.1 mW/cm^2 and a spatial resolution of 50 μm.

4:45 PM A18.6
PIEZORESISTIVE SENSORS ON PLASTIC SUBSTRATES USING DOPED μc-Si:H. P. Alpuim, V. Chu, INESC, Instituto de Engenharia de Sistemas e Computadores, Lisbon, PORTUGAL; J.P. Conde, Dept of Materials Engineering, Instituto Superior Técnico, Lisbon, PORTUGAL.

The piezoresistive behavior of optimized n-type and p-type microcrystalline silicon films deposited on PET (polyethylene terephthalate) by hot-wire (HW) and radio-frequency plasma-enhanced chemical vapor deposition (RF) at a substrate temperature of 100°C was studied. A 4-point bending jig allowed the application of positive and negative strains in the films. The piezoresistive response of the films when subjected to strain was evaluated from the formula $\Delta R/R=\eta\times\epsilon$, where R is the resistance of the sample, η the gauge factor and ϵ is the strain. Repeated measurements of the relative changes in the resistance of the samples, $\Delta R/R$, during the strained condition showed reversible behavior, with p-type microcrystalline films having positive gauge factor in the range from 15 to 30 and n-type μc-Si:H films having negative values of gauge factor from -52 to -17. The induced strain in the films was in the range between 0 and $\pm0.3\%$. The resistance of the doped μc-Si:H samples was of the order of 100 kΩ. The crystallite size was 10 nm for HW films and 6.5 nm for RF films and the crystalline fraction was between 50 and 80%. The microscopic origin of the piezoresistance in doped microcrystalline silicon will be discussed. The comparative behavior of HW and RF samples as well as p- and n-type will be related to their structural and optoelectronic properties. The absolute value and the sign of the gauge factor will be compared to those for polycrystalline silicon and crystalline silicon from the literature. This piezoresistive property can be exploited to make sensors which detect shape changes in flexible surfaces.

SESSION A19: POSTER SESSION
METASTABILITY III
Chair: Howard M. Branz
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A19.1
MODEL OF HYDROGEN-MEDIATED METASTABLE CHANGES IN A TWO-PHASE AMORPHOUS SILICON NETWORK. Jonathan Baugh, Daxing Han, Dept of Physics and Astronomy, Univ of NC, Chapel Hill, NC.

A phenomenological model for the light-induced metastability of a-Si:H is proposed in which a two-phase model of the amorphous network plays a central role. Boundaries between high and low density phases are postulated to be associated with the majority of the clustered Si-H detected by NMR in a-Si:H. Weakly bonded hydrogen at these boundaries catalyzes microstructural changes in the Si network in the presence of high carrier concentrations, leading qualitatively to both the gross structural changes and the increase in electronic defect density that are observed experimentally. Such changes are analogous to H-mediated structural changes that have been observed experimentally in a-Si:H and μc-Si:H [1]. Entropy increase and reduction of lattice-strain energy drives structural change under light-soaking, whereas minimization of local atomic-positional energy effectively reverses the changes during annealing. [1] I. Kaiser, N.H. Nickel, W. Fuhs and W. Pilz, Phys. Rev. B 58, R1718 (1998).

A19.2
DEFECT DENSITY PROFILING IN LIGHT-SOAKED AND ANNEALED HYDROGENATED AMORPHOUS SILICON SOLAR CELLS. Richard S. Crandall, National Renewable Energy Laboratory, Golden, CO; Jeffrey Yang and Subhendu Guha, United Solar Systems Corp., Troy, MI.

The fundamental ingredient lacking in solar cell modeling is the spatial distribution of defects. To correct this deficiency we have used drive-level capacitance profiling (DLCP) on hydrogenated amorphous-silicon (a-Si:H) n-i-p solar-cells. We find the following: Near the p-i interface the defect density is high, decreasing rapidly into the interior, reaching low values in the central region of the cell, and rising rapidly again at the n-i interface. The states in the central region are neutral dangling-bond defects whose density agrees with those typically found in similar films. However, those near the interfaces with the doped layers are charged dangling bonds in agreement with the predictions of defect thermodynamics.[1] We correlate the changes in solar cell efficiency owing to intense illumination with changes in the defect density throughout the cell. Defects in the central region of the cell increase to values typically found in companion films. In this presentation we will describe the measurements and interpretation of DLCP for solar cells with the aid of solar cell modeling using AMPS[2]. 1. H.M. Branz and R.S. Crandall, Solar Cells, 27, 159, (1989). 2. J.K. Arch, F.A. Rubinelli, and S.J. Fonash, J. App. Phys., 69, 7057, (1991).

A19.3
LAPLACE-TRANSFORM TRANSIENT PHOTOCURRENT SPECTROSCOPY AS A PROBE OF METASTABLE DEFECT DISTRIBUTIONS IN HYDROGENATED AMORPHOUS SILICON. M.J. Gueorguieva, C. Main and S. Reynolds, School of Science and Engineering, Univ. of Abertay Dundee, UNITED KINGDOM.

Recently, several methods employing Laplace transformation of transient photocurrent data for determination of the density of electronic states in disordered semiconductors have been developed. The starting point in all such analyses is the linearised system of rate equations arising from the well-known multiple-trapping model. Upon Laplace transformation a Fredholm integral equation of the first kind is obtained, which is difficult to solve for the DOS due to its ill - posed nature. Several solution methods have previously been reported and investigated primarily by application to computer-simulated photocurrent decays. Some, employing mathematical approximations, are robust but suffer from diminished accuracy and are subject to an energy resolution limit of order kT [1,2]. An exact method developed by the authors [3], although capable of high accuracy and resolution, is more severely affected by the quality of the experimental data. Tikhonov regularisation [4], one of the most reliable methods for extracting physically important model functions from noisy experimental data, has also been brought to bear on the problem [5]. In order to assess the prospects for practical application of these various methods, we have analysed a set of photocurrent transients obtained from a PECVD-prepared hydrogenated amorphous silicon film subjected to increasing degrees of light-soaking. The results illustrate the compromise between energy resolution and sensitivity to fluctuations in the input data. [1] T. Nagase and H. Naito, J. Non-Cryst. Solids 227-230, 824 (1998). [2] N. Ogawa, T. Nagase and H. Naito, J. Non-Cryst. Solids 266-269, 367 (2000). [3] M.J. Gueorguieva, C. Main and S. Reynolds, MRS Spring 2000 meeting. [4] J. Weese, Computer Physics Communications 69, 99 (1992). [5] T. Nagase, K. Kishimoto and H. Naito, J. Appl. Phys. 86(9), 5026 (2000).

A19.4
DANGLING BONDS, HYDROGEN DISTRIBUTIONS, AND MODEL LINESHAPES OF ESR SIGNALS IN a-Si:H. P.A. Fedders, Department of Physics, Washington University, St. Louis, MO.

For many years it has been assumed widely that hydrogen is involved in some way in the formation of light induced defects. However recently some doubt has been cast on this because of experimental evidence that there is little H near light induced dangling bonds. In this paper we present a number model calculations comparing ESR spectra of dangling bonds with and without correlations with H positions. The above models include distributions of with H with correlations or anti correlations of nearby H, clustering of H, and

other features. In all cases the spectra are compared to those with no correlations or clustering. Our results coupled with published experimental data strongly suggest that dangling bonds are not correlated positively with the presence of nearby H and, in fact, it appears that light induced dangling bonds are negatively correlated with nearby H. Further we suggest how detailed information about the amounts, species, and clustering of hydrogen might be extracted from ESR measurements.

A19.5
FAST LIGHT-INDUCED CHANGE IN SPECTROSCOPIC ELLIPSOMETRY SPECTRA OF HYDROGENATED AMORPHOUS SILICON MEASURED THROUGH TRANSPARENT SUBSTRATE UPON BIAS LIGHT ILLUMINATION. Nobuhiro Hata, Electrotechnical Laboratory, Tsukuba, JAPAN; Charles M. Fortmann, State University of New York at Stony Brook, Dept. Applied Mathematics, Stony Brook, NY; Akihisa Matsuda, Electrotechnical Laboratory, Tsukuba, JAPAN.

We describe light bias induced change in the pseudo dielectric functions of a-Si:H, which were measured with spectroscopic ellipsometry using the through-the-substrate measurement technique [1]. The a-Si:H sample used were deposited at 16°C on fused-silica substrate by plasma-deposition technique from silane. The spectrum ranging from 1.5 - 5.0 eV photon energies was investigated using an incident angle of 70 degrees onto the substrate. The a-Si:H side of the sample was bonded to a temperature-controlled heater block. For measurements under illumination a 4 W cm^{-2} white or a 2 W cm^{-1} red bias light at normal incident to the (substrate) surface was used. The measured pseudo dielectric functions exhibited the well-known characteristic temperature dependencies in which the $< \epsilon 1 >$ and the $< \epsilon 2 >$ spectra were red-shifted upon heating corresponding to the temperature-dependent shift of the optical band-gap of a-Si:H, which was significant below the peak photon energy of $< \epsilon 1 >$ spectrum at $\sim$ 4 eV. On the other hand, in the higher photon energy range ($>$ 3.5 eV), a significant decrease of $< \epsilon 1 >$ was observed upon either white or red bias-light illumination, which disappeared upon termination of the bias light. The corresponding change in $< \epsilon 2 >$ spectrum was an increase that extended to lower photon energies. Little light-induced change could be observed when the measurement was done: from the free-surface side of the a-Si:H sample, on c-Si sample, or on bare (without a-Si:H deposited) fused-silica substrate. The direction of this fast change in $< \epsilon 2 >$ was opposite from and the magnitude was larger than the slow changes induced in $< \epsilon 2 >$ by prolonged illumination under intense light [1]. These optical changes provide numerous prospected for an a-Si:H based optical device technology. [1] N. Hata, P. Stradins, C.M. Fortmann, H. Fujiwara, M. Kondo, and A. Matsuda, J. Non-Cryst. Solids 266-269, 491 (2000).

A19.6
ILLUMINATION AND TIME DEPENDENT PHENOMENA IN MICROCRYSTALLINE PIN DIODES. Torsten Brammer, Helmut Stiebig, Heribert Wagner, Institut für Photovoltaik, Forschungszentrum Jülich GmbH, Jülich, GERMANY.

Light and time dependent measurements on microcrystalline silicon solar cells with pin deposition sequence realized by PECVD (95 MHz) for various silane concentrations (SC=$[SiH_4]/([SiH_4]\ [H_2])$) were performed to study the transport and recombination behavior. Diodes deposited with small SC (below 2%) show a distinct time dependent behavior when stored under atmosphere at room temperature. After annealing the dark current increases within several hours. Consequently, a reduction of the open-cicuit voltage (V_{OC}) by 50 mV and a smaller fill factor (FF) is observed. The quantum efficiency is also affected by the exposure time to ambient conditions. Under short-circuit conditions, the red response decreases exponentially in time and converges to a value of 15% below the annealed level caused by a reduced bulk extraction efficiency. All observed processes are reversible by annealing. Solar cells deposited with moderate SC ($\approx$5%) show the highest efficiency and do not show this drastic degradation behavior due to a better passivation of the crystalline phase. Current-voltage characteristics were measured under AM1.5, BG12 and OG630 filtered light for intensities ranging over five orders of magnitude. Generally, the intensity dependent V_{OC}-J_{SC} pairs match their respective dark I/V-curve. For SC$\lesssim$5%, FF increases with light intensity independent of the spectral composition since it is dominated by the dark current. For SC$\gtrsim$6.5%, however, the spectrum of the incident light becomes important. As a function of light intensity, FF is smaller for blue than for red illumination. This indicates a smaller extraction efficiency of photo-generated carriers in the front part of the device where blue light is absorbed. We attribute this to the nucleation region which extends deeper into the i-layer for large SC than for small SC. This is in agreement with temperature-dependent quantum efficiency measurements of solar cells with pin deposition sequence.

A19.7
DC-GATE-BIAS STRESSING OF a-Si:H TFTs FABRICATED AT 150°C ON POLYIMIDE FOIL. Helena Gleskova and Sigurd Wagner, Princeton University, Department of Electrical Engineering, Princeton, NJ.

With the growing interest in low-temperature a-Si:H thin film transistors (TFTs) on plastic substrates the electrical stability of these devices under prolonged dc gate bias becomes important. We investigated the stability of a-Si:H TFTs with mobility of $\sim$ 0.7 cm^2/Vs fabricated at 150°C on polyimide foil. Positive gate bias causes a positive shift in the threshold voltage that shows a power law dependence on time and on gate bias. The power law exponents are similar to those observed for a-Si:H TFTs fabricated at the conventional temperature of 250-350°C. We made a-Si:H TFTs with inverted staggered structure on 51 μm thick polyimide foil. The gate electrode was made of Ti/Cr and the source-drain contacts of Al. The SiN_x gate dielectric was 360 nm thick, the a-Si:H channel layer 100 nm, the (n)a-Si:H layer 50 nm, and the top SiN_x 180 nm. All recipes were optimized to provide good electrical performance and to minimize mechanical stress in the devices. Four different values of gate voltage were used in the stress experiments: 20, 40, 60, and 80 V. The bias stressing caused an increase in threshold voltage and inverse subthreshold slope, and a minor decrease in mobility. Annealing in forming gas substantially improved the stability of the TFTs. The threshold voltage shift exhibited a power law dependence on time with the exponent γ depending on gate bias V_g. For V_g = 20 V, γ = 0.45, while for V_g = 80 V, γ = 0.27. The threshold voltage shift also exhibited a power law dependence on gate voltage with the exponent β depending slightly on the stressing time. β = 2.1 for t = 100 sec and 1.7 for t = 5000 sec. This work is supported by the DARPA HDS program.

A19.8
AMORPHOUS SILICON WITH SMALL HYDROGEN CONTENT. S.M. Pietruszko, Institute of Microelectronics and Optoelectronics; M. Urbanski, Faculty of Physics, Warsaw University of Technology, Warsaw, POLAND.

We studied the effects of thermally-induced metastability a-Si deposited by LPCVD at high temperature (560°C). In as-grown films, the hydrogen content (CH) is 0.06 at.%. Films were post-hydrogenated by ion implantation in the in the range to 8 at.%. Special care was taken to investigate films with CH below 1 at.%. The temperature dependence of the dark conductivity vs inverse temperature was measured for slow cooled and quenched samples. The parameters (σ RT, EA1, σ01, EA2, σ02) of the carriers transport were found. The σRT of as-grown films is typically 10-6 ohm-1cm-1. The Arrhenius plot consists of two regimes. The high (above 450 K) temperature activation energy, EA2 is 0.82 - 0.85 eV. The conductivity activation energy in the low temperature region, EA1 is typically 0.17 to 0.20 eV. Introducing of hydrogen causes straightening of the lower part. It was found that only 0,26 at.% of CH causes drop of the room temperature dark conductivity by two orders of magnitude and increase of EA1 to 0,65 eV. It was observed that in the low temperature region the parameters EA1, sigma01 obey Meyer-Neldel rule with E0 = 30 meV if the CH is below 1 at.%. We have also observed the linear dependence of EA1, σ01, and EA2 vs logarithm of hydrogen content, in case of samples with CH below 1 at.%. The metastable changes in a-Si:H were induced by quenching samples from 675 K to liquid nitrogen temperature. The room temperature conductivity and the activation energy of conductivity are different after slow cooling and quenching. Magnitude of these changes depends on hydrogen content. Difference between the activation energy after slow cooling and quenching increases with increase of CH to 150 meV. The increase of relation σRTq/σRTc and in difference EA1c - EA1q indicates that CH has influence on magnitute of metastable changes. The changes induced by quenching are reversible.

A19.9
STRUCTURAL CHANGES IN AMORPHOUS SILICON ANNEALED AT LOW TEMPERATURES. B. Pivac, R. Boskovic Institute, Zagreb, CROATIA; P. Dubcek, Sinchrotron ELETTRA, Bassovizza (TS), ITALY; I. Zulim, FESB, Split, CROATIA.

The light-induced creation of dangling bonds in amorphous silicon, called Staebler-Wronski effect is major obstacle to the widespread technological application of this material. In order to stabilize solar cells characteristics, devices are exposed to the light soaking (aging) accompanied by low temperature annealing. We used FTIR, X-ray reflectivity and SAXS analysis to monitor the structural changes occurring during the low temperature annealing of undoped a-Si:H films. FTIR results show that hydrogen is moved from positions (voids) where it was accumulated unbonded to silicon and it was trapped at dangling bonds. SAXS measurements confirmed the existence of the voids of about 2.5 nm in diameter. Hydrogen removal from the voids was confirmed by SAXS and X-ray reflectivity

measurements showing that this treatment influenced their size and redistribution.

SESSION A20: POSTER SESSION HYDROGENATION AND OXIDATION

Chair: Yoshiyuki Nasuno
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A20.1
FORMATION OF NANOCRYSTALLINE LAYERS BY PLASMA HYDROGENATION OF MONOCRYSTALLINE SILICON. Reinhart Job, Alexander G. Ulyashin, Gunter Grabosch, Wolfgang R. Fahrner, University of Hagen, Hagen, GERMANY.

In this work a study of Si:H layers, which are formed by hydrogen plasma treatments of monocrystalline silicon wafers, is presented. The hydrogenation was done in a standard PECVD setup with 13.56 and 110 MHz at room temperature, 150 C and 250 C. For comparison a microcrystalline Si layer was deposited at 150 C on a c-Si substrate. The layers were analyzed by scanning electron microscopy and Raman spectroscopy. Mechanical beveling of the samples was done in order to provide depth resolved measurements, too. By such investigations it was shown that the layers which were formed at the surface of the wafer by hydrogen plasma treatments are structured in nano-scale dimensions. It was found that the thicknesses of such nano-structured subsurface layers are about 100 - 200 nm. The variations of structural and optical properties of these layers after the annealing at temperatures in the range of 150 - 600 C was also studied. The modifications of voids and the evolution of Si-H and H-H bonds in dependence on the annealing procedure were investigated by Raman spectroscopy. The voids are most probably located in the structured sub-surface layers and are filled by molecular hydrogen. Dangling Si bonds at the internal surfaces of the voids are passivated by hydrogen. Both, the H-H vibrations of the hydrogen molecules and the Si-H vibrations of the passivated dangling bonds can easily be detected by the Raman measurements. It can be concluded that the hydrogen plasma treatments can be used for the formation of nano-structured layers which have properties similar to the typical micro- (or nano-) crystalline Si layers, which are deposited by the conventional techniques. The applications of our nano-structured Si layers will be discussed.

A20.2
ROLE OF INTERFPHASES AND HYDROGEN SUBSURFACE REACTIONS IN THE MICROSTRUCTURAL AND OPTICAL MODIFICATIONS OF SILICON BASED HETEROSTRUCTURES BY SPECTROSCOPIC ELLIPSOMETRY. Maria Losurdo, Michelaria Giangregorio, Grazia Cicala, Pio Capezzuto, Giovanni Bruno, Plasma Chemistry Research Center CNR, Bari, ITALY; Franco Roca, Francesca Varsano, Mario Tucci, ENEA Research Center, Portici, Naples, ITALY.

In developing and optimizing silicon based heterostructures for solar cells, detailed characterization of surface processes is essential. This is particularly crucial for devices including an hydrogenated amorphous silicon thin film, where atomic hydrogen is known to play a crucial role in the surface and subsurface reactions during both the plasma enhanced chemical vapor deposition of the a-Si:H layer and postannealing treatments of device structures. For the optimization of c-Si,a-Si:H,ITO stacked solar cells, we have exploited the high sensitivity of real time spectroscopic ellipsometry to monolayer modifications to study the kinetics of subsurface reactions operated by hydrogen as a function of process procedures and variables. A series of c-Si,a-Si:H,ITO heterostructures including a 20nm a-Si:H layer with different hydrogen content were deposited on different doped (n-, p-) silicon by PECVD using both SiH4-H2 and SiF4-H2 mixtures, and were annealed at temperatures ranging from 250 to 600 C. The effect of the hydrogenation of the c-Si by both remote and direct plasma processes, and of the hydrogen content in the a-Si:H layer on the optical response of devices is investigated. The emphasis is on the kinetics of hydrogen induced c-Si,a-Si and a-Si,ITO interfaces degradation and passivation, and on the structure modifications involving the a-Si layers to detect the onset for any crystallites formation after the postdeposition annealing treatment. The effect of doping on the electronic nature of the silicon-hydrogen interaction is also discussed.

A20.3
EVALUATION OF THE ROLE OF HYDROGEN IN AMORPHOUS SILICON FILMS GROWN BY PECVD AND MBE. Whitney Mason, J.D. Benson, J.H. Dinan, US Army NVESD, Fort Belvoir, VA; A.J. Stoltz, E-OIR Measurements Inc., Spotsylvania, VA.

Amorphous silicon (a-Si) films have been studied for some time. Bolometers fabricated with doped a-Si are used as uncooled infrared imagers. The presence of hydrogen in a-Si lowers the defect density in the material but also lowers the detectivity of devices[1]. We have investigated the role of hydrogen concentration in boron-doped and undoped amorphous silicon films grown by plasma-enhanced chemical vapor deposition (PECVD) and undoped a-Si films deposited by e-gun evaporation under uhv conditions in a chamber used for molecular beam epitaxy (MBE)–a method we are calling MBE-growth. Films with thicknesses ranging from 100-600 nm were deposited on silicon substrates coated with either thermal oxide or nitride. Fourier transform infrared spectroscopy measurements[2] (FTIR) showed no intrinsic hydrogen in the MBE-grown material, a result to be expected from the UHV deposition conditions. FTIR measurements showed peaks in the PECVD-grown material at about 2100 cm^{-1}, which corresponds to the hydrogen bond-stretching mode and at about 700 cm^{-1}, which corresponds to a bond-bending-wagging mode[3]. X-ray diffraction showed that the material was amorphous rather than polycrystalline to a resolution of 10 nm. Resistivity measurements were performed using a standard four-point probe technique from room temperature to about 600K. The p-doped materials had an activation energy of about 0.2 eV; the undoped PECVD materials had an activation energy of about 0.9 eV. The MBE material had activation energies ranging from 0.04eV to 0.83eV. Additionally, as this material is heated, the resistivity increases over time until it reaches an equilibrium value, usually about three to four times greater than the original, whereas this type of behavior is not seen in PECVD material. Implications of these results for our understanding of the role of hydrogen in a-Si will be discussed. 1. M.H. Unewisse, B.I. Craig, R.J. Watson, O. Reinhold, K.C. Liddiard, SPIE 2554, 43 (1995) 2. K. Nakashima, M. Ishii, T. Hayakawa, I. Tajima and M. Yamamoto, JAP 74, 6936 (1993) 3. S.J. Pearton, J.W. Corbett, and T.S. Shi, Appl.Phys. A43, 153 (1987)

A20.4
SURFACE DERIVATIZATION OF AMORPHOUS SILICON BY GRIGNARD REAGENTS. Takashi Ehara, Arata Maruyama, Ishinomaki Senshu Univ, School of Science and Engineering, Ishinomaki, JAPAN.

Substitution reactions of hydrogen in amorphous silicon at room temperature have been studied. After the treatment of powdered hydrogenated amorphous silicon with Grignard reagent, the hydrogen atoms in the amorphous silicon have been substituted by organic groups. For example, use of $CH_3(CH_2)_9$-MgBr that is synthesized from 1-Bromodecan and Mg metal induced the alkylation of amorphous silicon. Treatment with the Grignard reagent with amorphous silicon followed by quenching by diluted HCl induces the change in infrared absorption spectra. After the treatment, new peaks of CH_n (n=1,2,3) bonding are observed at 2920 and 2850 cm^{-1} beside the Si-H peaks (2000 cm^{-1} and 640 cm^{-1}). The peaks did not disappeared after rising by hydrofluoric acid or various kinds of organic solvent. The spectra indicate that the Grignard reagent is enough reactive to form new covariant bonds of C and Si at the amorphous silicon surface by substitution reaction. In addition, peak intensity of the Si-H bond has not decrease. This means only small amount of hydrogen atoms has been substituted in the reaction. The results observed here is well consistent with the case of porous silicon. In the presentation, we will display the results using another kinds of Grignard reagents and results in the case of microcrystalline silicon instead of amorphous silicon. The effects of surface substitution to the electrical or optical properties of the amorphous silicon films are also discussed.

A20.5
Abstract Withdrawn.

A20.6
PHOTOLUMINESCENCE STUDY OF THE SELF-LIMITING OXIDATION IN NANOCRYSTALLINE SILICON QUANTUM DOTS. Kenta Arai, Jyunichi Omachi, Katsuhiko Nishiguchi and Shunri Oda; Res Cen for Quantum Effect Electronics, Tokyo Inst of Tech and CREST, JST, Tokyo, JAPAN.

Recently, nanocrystalline silicon (nc-Si) quantum dots (QDs) have attracted attention for possible applications in the next generation of computation devices. By employing a gas-phase crystal growth process of VHF PECVD, the nc-Si QDs of 8 ± 1 nm in size can be fabricated[1]. However, in order to realize the devices featuring the quantum effect at room temperature, the size of the nc-Si QDs must be reduced to $\sim$3 nm. A self-limiting oxidation of cylindrical silicon structures (radius: $\sim$0.5 μm) with a good reproducibility was first reported by Kao *et al*[2]. The mechanism for the self-limiting oxidation is proposed to be from the reduction of the surface reaction rate at the Si-SiO_2 interface due to the stress normal to the interface. By transmission electron microscopy (TEM) observation of the size of the nc-Si QDs, we have similarly observed the self-limiting oxidation of

the nc-Si QDs with increasing the oxidation time[3]. Photoluminescence (PL) spectrum is sensitive to not only the quantum confinement of the nc-Si QDs size but also the strain on the nc-Si QDs. We present further evidence for the role of strain in the self-limiting oxidation of the nc-Si QDs by PL spectroscopy. The nc-Si QDs deposited on the quartz substrate were oxidized at 800°C in a dry oxygen atmosphere. The oxidation time was varied ranging from 10 minute to 10 hour. An emission band from the nc-Si QDs showed a blueshift from ~1.4 eV to ~1.7 eV with increasing the oxidation time from 10 minute to 40 minute. For further oxidation, the emission band showed a redshift from ~1.7 eV to ~1.6 eV with increasing the oxidation time from 40 minute to 3 hour. This blueshift is attributed to the enhancement of the quantum confinement by reducing the size of the nc-Si QDs from ~7 nm to ~4 nm, which is supported by the TEM observation. It is well known[4] that the indirect bandgap of bulk crystalline Si has a pressure coefficient of about −1.4 meV/kbar. Therefore, the redshift is a direct observation of the effect of the compressive strain on the nc-Si QDs, responsible for the self-limiting oxidation.

[1] T. Ifuku *et al.*, Jpn. J. Appl. Phys. Part 1 **36**, 4031 (1997).
[2] D.B. Kao *et al.*, IEEE, Trans. Electron. Device. ED-**34**, 1008 (1987).
[3] J. Omachi *et al.*, 2000 MRS Fall Meeting, F5.3.
[4] B. Welber *et al.*, Solid State Commu. **17**, 1021 (1975).

A20.7
PLASMA OXIDATION OF SILICON USING AN ELECTRON CYCLOTRON WAVE RESONANCE (ECWR) PLASMA SOURCE.
D.F. Lai, J. Robertson, W.I. Milne, Engineering Department, Cambridge University, UNITED KINGDOM.

High quality dielectrics made at low temperatures are needed for gate insulators in applications such as thin film transistors in active matrix liquid crystal displays. Silicon dioxide is the preferred gate dielectric when n- and p-type transistors are needed. We have grown thin SiO_2 films (20-100nm) on silicon by plasma oxidation at 483 to 673K using a high density plasma source, the electron cyclotron wave resonance (ECWR). The ECWR is a RF powered, inductively-coupled source. At these low temperatures, the ECWR gives oxidation rates comparable to thermal oxidation. The oxidation efficiency, defined as the ratio of initial growth rate to anodisation current, is very high compared to other plasma oxidation methods. Oxides were grown under floating, anodic and cathodic bias. The density, stoichiometry and bonding in the oxide was characterised by refractive index, infra-red and X-ray photoemission. The refractive index at 632.8 nm is ~ 1.47, while the Si-O bond stretching mode lies around 1066 cm^{-1}, lower than in thermal oxide. As-grown oxides have breakdown fields over 7 $MVcm^{-1}$. High frequency and combined high-low frequency capacitance-voltage measurements show that the as-grown oxides have high interface state densities due to plasma damage, but these can be reduced by annealing at moderate temperatures.

SESSION A21: POSTER SESSION
THEORY AND COMPUTER MODELLING
Chair: Gerard T. Barkema
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A21.1
COMPUTATIONAL GROWTH AND CHARACTERIZATION OF PLASMA-DEPOSITED HYDROGENATED AMORPHOUS SILICON THIN FILMS THROUGH ATOMISTIC SIMULATIONS.
Saravanapriyan Sriraman, Shyam Ramalingam, Eray S. Aydil and Dimitrios Maroudas, Department of Chemical Engineering, University of California, Santa Barbara, CA.

Hydrogenated amorphous silicon (a-Si:H) thin films grown by plasma-assisted deposition from silane-containing discharges are used widely in photovoltaic and flat-panel display technologies. In spite of the extensive experimental research on a-Si:H deposition, the elementary surface processes that lead to film deposition, H incorporation, and defect generation are still not well understood. Developing deposition strategies for improving film quality requires a fundamental understanding of the interactions of radicals, such as SiH_x (0<x<4) and H, with the deposition surface. Toward this end, we have developed a hierarchical atomic-scale modeling approach based on molecular-dynamics (MD), molecular-statics, and Monte Carlo methods to identify and analyze the interactions between silane fragments and the silicon growth surfaces and to characterize systematically the computationally generated a-Si:H films. These computational characterization results are directly comparable to surface diagnostics measurements. Specifically, we simulated through MD the growth of a-Si:H films on H-terminated Si(001)-(2x1) substrates by impinging on the growth surface repeatedly SiH_3, SiH_2, and SiH radicals, separately, as precursors. Analysis of the MD trajectories identified the surface chemical reactions that govern the deposition process. The effects of these reactions on the growth mechanism are examined by analyzing local structural configurations and surface chemical reactivity in the vicinity of the surface reaction sites. Systematic comparative studies are presented of the evolution of the films' structure, surface morphology and roughness, surface reactivity, and surface composition for films deposited from individual SiH_3, SiH_2, and SiH precursors. Experimental measurements of the surface H coverage and silicon hydride composition, as well as their temperature dependence, will be used synergistically with the atomistic simulation results to elucidate elementary processes occurring on the surface and discuss our current understanding of the a-Si:H deposition process.

A21.2
A TIGHT BINDING STUDY OF POINT DEFECTS AND NETWORK CONNECTIVITY IN a-Si.
Cristiano L. Dias, Laurent J. Lewis, and S. Roorda, Département de Physique et Groupe de Recherche en Physique et Technologie des Couches Minces (GCM), Université de Montréal, Montréal, Québec, CANADA.

High-precision x-ray diffraction measurements of the radial distribution function (RDF) of *a*-Si prepared by ion implantation were recently reported by Laaziri *et al.*[†] The data indicates that the coordination number increases from 3.786 ± 0.01 to 3.88 ± 0.01 upon annealing the as-prepared material at room temperature, while the density remains constant at a value below that of the crystal. These observations have been interpreted in terms of the recombination of vacancies and interstitials, the former being more numerous than the latter, thus explaining both the deficit in coordination and in density. In order to verify this conjecture, we have carried out a detailed tight-binding molecular-dynamics study of point defect relaxation in a highly-relaxed model of *a*-Si prepared using a modified version of the Wooten-Winer-Weaire (WWW) algorithm;[‡] defects are introduced "by hand" so as to mimic the as-implanted material, and the results are compared to the "perfect" material. The defects are identified using an algorithm based on an analysis of the charge associated with gap states. Our simulations indicate that, fully consistent with experiment, the coordination number of a continous random network decreases linearly with the density of defects, and that the undercoordination of *a*-Si is well accounted for by the presence of a residual number of vacancies. Vacancies, therefore, would appear to be intrinsic to the material. [†]Laaziri *et al.*, Physical Review B, 60,13520 (1999) [‡]G.T.Barkema and Normand Mousseau, Physical Review B, 62, 4985 (2000)

A21.3
CRYSTALLINE AND NONCRYSTALLINE STRUCTURES OF Si-NANOWIRES.
Shudun Liu, C.S. Jayanthi, Shi-Yu Wu, Dept. of Physics, University of Louisville, Louisville, KY; Zhenyu Zhang, Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN.

Crystalline and noncrystalline structures of Si-nanowires of different radii (from a few angstroms to 80 nm) are studied using molecular dynamics simulations and within the non-orthogonal tight-binding model. Substantial re-arrangement of atoms near the surface is found to occur in order to reduce the number of dangling bonds, and as a result, the total energy of the system. Such surface effect, however, is found to be confined to a region within about 1.5 nm of the surface, regardless of the sizes of the wires. When the radius of a wire is larger than this critical thickness, it is found that it can maintain a crystalline structure in its core region. For a wire of smaller radius, no such core region exists and noncrystalline structure is formed. The transition from a crystalline structure to a noncrystalline one is thus directly connected to the onset of the surface-surface interaction. We believe such a simple connection exists in many other nanosystems. The change of the mechanical properties of Si-nanowires as its radii decreases will also be discussed.

A21.4
DEPOSITION OF SILICON CLUSTERS. A MOLECULAR DYNAMICS STUDY OF CLUSTER FRAGMENTATION AND SURFACE DISORDERING.
A.M. Mazzone, CNR, Bologna, ITALY.

Cluster deposition is a promising technique for nanostructure growth in a variety of applications. Therefore many efforts, in theories and experiments, are dedicated to the understanding of the optimal conditions for film growth. These studies indicate that a major problem of these techniques is that the requirements needed to achieve cluster fragmentation, which favors a smooth film growth, are generally in conflict with the ones necessary to obtain a film-substrate interface of good quality. Therefore the understanding of the damaging effects, due to cluster-surface interaction, is an important step for a further development of cluster-based techniques. This understanding is, however, complicated by a wealth of new phenomena with little or no commonality with the ones occurring during epitaxial growth. In fact, experiments and molecular dynamics

simulations on deposition of metallic clusters have shown that complex mechanisms, such as cluster rolling, site-exchange between cluster and surface atoms and channelling of the cluster atoms, have to be taken into account. The purpose of this contribution is to investigate if these effects also take place during deposition of silicon clusters. Therefore a study, based on molecular dynamics simulations, has been conducted by depositing clusters of small size (30 atoms or smaller) with a deposition energy in the range from 0.1 to 1eV/atom on a crystalline silicon substrate. The results describe diffusion and channelling of the cluster atoms and formation of defects in the impact region in dependence of the cluster size, of the deposition energy and of the alignment of the cluster with the crystal channels.

A21.5

VIBRATIONAL BOND-STRETCHING MODES OF THE Si-H AND Si-D BONDS IN AMORPHOUS SILICON NITRIDE. Shu-Ya Lin, Department of Electrical Engineering, National Tsing Hua University, Hsinchu, Taiwan, REPUBLIC OF CHINA.

The theoretical cluster-Bethe-lattice method is used to study the vibrational local modes induced by the Si-H and Si-D bonds in amorphous silicon nitride. The four-fold rotation-reflection, S_4, symmetry is used to build the Si_3N_4 Bethe lattice. The vibrational density of states for the Si_3N_4 Bethe lattice, SiH(D) and $SiH_2(D_2)$ groups in amorphous silicon nitride are calculated. The bond-stretching modes of the Si-H bond of the SiH group and Si-D bond of the SiD group are at 2160 and 1554 cm^{-1}, respectively. The Si-H bond-stretching mode of the SiH_2 group is split into a symmetrical and an asymmetrical mode at 2176 and 2190 cm^{-1}, respectively. The Si-D bond-stretching mode of the SiD_2 group is split into a symmetrical and an asymmetrical mode at 1558 and 1584 cm^{-1}, respectively. The Si-D bond-stretching mode has larger splitting. The difference between the Si-D bond-stretching frequency of the SiD group and the Si-D asymmetrical stretching frequency of the SiD_2group has about the same value as that of the Si-H bonds. The result is consistent with the experimental data [1]. The difference in the effective masses of the Si-H and Si-D bonds causes the Si-D bond-stretching modes to have less frequency difference between the SiD and SiD_2 groups compared with that of the Si-H bond-stretching modes. The larger splitting of the Si-D bond-stretching mode of the SiD_2 group has compensating effect. This study proposes that the asymmetric Si-H bond-stretching mode of the SiH_2 group is responsible for the Si-H bond-stretching frequency beyond 2160 cm^{-1}.
[1] G. Lucovsky, P. Santos-Filho, A. Banerjee, and Z. Jing, Mater. Res. Soc. Symp. Proc. 420, 503 (1996).

A21.6

A NEW APPROACH TO THE CLASSIFICATION OF NON-CRYSTALLINE SOLIDS: APPLICATIONS TO ELEMENTAL AND BINARY OXIDES AND CHALCOGENIDES. Gerald Lucovsky, NC State Univ, Dept of Physics, Raleigh, NC.

The scheme was developed for silicon CMOS scaling which requires replacement of thermally-grown silicon dioxide by non-crystalline insulators with significantly increased dielectric constants. Elemental and binary oxide replacements including aluminum and tantalum oxide, and transition metal silicates are considerably more ionic than silicon dioxide, nitride and oxynitride alloys. This suggested a classification based on bond-ionicity in the context of the Pauling electronegativity scale. Extension to binary silicate and aluminate alloys would then rely on compositionally-averaged bond-ionicities. Application of this scheme revealed interesting correlations between bond-ionicity and solid state structure that separated non-crystalline oxides into three groups with qualitatively different properties. The scaling variable is the electronegativity difference for elemental oxides and compositionally-average difference for binary oxide alloys. The first group includes oxides in which the average electronegativity is less than 1.6, or $\sim$ 47% ionicity using the Pauling definition. These materials have a continuous random network structure, and include group III (B), IV (Si,Ge) and V (As,P) oxides and their alloys, as well as silicon nitride and oxynitride alloys. The second group includes aluminum and tantalum oxide, and transition metal silicates and aluminates, and is being focused on for replacement gate dielectrics. The local structures are comprised of a network component with two or three fold coordinated oxygen, and metal atoms and silicon atoms with different degrees of covalency in their bonding. This group has electronegative differences between about 1.6 and 2.1, or ionicities between 47 and 67%. The final group is comprised most of metal oxides, e.g., zirconium, hafnium, yttrium and lanthanum, and the solid state structure is a random close packing of oxygen and metal ions. Properties including effective crystallization temperature scale with electronegativity difference, increasing with decreasing ionicity. This scheme is readily extended to chalcogenide materials and their alloys.

SESSION A22: POSTER SESSION
DEFECTS AND DEFECT SPECTROSCOPY
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A22.1

NEUTRAL DANGLING BONDS ARE NOT THE DOMINANT RECOMBINATION CENTERS FOR PHOTOCONDUCTIVITY IN HOT-WIRE A-Si:H. Daxing Han, Guozhen Yue, Dept of Physics & Astronomy, Univ of North Carolina at Chapel Hill, Chapel Hill, NC; Qi Wang, National Renewable Energy Laboratory, Golden, CO.

It is commonly observed that the phtoconductivity (PC) decay upon light-soaking in device quality a-Si:H prepared by hot wire chemical vapor deposition (HWCVD) is relatively small. However, there were the same photodegradation effects in its device structures, why? We question whether the recombination centers are different in HW from regular glow discharge (GD) films. We explore the properties of the recombination centers by conducting thermostimulated conductivity (σ_{TSC}) and temperature dependence of PC in both GD and HW films. Device-quality intrinsic a-Si:H films were prepared by HW, rf-GD, and dc-GD CVD at the National Renewable Energy Lab (NREL), BP-Solarex (BP-SLX), and United Solar Systems Corp (USSC), respectively. PC was generated by a 632.8 nm laser beam at a generation rate of G = 5×10^{15} photons cm^{-3} s^{-1}. In the σ_{TSC} study, the sample was first cooled down to 120 K and then exposed to the light with an exposure time of t_e = 60 s, after a delay time of to = 30 min σ_{TSC} was measured in a step-heating process with a constant heating rate b=1.5 K/min in the dark. Light soaking was performed in situ by a 200 mW/cm^2 white light through a water filter. The sample temperature was kept at 35°C during light soaking. State A was reached after the sample was annealed in a vacuum for one hour at 160°C; state B was reached after light soaking of 4 hours. We observed a sudden rise of σ_{TSC} near the transition from the initial rise to the steady-state regime of σ_{TSC} in HW films. This feature has never been observed in any a-Si:H based materials, which is evidence of strong-recombination. The strong recombination centers such as positive charged defects (D^+) rather than neutral dangling bonds (D^o) dominate the electron lifetime in HW films. Therefore, the PC shows a relative stable value in HW films upon light-induced D^o creation. The work is supported by NREL subcontract XAK-8-17619-11 and thin film PV partnership. Yue is partially supported by NSF-Int-9604915. Wang is supported by DOE subcontract DE-AC36-99G010337.

A22.2

SENSITIZATION OF THE HOLES LIFETIME BY DANGLING BONDS IN a-Si:H. L.F. Fonseca, S.Z. Weisz, Univ of Puerto Rico, Dept. of Physics, San Juan, PR; I. Balberg, The Hebrew University, The Racah Institute of Physics, Jerusalem, ISRAEL.

It is generally accepted that at room temperature the dangling bonds are the dominant recombination centers in intrinsic hydrogenated amorphous silicon (a-Si:H). Correspondingly, it is expected that the increase of the dangling bond concentration Ndb will yield a monotonic decrease of the mobility-lifetime products of both the majority carriers (the electrons $\mu_e t_e$) and the minority carriers (the holes $\mu_h t_h$). While such a decrease is commonly observed for electrons[1], our data[2] as well as data of others[3] for the holes, has revealed a maximum in the dependence of $\mu_h t_h$ on Ndb around Ndb $\approx 10^{16}$ cm^{-3}. That this is a genuine effect of intrinsic a-Si:H can be concluded from its observation in computer simulations of the standard model of a-Si:H [3]. However, in spite of these findings and their importance for the bipolar action of devices based on a-Si:H, no discussion of this effect has been presented previously. In this paper we report comprehensive computer simulations as well as analytical arguments that explain the mechanism responsible for the above-described effect. Basically, we demonstrate clearly that this, rather unexpected, minority carrier sensitization by dangling bonds, is a result of the well known1 transition of the major recombination channel from that of the valence band tail to that of the dangling bonds. The general physical basis of this effect and its importance for a-Si:H applications in general, and for solar cells in particular, will be discussed in detail. [1] For a review, see for example, M.Q. Tran, Phil. Mag. B 72, 35 (1995). [2] R.S. Crandall, A.H. Mahan, B. Nelson, M. Vanecek and I. Balberg, Proc. of the 6th Int'l PVSEC, B.K. Das and S.N Singh, Editors (Oxford, & IBH, New Delhi, 1992), p. 879. [3] F. Wang and R. Schwarz, Phys. Rev. B 52, 14586 (1995) .

A22.3

DEFECTS IN LOW TEMPERATURE EPITAXIAL SILICON FILMS FROM ION-ASSISTED DEPOSITION. Thomas A. Wagner, Lars Oberbeck, Ralf B. Bergmann, Institut für Physikalische Elektronik, University of Stuttgart, GERMANY.

High-quality, low-temperature epitaxy of silicon is of great importance for microelectronic devices and solar cells on foreign substrates. The understanding of defect formation and the engineering of defects in low-temperature thin films is of crucial importance for device application. We investigate the growth of thin epitaxial silicon films prepared by ion-assisted deposition at low deposition temperatures $T_{dep} < 650°C$ and very high deposition rates of up to 0.8 μm/min. We correlate majority and minority carrier properties with the presence of extended and point defects. Defect spectroscopy, such as deep level transient spectroscopy and photoluminescence, as well as internal quantum efficiency (IQE) and etch pit density measurements serve for structural and electronic characterization. Apart from deposition parameters such as temperature and deposition rate, the substrate orientation plays an important role for the electronic and structural properties of the films. In (100)-oriented films, defect spectroscopy reveals point defects with a concentration of up to 1.6×10^{14} cm^{-3}, while in (111)-oriented films defects reach a concentration of 2×10^{18} cm^{-3}. (100)-oriented samples display several discrete defect bands, while (111)-oriented samples show a broad defect distribution. The energetic levels of the defect bands indicate copper decorated dislocations and C-O-defect complexes as the major impurities. Minority carrier properties correlate well with band-edge-photoluminescence intensity and point defect densities. For deposition temperatures below 650°C, the minority carrier diffusion length L_{diff} obtained from IQE-measurements is around one order of magnitude lower in (111)-oriented films than in (100)-oriented films. The strong influence of the substrate orientation on the electronic properties limits applications of low temperature epitaxy to polycrystalline films for thin film solar cells. However, a diffusion length of $L_{diff} = 50$ μm in (100)-oriented films demonstrates the high quality of our silicon films for electronic devices that require low temperature epitaxy.

A22.4
HYDROGENTED AMORPHOUS SILICON SUB-BAND GAP ABSORPTION MEASUREMENTS USING THE CAVITY RING DOWN TECHNIQUE. Arno Smets, Jean-Pierre van Helden, Daan Schram, Richard van de Sanden, Eindhoven Univ of Technology, Dept of Appl Phys, Eindhoven, THE NETHERLANDS.

The study of defects in hydrogenated amorphous silicon (a-Si:H) is of great importance for the following two reasons. First the performance of a-Si:H solar cells and other devices strongly depends on the defect density. Secondly in situ monitoring of dangling bonds (defects), can play a crucial role in understanding the a-Si:H growth mechanism, as the dangling bonds are believed to be reaction sites for precursors to bond to the surface. Because the sub-band gap states correspond to defect states, the investigation of sub-band gap states has been subject of numerous ex situ studies. In this contribution we will introduce a new sensitive absorption measurement technique called the cavity ring down (CRD) technique to measure directly the sub-band gap absorption. The main advantage of the CRD technique is the fact that it can be applied in situ. CRD is based upon the measurement of the intensity decay rate of the absorption of a light pulse in an optical cavity. We will show that the CRD absorption spectroscopy is sufficient to measure the sub-gap absorption for various film thickness (10 nm - 3 μm) on Corning 7059 substrates. Single wavelength and spectral ex situ measurements are performed as function of the a-Si:H thickness for various deposition conditions and show that the surface morphology correlates with the surface defect density ($\sim 10^{12}$ cm^{-2}). Comparison of CRD results (α = 10 to 200 cm^{-1}) with dual beam photoconductivity (DBP) results (α = 0.5 to 20 cm^{-1}), show that not every sub-band gap absorption results in a charge, contributing to the DBP current. The first results of in situ a-Si:H sub-band gap CRD absorption measurements on a suprasil quartz prism together with in situ ellipsometry measurements will be presented and the a-Si:H growth mechanism will be discussed.

A22.5
COMPARATIVE STUDY OF THE DEFECTS STRUCTURE IN A-Si:H FILMS BY CPM AND POSITRON ANIHILATION. A. Amaral, C. Nunes de Carvalho, G. Lavareda, CFM, Complexo I, IST/UTL, Lisboa, PORTUGAL; P.M. Gordo, V.S. Subrahmanyam, C. Lopes Gil, A.P. de Lima ICEMS, Departamento de Física, U. C., Coimbra, PORTUGAL; M. Duarte Naia, Secao de Física da U.T.A.D., Vila Real, PORTUGAL.

Thin films of hydrogenated amorphous silicon deposited on glass and crystalline silicon substrates by rf PECVD at different rf power densities were studied using slow positron beam in order to verify the influence of that deposition parameter on the film defect structure. Other techniques, namely, constant photocurrent method (CPM), infrared spectroscopy (IR) and conductivity measurements, were used to determine the density of states (DOS), the relative concentration of the SiH_n radicals and the photo-to-dark conductivity ratio of the films, respectively. It was found that mainly two kinds of vacancy type defects are present in the films: large vacancy clusters or voids and small vacancy type defects. Correlations observed between the positron results and the information obtained from the other techniques show that positron annihilation technique can give significative information on the a-Si:H structure characteristics. Films with high Doppler parameter (S) values, present large voids, leading to a less dense material. For very thin film applications this morphology can be a drawback. However, for thicker films, the optoelectronic properties seem not to be affected by this structure.

A22.6
EFFECT OF EXPERIMENTAL NOISE ON RECOVERY OF THE ELECTRONIC DENSITY OF STATES FROM TRANSIENT PHOTOCURRENT DATA. S. Reynolds, C. Main and M.J. Gueorguieva, School of Science and Engineering, Univ. of Abertay Dundee, UNITED KINGDOM.

Over the past decade, sophisticated analytical procedures for recovering the density of states (DOS) from transient photocurrent (TPC) data have been developed, and evaluated through the use of simulated ideal (i.e. noise-free) transient photocurrent data. In this paper we investigate the effects of sample and instrumental noise on their performance. We begin by measuring the fluctuations present in typical experimental current-time data obtained from amorphous silicon and pentacene thin films, arising from intrinsic sample noise and instrumental contributions. From this information, data appropriate to a range of TPC experimental conditions are generated by superimposing noise on decays simulated from, for example, an amorphous silicon-like model DOS, consisting of an exponential tail of states plus a distribution of deep defects. These data sets are then processed to recover the DOS, by approximate Fourier [1] and Laplace [2] methods, an exact Laplace method [3], and a method based on Tikhonov regularisation [4]. Our results indicate that approximate methods are capable of attaining an energy resolution of better than kT when used at noise levels typical of those found in experimental work on amorphous silicon. The exact Laplace method is less tolerant of noise and may require further data processing if its inherently higher resolution is to be realised. The method employing Tikhonov regularisation allows a trade-off between data quality and resolution to be achieved. [1] C. Main, MRS Symp. Proc. 467, 167 (1997). [2] N. Ogawa, T. Nagase and H. Naito, J. Non-Cryst. Solids 266-269, 367 (2000). [3] M.J. Gueorguieva, C. Main and S. Reynolds, MRS Spring Meeting (2000). [4] T. Nagase, K. Kishimoto and H. Naito, J. Appl. Phys. 86, 5026 (2000).

SESSION A23: POSTER SESSION STRUCTURAL AND ELECTRONIC PROPERTIES OF THIN SILICON

Chair: Eric A. Schiff
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A23.1
PROPERTIES OF SILICON FILMS DEPOSITED UNDER ARGON DILUTION. C. Longeaud, D. Roy, Laboratoire de Génie Electrique de Paris, Gif sur Yvette, FRANCE; P. Chaudhuri, N. Dutta Gupta, P. Pratim Ray, Energy Research Unit, IACS, Calcutta, INDIA; S. Vignoli, R. Meaudre, M. Meaudre, Dept. Physique des Matériaux, Université Lyon I, Villeurbanne, FRANCE.

We have studied transport properties of four different series of a-Si:H samples prepared at 250°C by decomposition of a mixture of silane and argon in a radio-frequency powered deposition system (RF-PECVD). The dilution ratios were respectively 1%, 1.5%, 5% and 10% of silane, the total pressure was 0.5 Torr for the first series and 0.2 Torr for the others and the RF power density scaled from 16 to 570 mW/cm^2. The samples were deposited onto glass and fitted with two coplanar parallel ohmic electrodes. For all the samples we have measured the dark and photo-conductivity, the density of states above and below the Fermi level by means of the modulated photocurrent technique and the constant photocurrent method respectively and the minority carriers diffusion length L_d by means of the steady state photocarrier grating technique. All these measurements were performed in the as-deposited, light-soaked and annealed states. The measured parameters were compared with those obtained on state-of-the-art material. For all the series the transition from purely amorphous materials toward microcrystalline materials with increasing RF power was put into evidence. This transition is dilution dependent. In all the series we have found optimum deposition conditions leading to device grade samples. Depending of the series we have obtained i/ samples as ≪good≫ as standard material - i.e. same density of states, similar $\mu\tau$ product for the electrons and L_d of the minority carriers- but with a much higher deposition rate or ii/ material presenting enhanced transport properties, higher $\mu\tau$ and larger L_d , but deposited at the same rate as standard a-Si:H. After

light-soaking these last samples exhibited values of L_d higher than measured on as-deposited standard a-Si:H, an interesting behaviour for solar cells applications. As a conclusion argon dilution allows to tailor the material for a given application.

A23.2
THE DETERMINATION OF OPTOELECTRONIC PROPERTIES OF MICROCRISTALLINE AND AMORPHOUS SILICON FILMS.
M. Kunst, S. von Aichberger, W. Thom, F. Wunsch, Hahn-Meitner-Institut, Dept Solare Energetik, Berlin, GERMANY.

Thin amorphous silicon (a-Si:H) and microcristalline silicon (μc-Si) films are increasingly used in (opto-) electronic and photovoltaic devices. The knowledge of the (opto) electronic properties of these films is important for the devices. Unfortunately, the determination of these properties, as for example the mobility from Hall measurements, is by no means trivial. In this work the determination of the mobility by contactless transient photoconductivity measurements is reported. A-Si:H films were produced by plasma enhanced chemical vapor deposition (PECVD). μc-Si films were produced by PECVD, Hot Wire deposition and by laser induced crystallization of a-Si:H films. Contacless transient photoconductivity measurements were performed by the time resolved microwave conductivity (TRMC) technique, using 10ns (FWHM) 1064nm and 532nm laser pulses for the excitation of excess charge carriers in the light absorbing film. The mobility is determined from the amplitude of the TRMC-signal induced by 532nm light. In the range where the amplitude is proportional to the excitation density. This means that the mobility determined in this way is only sensitiv e to deep trapping during the excitation of 10ns. For state of the art intrinsic a-Si:H an electron mobility of 0.5 cm^2/Vs is determined for films produced in different laboratories. In μc-Si films the largest electron mobilities do not exceed 3 cm^2/Vs.The largest electron mobilities up to 50cm^2/Vs have been observed in films produced by laser cristallization of a-Si:H films. The values are discussed with respect to other film properties such as doping level, impurity diffusion during annealing and grain size.

A23.3
NANOSTRUCTURAL AND OPTICAL FEATURES OF SILICON FILMS PREPARED BY PECVD AND RF MAGNETRON SPUTTER TECHNIQUES. N.-H. Cho, M.-B. Park, J.-S. Lee, Inha University, Dept. of MS&E, Inchon, KOREA.

We investigated the nanostructural and optical features of silicon thin films; the nano-crystalline Si films were prepared by plasma enhanced chemical vapor deposition(PECVD) and rf-magnetron sputter techniques as a function of substrate temperature and post-deposition heat-treatment conditions. The crystallinity, structural and chemical features of the films were examined by SAXS, XRD, RBS and TEM with an EDS detector. The PL phenomena of the films were analyzed using a spectro-fluoro-photometer. The phase of the films prepared at room temperature by PECVD is somewhere between amorphous and crystalline states, consisting of 5.0 nm nano-crystallites with {100} orientation preference. These films exhibit significant PL intensities near blue light region. The films prepared at 500°C by PECVD are composed of about 6.0 and 150 nm crystallites, exhibiting little PL phenomena. On the other hand, owing to the increase of the crystallinity, the PL phenomena of the films prepared by sputter techniques were observed to be enhanced by annealing treatments. The relations of the photoluminescence (PL) phenomena of the films with process variables are discussed in detail.

A23.4
ELECTRONIC TRANSPORT STUDY OF HIGH DEPOSITION RATE HWCVD a-Si:H BY THE MICROWAVE PHOTOMIXING TECHNIQUE. S.R. Sheng, R. Braunstein, Department of Physics and Astronomy, University of California, Los Angeles, CA; B.P. Nelson, Y.Q. Xu, National Renewable Energy Laboratory, Golden, CO.

The electronic transport properties of high deposition rate a-Si:H films prepared by HWCVD has been investigated in detail by employing the microwave photomixing technique. This technique enables us to determine the drift mobility and lifetime separately; from the electric field dependence of these quantities, the range and the depth of the long range potential fluctuations, and subsequently the relative changes in the charged defect density in the films can be determined. The high deposition rate (up to 1 μm/min.) was achieved by increasing deposition pressure, silane flow rate, and decreasing filament-to-substrate distance. The effect of the deposition rate on the resultant film properties with respect to the substrate temperature, deposition pressure and silane flow rate was studied. It was found that the film transport properties do not change monotonically with increasing deposition rate. The photoconductivity peaks at ~70-90 Å/s, where both the drift mobility and lifetime peak, consistent with the deposition rate dependence of the range and depth of the potential fluctuations. High quality, such as a photoconductivity-to-dark-conductivity ratio of $\sim 10^5$ and nearly constant low charged defect density, can be maintained at deposition rates up to ~130 Å/s, beyond which the film properties deteriorate rapidly as a result of an enhanced effect of long-range potential fluctuations due to a considerable increase in the concentration of the charged defects. Our present results indicate that medium silane flow rate, low pressure, and higher substrate temperature are generally required to maintain high quality films at high deposition rates.

A23.5
STUDY OF ELECTRICAL PROPERTIES OF MICROCRYSTALLINE SILICON FILMS USING AC MEASUREMENTS.
Ely A.T. Dirani[a,b], Alexandre Mantovani Nardes[a], Adnei M. de Andrade[a], Fernando J. Fonseca[a]; [a]LME, Dept Eng Sist Eletr, Escola Politécnica da USP, São Paulo, SP, BRAZIL; [b]Dept de Eng Eletr - PUCSP, São Paulo, SP, BRAZIL.

Hydrogenated amorphous (a-Si:H) and microcrystalline (μc-Si:H) silicon films are indispensable materials for large area electronic devices like solar cells, image sensors and thin film transistors (TFTs). Microcrystalline silicon consists of an amorphous silicon matrix in which silicon nanoparticles are embedded. The interest of the μc-Si:H films arise from the fact that they combine the high optical absorption of a-Si:H and the electrical transport properties close to those of crystalline silicon. In this work we show the correlation among substrate deposition temperature, crystallinity and electrical properties of a-Si:H and μc-Si:H films. The films were prepared by a conventional PECVD (13.56 MHz) RF system from $PH_3/SiH_4/H_2$ gas mixtures in the temperature range of 100 to 250°C. While phosphorus doped (n+) a-Si:H are deposited yielding conductivity values no better than 10^{-2} S/cm, (n+) μc-Si:H layers deposited at substrate temperature of 250°C show conductivity values higher than 10^1 S/cm, crystalline fraction up to 80% and Hall mobility of about 0.9 $cm^2.V^{-1}.s^{-1}$. It was observed that a change in the dark conductivity behavior occurs around 140°C, with a large increase in the conductivity values. A correspondent increase is not seen in the average grain size and in the crystalline volume fraction, which show an almost linear increase with the deposition temperature. This stronger influence of the temperature in the electrical characteristics of the μc-Si:H films may be related to the phosphorus activation, which occurs in higher degree at higher deposition temperatures. The correlation among Raman spectroscopy, Hall effect and AC conductivity measurements (frequency range 6 Hz to 13 MHz) showed that crystalline phase domains the electrical transport mechanism on μc-Si:H films. The AC measurements allowed determining the electrical resistivity of each phase of this material.

A23.6
ENHANCING THE DARK CONDUCTIVITY ACTIVATION ENERGY IN UNDOPED MICROCRYSTALLINE SILICON BY POST-GROWTH ANNEALS. Jong-Hwan Yoon, Kangwon National University, Department of Physics, Chunchon, KOREA.

Hydrogenated microcrystalline silicon (μc-Si:H) has a high potential in thin film electronic devices such as solar cells and thin film transistors (TFTs). Especially, the stable electronic properties of mc-Si:H against light exposure and the high mobility, as compared to amorphous silicon, make it be of growing interest for solar cell applications. However, the strong n-type character of about 0.2 eV dark conductivity activation energy, usually observed in undoped mc-Si:H films grown by a conventional plasma-enhanced chemical vapor deposition (PECVD) from high dilution of silane in hydrogen, is one of the main properties to be improved for device applications. There are a few research works on n-type character. In this work, we report experimental results that the n-type character may be reduced by a post-growth anneal. Hydrogenated microcrystalline silicon (μc-Si:H) films were grown by a conventional plasma-enhanced chemical vapor deposition from high hydrogen-diluted silane. Annealing was performed by increasing the temperature from 25°C to 450°C at a constant rate of 12°C/min (one annealing cycle), and repeating this process. Dark-conductivity activation energy gradually increases with increasing the number of annealing cycle to a saturation value of about 0.6 eV, observed in truly intrinsic mc-Si:H films of about 1.2 eV optical gap. For the saturated state, the dark conductivity of the order of 10^{-8} S/cm was obtained. Little or no change in the oxygen content and microcrystalline structure is observed after the annealing.

A23.7
GENERATION-RECOMBINATION NOISE IN AMORPHOUS SEMICONDUCTORS. C. Main, S. Reynolds, School of Science and Engineering, Univ of Abertay Dundee, UNITED KINGDOM; R.I. Badran, Dept of Physics, The Hashemite University, JORDAN.

We examine different approaches to the analysis of noise in amorphous hydrogenated silicon associated with trapping and generation - recombination processes, which appear to predict very different noise spectra. In one approach the broad noise spectrum observed is assumed to be composed of a distribution of Lorentzian

noise spectra [1,2], each associated with traps at a given energy depth, with appropriate weighting according to the energy distribution of characteristic time constants. This latter weighting is taken to mirror the energy distribution of states in the gap. This represents a linear superposition of the (weighted) contribution from individual trapping levels, each with its own characteristic time constant. This approach thus assumes that each trap level is an independent source of fluctuation in free carrier number, unaffected by the presence of other traps in the material. At first sight this assertion seems plausible, since in the multi-trapping situation envisaged, cross-correlation effects must be very small. However, the presence of several groups of traps, or, in the limit, a continuum, results in a distribution of characteristic time constants, which is not a simple linear superposition of the time constants for each level. Thus the assertion that a flat density of states, or a region which is flat, such as the top of a broadened level, results in a region of 1/f slope in the noise spectrum, may not be valid. We present an alternative model [3] in which the distribution of time constants is appropriately incorporated, and compare the predictions of this model with the 'superposition' approach, using computed noise spectra. [1] P.A.W. Verleg and J.I. Dijkhuis, J. Non-Cryst Solids 266-269, (2000) 232. [2] P. Dutta, P. Dimon and P.M. Horn, Phys. Rev. Lett. 43, (1979) 646. [3] C. Main, S. Reynolds and M.J. Rose, J. Non-Cryst. Solids 227-230, (1998) 233.

A23.8

CORRELATION BETWEEN p^+ a-Si:H AND n^+ a-Si:H FILMS AND SCHOTTKY CELL STRUCTURE PROPERTIES FOR VARIOUS OBTAINING METHODS. Andrzej Kolodziej, Pawel Krewniak, Stanislaw Nowak, Univ of Mining and Metallurgy, Dept of Electronics, Krakow, POLAND.

Effectiveness of the n^+/i a-Si:H as well as p^+/i a-Si:H junctions based on n^+ and p^+ a-Si:H layers obtained by sputtering of Si:B and Si:P targets apparently increases under conditions of fast deposition and of high hydrogen dilution with simultaneous lowered temperature. This leads to a conclusion that temperature of the substrate rather than energy of sputtered particles determines junction creation process (diffusion of dopants). On the other hand, the microcrystallization of doped layers with simultaneous amorphous phase of i layer is profitable. Analyzing those processes we compare them to the p^+/i a-Si:H and n^+/i a-Si:H junctions obtained in the PECVD process at high dilution conditions for the p^+ and n^+ a-Si:H layers, as well as in condition of protocrystalline properties for the i a-Si:H films. The analysis is performed by systematic research of the I-V characteristics and Schottky type fill factor in the structure: half-transparent Ni / i / n^+ / Al or .../ p^+ / Al. Based on them the role of above junctions, the gap state distribution and the charge defects are determined. The quality differences of inter-surfaces between n^+/i and p^+/i a-Si:H layers for structures manufactured by means of the RMS (Reactive Magnetron Sputtering) and PECVD technologies are visible after systematic analysis of the high resolution cross-section TEM and AFM images. X-ray small angle spectroscopy and also fluorescent spectroscopy are employed to the analysis of densities and defects of layers, as well as to determine amount of dopes. Layers and the Schottky structures are manufactured on the polyimide covered and clean Al and Cu foils at temperature 120°C and 250°C, respectively. At the same time, we present the performance of x-ray matrix image sensor structure made after optimization of the n^+/i and p^+/i a-Si:H junctions.

SESSION A24: POSTER SESSION HETEROJUNCTIONS

Chair: Markus B. Schubert
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A24.1

CHARGE CARRIER TRANSPORT IN a-Si:H/cSi HETERO-JUCTIONS. S. von Aichberger, F. Wunsch, M. Kunst, Hahn-Meitner-Institut, Dept Solare Energetik, Berlin, GERMANY.

Charge Carrier Transport in amorphous silicon (a-Si:H) / crystalline SI (c-Si) heterojunctions is essential for the performance of optoelectronic devices based on these junctions. In this work these junctions will be studied by contactless transient photoconductivity measurements in the microwave frequency range (TRMC measurements). The TRMC technique enables the study charge carrier dynamics after surface excitation (by 532 nm light) and volume excitation (by 1064 nm light). TRMC signals induced by 1064 nm light refer only to excess charge carriers in the c-Si substrates. The surface recombination velocity at the a-Si:H/c-Si interface is clearly lower than at the c-Si surface before deposition. The passivation of the c-Si surface was found for all heterojunctions studied in this work, i.e. i a-Si:H/n c-Si, i a-Si:H/p c-Si, n a-Si:H/n c-Si, n a-Si:H/p c-Si and p a-Si:H/n c-Si. However the best passivation was observed for i a-Si:H films. The surface recombination velocity decreases with increasing thickness of the a-Si:H film but saturates beyond a certain thickness. In the space charge field of the heterojunctions examined, excess electrons and holes are separated and stored at this interface and cant recombine, therefore exhibiting a very long lifetime. This phenomenon is clearly observed in n a-Si:H/p c-Si samples with a highly recombining rear face of the c-Si .The a-Si:H deposition results in a tail with a very long decay time from which information on the band bending in theses samples can be obtained. The comparison of the TRMC-signal excited through the a-Si:H film from the c-Si-substrate before and after the a-Si:H deposition determines the film thickness of the a-Si:H. TRMC measurements induced by 532 nm light lead to the same results as those induced by 1064 nm light for thin a-Si:H films, until a considerable part of the light is absorbed in the a-Si:H films (> 500 nm). Then charge carriers in the a-Si:H film contribute to the TRMC signal and minority carrier injection from the a-Si:H film into the c-Si substrate can be observed.

A24.2

DEFECTS IN a-Si/c-Si HETEROJUNCTION DEVICES. Thomas Unold, Max Roesch, Karsten Brendel, Gottfried H. Bauer, Dept of Physics, Univ of Oldenburg, GERMANY.

The role of the bulk and interface defects in amorphous/crystalline silicon heterojunctions is still not clearly understood. This is due to the complicated band structure and defect occupation at the interface which prohibits a simple analysis of measurement results. We have measured the frequency and temperature dependent admittance on a number of differently prepared a-Si/c-Si devices. The data were analysed by computer modeling using an improved implementation. In difference to conclusions from previous analyses our simulations show only a small influence of interface defects on the capacitance spectra, although some of the devices yield a large increase in the low frequency capacitance by more than a factor of two. Therefore it is concluded that in these devices a significant density of defects must be present in the crystalline wafer. Since this also occurs in devices based on float-zone wafers, the amorphous silicon deposition seems induce defects in these wafers under certain conditions. Analysis of the activation energies and prefactors of the steps in the admittance spectra indicate a tunneling of carriers at or near the heterointerface.

A24.3

OPTIMIZATION OF DRY SURFACE CONDITIONING OF TEXTURIZED CRYSTALLINE SILICON WAFERS FOR THE GROWTH BY PLASMA ENHANCED CHEMICAL VAPOR DEPOSITION OF AMORPHOUS SILICON THIN LAYERS. Francesco Roca, M. Luisa Addonizio, Ivana Nasti, Mario Tucci, Francesca Varsano, ENEA Portici Research Centre, Portici, Naples, ITALY.

In the last year, remarkable progress has been observed in the development of a cost-effective, high output-conversion efficiency solar cells based on a "hybrid" heterojunction (HJ) fabricated by growing a ultra thin amorphous silicon layer on a crystalline base at temperature less than 250°C using Plasma Enhanced Chemical Vapor deposition. The technology is not only strategic for the actual PV market to increase the output and decrease the costs including those coming from energetic aspects, but also for the PV of the next future for the high compatibility with thin silicon grown on glass or similar substrates. One of the more limiting step is bonded to the surface conditioning of crystalline base in spirit of removing the damage on silicon surface leaving an atomically flat and uncontaminated surface suitable for the deposition of amorphous layer. We present the results of our studies using dry cleaning procedures of p-type c-Si, multi-Si, and thin silicon films growth on glass. Particulary we investigated a dry cleaning procedures using a CF_4/O_2 8% mixture in a commercial single UHV chamber 13.56 MHz capacitive coupled glow discharge system. The temperature was changed in the range 40°C -320°C, the mixture flow between 10sccm-50sccm, the etching time from 30 sec. to 20 min. The partial pressure of mixture between 35 mTorr - 500 mTorr. We found evidence applying the process on texturized cSi that the incoming flux acts on the lateral faces piramides and poorly on the tip, so there is a change in the shape depending from the etching time. A detailed analysis using I-V dark, yield, total-diffused reflectance, SEM analysis, C-V-F-T showing the best condition to increase the performance of the devices. By using the optimised process on cast silicon for solar applications we obtained PV conversion efficiency of 12.9% on 51 cm^2 and 9.2% on 45 cm^2 aperture area respectively for HJ solar cells on cSi and m-Si

A24.4

BUFFER LAYERS FOR IMPROVING THE CELL PERFORM-ANCE OF HYDROGENATED AMORPHOUS SILICON SOLAR CELLS DEPOSITED WITH AN EXPANDING THERMAL PLASMA. B.A. Korevaar, C. Smit, R.A.C.M.M. van Swaaij, Delft University of Technology, DIMES, Delft, THE NETHERLANDS; D.C.

Schram, M.C.M. van de Sanden, Eindhoven University of Technology, Eindhoven, THE NETHERLANDS.

A cascaded arc expanding thermal plasma is used to deposit intrinsic hydrogenated amorphous silicon at growth rates larger than 10 Å/s. Implementation into a single junction p-i-n solar cell resulted in initial efficiencies of ~7%, whereas all the optical and initial electrical properties of the individual layers are comparable with RF-PECVD deposited films. Spectral response measurements indicate that the p-i interface is responsible for the lower efficiencies than obtained for conventional low rate RF-PECVD. As there is no deterioration of the p-layer by the plasma, the initial growth is a likely candidate in the sense that the first nanometres might contain more defects at higher growth rates. A low growth rate buffer layer is implemented between the p- and i-layer to increase the efficiency of the expanding thermal plasma solar cell. This increase in efficiency is achieved by a better initial defect density near the p-i interface resulting in a higher fill-factor, a better carrier collection, and less degradation. Results will be compared with simulations of the solar cell to interpret the obtained results if buffer layers are implemented.

A24.5
AMORPHOUS SILICON DEPOSITION ON ZnO SUBSTRATES WITH DEEP NANOSTRUCTURE. R. Könenkamp, M. Poschenrieder and M.-Ch. Lux-Steiner, Hahn-Meitner Institut Berlin, GERMANY; S. Wagner, Department of Electrical Engineering, Princeton University, Princeton, NJ; F. Zenia, C. Levy-Clement, Laboratoire de Chimie Metallurgique des Terres Rares, CNRS Thiais, FRANCE.

We report results of a-Si:H deposition on novel ZnO films consisting of free standing single crystalline columns of several micrometer height and approximately 100 nanometer diameter. The ZnO films have considerable potential for use in photoelectric thin film devices. Morphology, electronic parameters, and basic optical behavior, such as reflectance and light trapping efficiency, are reported. Amorphous silicon is deposited on the columns as a continuous smooth film with conformal coverage. Some possibilities of using these films in devices are discussed.

A24.6
OPTICAL ANALYSIS OF SPECULAR AND TEXTURED SnO_2 FOR APPLICATIONS IN a-Si:H SOLAR CELLS. Joungchel Lee, Andre S. Ferlauto, Randy J. Koval, Joshua M. Pearce, Gelio M. Ferreira, Chi Chen, Christopher R. Wronski and Robert W. Collins, Materials Research Laboratory and Center for Thin Film Devices, Pennsylvania State University, University Park, PA.

We have applied Stokes vector spectroscopy to characterize the optical properties, microscopic structure, and macroscopic structure of several specular and textured conducting SnO_2 films on glass substrates. The measured characteristics have been correlated with atomic force microscopy (AFM) and with the quantum efficiencies of a-Si:H p-i-n solar cells deposited on the same glass/SnO_2 surfaces. A number of different doped SnO_2 films have been studied in this way, including Asahi types A, B, and U, each exhibiting differing amounts of "haze" from 5 to 10%. With the Stokes vector spectroscopy, we measure changes in three different characteristics of a light beam upon its reflection from the glass/SnO_2 surface [1]. These include changes in (i) the polarization ellipse of the beam, including the ellipticity and tilt angles, (ii) the degree of polarization of the beam, and (iii) the irradiance or power per unit cross-section of the beam. From the change in the polarization ellipse, the spectroscopic optical properties (index of refraction and extinction coefficient) as well as the microscopic structure of the film (bulk, surface, and interface layer thicknesses) can be obtained. From the change in the degree of polarization, information on geometric scale structure (non-uniformity) and multiple scattering can be obtained. From the change in irradiance (i.e., the reflectance), properties of the macroscopic roughness can be determined. A key characteristic of the SnO_2 film is the total integrated scattering (TIS) that it generates, determined by combining information from the changes in the polarization state and irradiance. The TIS is resolved spectroscopically and describes the losses from the specular beam via non-specular scattering. Correlation of these losses with the quantum efficiency gains in the solar cell allows us to extract basic spectroscopic information on the effectiveness of different SnO_2 films for optical enhancement. [1] P.I. Rovira and R.W. Collins, J. Appl. Phys. 85, 2015 (1999).

SESSION A25: POSTER SESSION AMORPHOUS AND MICROCRYSTALLINE SOLAR CELLS

Chair: Arthur Yelon
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A25.1
INTEGRATED OPTICAL AND ELECTRICAL MODELING OF a-Si:H BASED SOLAR CELLS. Miro Zeman, Joost van den Heuvel, Rene van Swaaij, and Wim Metselaar, Delft University of Technology, DIMES, Delft, THE NETHERLANDS.

Current amorphous and microcrystalline silicon solar cells use textured substrates for enhancing the light absorption and buffer and graded layers in order to improve the overall performance of the cells. The resulting solar cell structures are very complex and for understanding the role of these layers and for further optimization of the solar cell structures computer modeling is a useful tool. In this paper we describe some of the new features of the ASA (Amorphous Semiconductor Analysis) software package and demonstrate its applications to a-Si:H based solar cells. Simulated results obtained using ASA program are compared to experimental results in order to give insight into the behavior of the internal parameters of the solar cells. Improved understanding of the following issues will be presented in detail: 1. The effect of the front and back contact roughness on the external quantum efficiency and the absorption of light in the individual layers of a-Si:H solar cells and 2. The role of band gap grading of the intrinsic a-SiGe:H layer in a solar cell with the aim to improve the cells external parameters.

A25.2
ANNEALING KINETICS OF AMORPHOUS SILICON ALLOY SOLAR CELLS MADE AT VARIOUS DEPOSITION RATES. Baojie Yan, Jeffrey Yang, Kenneth Lord, and Subhendu Guha, United Solar Systems Corp., Troy, MI.

It is well known that the performance of amorphous silicon (a-Si) alloy solar cells depends critically on the deposition rate, and has been shown to correlate with the microvoid density of the intrinsic layer. Using RF glow discharge, solar cells deposited at rates > 3 Å/s exhibit lower initial efficiencies and poorer stability than those made at lower rates. The stabilized efficiency is determined by an equilibration between light-induced degradation and thermal annealing. In this paper, we present results on the annealing kinetics of a-Si alloy solar cells made with four different deposition conditions. Three cells were made at 1 Å/s, 3 Å/s, and 10 Å/s using RF glow discharge, and one cell at 8 Å/s with VHF. The nip cells having an intrinsic layer thickness of ~2200 Å were deposited on stainless steel substrates. The cells were light-soaked at room temperature using white light with an intensity of 30 suns to quickly reach the degraded state. The cells were then annealed at elevated temperatures for selected time intervals ranging from 1 minute to 110 hours. The correlation of J-V characteristics and defect density was obtained by computer simulation using AMPS. By fitting the annealing kinetics of defect density, the annealing activation energy distribution is obtained. We find that the cell deposited at 1 Å/s has the highest annealing rate, having the lowest annealing activation energy with the narrowest distribution. The cell deposited at 10 Å/s exhibits the lowest annealing rate with the highest annealing activation energy and the broadest distribution. The cell made with VHF at 8 Å/s displays a higher annealing rate than the 3 Å/s cell made by RF, consistent with the observed, improved stability of the VHF cells.

A25.3
CORRELATION BETWEEN FILM AND CELL PROPERTIES FOR DC PLASMA DEPOSITED AMORPHOUS SILICON. Jennifer T. Heath, J. David Cohen, Yoram Lubianiker, Univ of Oregon, Dept of Physics, Eugene, OR; Gautam Ganguly, BP Solarex Corp, Toano, VA.

We have carried out measurements to try to correlate amorphous silicon film properties with companion solar cell device performance. In a series of samples deposited at increasing growth rates we observed that decreasing cell efficiencies were not clearly correlated with an increase in defect density. In fact, these parameters appear to be anti-correlated, indicating that intrinsic layer defects are not the limiting factor to cell performance in this series of samples. The films and devices were deposited at Solarex in a double-load lock research reactor using dc plasma decomposition. The films were i-layers deposited onto p^+ -type crystalline Si substrates or onto SnO_2 coated specular glass, and the device structure was glass/SnO_2/p/i/n/ ZnO/Al. For the devices only the i-layers were varied to match the growth conditions of the corresponding films. The film properties were determined using drive-level capacitance profiling (DLCP) and transient photocapacitance spectroscopy. The DLCP technique established quantitative values of the deep defect densities in the films as well as the spatial uniformity of the electronic properties. The photocapacitance measurements indicated Urbach energies of 49±1 meV and optical gaps of 1.81±0.05 eV. Because these thin film characterization methods employ a sandwich device structure very similar to the working solar cell devices, the material properties and cell parameters are more likely to exhibit clear correlations across the wide range of growth conditions employed. Cell and film performance

were explored in both the as-grown and light-soaked states. Cell efficiency in the degraded state decreased from a maximum of 5.4% to 3.3% as the i-layer growth rate was increased by a factor of 10 by adjustment of the plasma power and hydrogen dilution. Meanwhile, the defect density of the degraded films, as determined by DLCP, decreased by a factor of 3. Other possible factors influencing the change in device performance will be discussed.

A25.4
EFFECTS OF LOW TEMPERATURE, REVERSE BIAS ANNEALING ON THE INITIAL AND STABILIZED PERFORMANCE OF AMORPHOUS SILICON SOLAR CELLS. David Carlson, Gautam Ganguly, Guang Lin, BP Solar, Toano, VA.

The performance of amorphous silicon solar cells has been improved by annealing the cells at successively lower temperatures for successively longer times. For tandem cells, the improvement is typically 3-6 percent as compared to cells that received only a thirty-minute annealing treatment at about 170C. For single-junction cells, the improvement in initial performance is usually on the order of 1-3 percent. The initial performance is also improved by the application of a strong reverse bias while annealing at low temperatures (60C-150C). Some of this improvement in performance is evident after light soaking, but the effect is small and not always statistically significant. We also studied the effects of reverse bias annealing treatments on single-junction a-SiC:H cells with a high density of metastable defects. These cells degraded by as much as 80 percent after several hundred hours of 1 sun light soaking, and the light-soaked cells exhibited a large improvement in performance when a strong reverse bias was applied at relatively low temperatures (60C-100C). The bias treatment caused a dramatic improvement in the fill factor and in the short-wavelength spectral response of the cells. Moreover, the bias-treated cells exhibited an improved short-wavelength spectral response after a second light soaking indicating that some of the metastable defects had been permanently removed by the bias treatment. The low temperature annealing effect can be explained in terms of a re-equilibration of thermally generated defects due to a redistribution of hydrogen atoms. The effects of reverse bias annealing on light-soaked cells can be explained using a model based on hole trapping at partially hydrogenated microvoids containing molecular hydrogen.

A25.5
MICROCRYSTALLINE SILICON SOLAR CELLS PREPARED BY 13.56 MHZ PECVD AT HIGH GROWTH RATES: SOLAR CELL AND MATERIAL PROPERTIES. Tobias Roschek, Tobias Repmann, Bernd Rech, Wolfhard Beyer, Institut für Photovoltaik, Forschungszentrum Jülich, Jülich, GERMANY; Peter Werner, Max-Planck-Institut für Mikrostrukturphysik, Halle, GERMANY; Felix Edelman, Albert Chack, Raoul Weil, Robert Beserman, Solid State Institute, Technion, Haifa, ISRAEL.

In the past years intrinsic microcrystalline silicon (μc-Si:H) has found growing attention as an absorber material in thin film solar cells. However, for sufficient absorption of red and infrared light, thicknesses of more than one μm are required for the μc-Si:H layer, and hence high deposition rates are essential. We prepared microcrystalline silicon based p-i-n solar cells using 13.56 MHz excitation frequency in the deposition regime of high plasma power resulting in high deposition rates. The deposition pressure turned out to play a key role for device performance. Only at high deposition pressures we could achieve both high efficiencies up to 8.1% and high growth rates of 5-6 Å /s. These cells exhibit FF and V_{OC} of about 70% and >500 mV, respectively, indicating good transport properties of the μc-Si:H i-layer material. At an increased growth rate of 10 Å /s we still achieved an efficiency of 6.6%. These empirically optimized solar cells as well as i-layer material deposited on glass or crystalline Si substrates were further characterized by various techniques including cross-sectional TEM, Raman spectroscopy, infrared absorption and hydrogen effusion. The results suggest that the increase in solar cell efficiency correlates with the structural i-layer properties. The results will be compared to issues of a recent study of μc-Si:H solar cells prepared by VHF-PECVD [1]. 1. O. Vetterl et al., MRS Symp. Proc. 609 (2000).

A25.6
GUIDING PRINCIPLE TO DEVELOP INTRINSIC MICRO-CRYSTALLINE SILICON ABSORBER LAYER FOR SOLAR CELLS BY HOT-WIRE CVD. A.R. Middya, Urban Weber, C. Mukherjee and B. Schroeder, Department of Physics and Center of Materials Research, University of Kaiserslautern, Kaiserslautren, GERMANY.

In last five years it has been established that hot-wire CVD (HWCVD) is a viable low-cost technique for one-step deposition of micro/polycrystalline silicon thin films on glass substrates with superior crystallographic quality and high growth rate ~1.5 nm/s. Recently scale up potential of this technique has also been demonstrated[1]. Here we report on importance of controlling impurities particularly oxygen-related and crystallographic orientation in microcrystalline intrinsic layer of HWCVD for its application in solar cells. Impurities severely affect electronic properties of microcrystalline samples since both metallic impurities and O-related SiO_2 defect-complex in crystalline Si acts as efficient recombination centers. Controlling filament temperature is one way to reduce metallic impurities, however reduction of oxygen in the films is not easy since its originates from residual water vapor (H_2O) in the reactor, out-gassing from chamber wall and post-oxidation. In our multi-chamber system, gas purifiers are attached to H_2 and SiH_4 gas lines to remove the possibility of contamination from the process gases. We adapted a special procedure before deposition to reduce H_2O vapor and wall out-gassing to reduce the oxygen content in the films. Additionally we varied hydrogen dilution (H_2/SiH_4) from 0 to 25 expecting structure of the films will undergo a smooth transition from amorphous to polycrystalline phase. With this combine approach, we developed a highly photosensitive ($10cm^3$) microcrsytalline Si films with high growth rate more than 1 nm/s, whose microstructure is close to amorphous phase ($f_c \approx 46 \pm 5\%$), as confirmed by X-ray diffraction. It has been observed that with the increase of f_c, photosensitivity continuously decrease to 10 for films with $f_c > 70\%$. Thus microcrystalline Si films close to amorphous phase is more suitable for absorber layer than materials with high f_c. The experiment to estimate the bulk defect density by CPM, its dependence on f_c and the study of recombination process in these high photosensitivity nano/microcrystalline films by photoluminescence spectroscopy are underway. However on application of these materials in pin devices did not result in expected performance[2]. Out of several possibilities, one could be, absence of (220) crystallographic orientation in these materials. We will develop (220) orientation by controlling chamber pressure and substrate temperature and verify above mentioned hypothesis. We will discuss the importance of reduction of oxygen content, metallic impurities and presence of (220) orientation having inactive grain boundary to achieve efficient microcrstalline solar cells on glass substrate. We will also outline the insight for future directions to achieve low cost a-Si:H/μc-Si:H tandem cells by HWCVD. 1. A. Ledermann, U. Weber, C. Mukherjee, and B. Schroeder, to be published in Proc. 1st Int. CAT CVD Conference (Kanazawa, Nov. 2000, to appear in Thin Solid Films). 2. U. Weber, A.R. Middya, C. Mukherjee and B. Schroeder, Proc. of the 28th IEEE PVSC (2000) (in press).

A25.7
CHARACTERISTICS OF POLY-Si SOLAR CELL USING GRAIN BOUNDARY ETCHING AND TRANSPARENT CONDUCTING OXIDE. In Lee, Dong Gun Lim, Uk-Jae Lee and Junsin Yi, School of Electrical and Computer Engineering, Sungkyunkwan University, Kyunggi-do, KOREA.

This paper deals with a novel structure of polycrystalline silicon (poly-Si) solar cell for terrestrial applications. Grain boundary (GB) in poly-Si degrade a conversion efficiency of poly-Si solar cell. To reduce the GB side-effect, we investigated various parameters such as the preferential GB etch, etch time, ITO electrode, heat treatment, and emitter layer effect. Among various preferential etchants such as Sirtl, Yang, Secco, and Schimmel, a Schimmel etchant illustrated an excellent preferential etching properties. We clearly observed a deep trench along grain boundaries and randomly textured grain surface with pyramid structure. We used rf magnetron sputter grown tin doped indium oxide (ITO) film as a top contact metal. ITO films showed a resistivity of 1.14×10^{-4} $W\Omega\cdot$cm and transmittance of 90.5% for the wavelength of 594 nm. ITO films served not only as a top electrode but also as an effective AR coating layer. ITO film properties were strongly influenced by the preparation temperatures. Substrate temperature of 400°C gave the highest conversion efficiency of poly-Si solar cell. With well-fabricated poly-Si solar cells, we were able to achieve conversion efficiency as high as 16% at the input power of 20 mW/cm^2.

A25.8
PREPARATION TEMPERATURE EFFECTS IN MICRO-CRYSTALLINE SILICON THIN FILM SOLAR CELLS. Helmut Stiebig, Oliver Vetterl, Andreas Lambertz, Reinhard Carius, Friedhelm Finger, Heribert Wagner, Institut für Photovoltaik, Forschungszentrum Jülich GmbH, Jülich, GERMANY; Arup Dasgupta, Energy Research Unit, IACS, Calcutta, INDIA.

In recent years the conversion efficiencies of microcrystalline silicon (μc-Si:H) thin film solar cells have been continuously improved. An important prerequisite for this advance is the ability to produce high quality intrinsic μc-Si:H material by optimized preparation processes. However, the connections between material properties on the one hand and the device performance on the other hand must be further explored. Based on the findings of previous works, which demonstrated effects on solar cells caused by the structural and electrical transport properties of material prepared at different silane concentrations and

discharge powers, we now extended the investigation to a variation of substrate temperature. For this purpose, $1\mu m$ thick μc-Si:H pin and nip solar cells have been prepared using a PECVD process at 95MHz. For the nip device design increasing the substrate temperatures above the standard 200°C leads to a clear improvement of device performance, resulting in maximum efficiencies of 8.7% at 250°C. Important to note, the improvement does not depend on the preparation temperature of the doped layers. Surprisingly, pin devices show no performance improvement upon increase of the temperature. The highest efficiencies in this case are obtained at the standard value of 200°C and slightly below. From the reduction of short wavelength response, which is the most deteriorating effect at high deposition temperatures, it can be assumed, that the properties of the p-doped/intrinsic interface zone are affected. This part of the pin solar cell is especially critical, since it is located on the light entering side and the crystalline nucleation zone is located there. In contrast to this, the nucleation zone of nip devices is located in the rear part and is less critical. The results emphasize the importance of the preparation temperature with respect to the device performance, but also show up possible interference with the device design.

A25.9
SOLAR CELL PERFORMANCE UNDER DIFFERENT ILLUMINATION CONDITIONS. Christian Gemmer and Markus B. Schubert, University of Stuttgart, Institute of Physical Electronics, Stuttgart, GERMANY.

The optimization of solar cells usually proceeds with regard to the standardized illumination spectrum air mass 1.5 (AM 1.5). In many cases, however, the illumination conditions deviate from the standard, resulting in substantially different cell performance. Typical examples are i) indoor applications, where the total power density P_{total} of predominantly red halogen light equals $P_{total} = 1$ Wm^{-2}, and ii) outdoor applications, where cloudy skies exhibit a blue-shifted spectrum and $P_{total} = 100$ Wm^{-2}. Thus, studying the performance of solar cells under low light conditions and different illumination spectra is of high relevance for hybrid electronic systems, like smart cards, wrist watches, transponder systems, and mobile sensors. Here we numerically study amorphous silicon (a-Si:H) and copper indium gallium diselenide (CIGS) based solar cells, and evaluate their feasibility for different application scenarios. For ease of comparison, we model solar cells of both material systems with the same "first principles" software, called ASA [1]. After successful transfer of input parameters from other modeling software to ASA, we apply i) black body radiation spectra with different maximum emission wavelengths, ii) the AM 1.5 wavelength distribution and, iii) the standardized D 65 spectrum, representing cloudy northern sky irradiance at noon. The total power density ranges between $P_{total} = 1$ mWm^{-2} and $P_{total} =$ 1 kWm^{-2}. One of our first results is that with lowering P_{total} the performance of the CIGS cell decreases more than the characteristics of the a-Si:H cell independent of the illumination spectrum.
[1] M.B. von den Linden, R.E.I. Schropp, W.G.J.H.M. van Sark, M. Zeman, G. Tao, and J.W. Metselaar, in: Proc. of EPVSEC-11, Montreux, Switzerland (1992), p. 647.

A25.10
CARRIER TRANSPORT AND PHOTOGENERATION IN LARGE AREA P-I-N Si/ Si C HETEROJUNCTION. P. Louro, Yu. Vygranenko, M. Fernandes and M. Vieira, Electronics and Communications Dept, ISEL, Lisbon, PORTUGAL; M. Schubert, Institut fur Physikalische Elektronik, Universitat Stuttgart, Pfaffenwaldring, Stuttgart, GERMANY.

A series of large area (4 x 4 cm^2) single layers and heterojunctions cells in the assembly glass/ZnO:Al/p (Si_xC_{1-x}:H)/i(Si:H)/ n(Si_xC_{1-x}:H)/Al (0<x<1) were produced by PE-CVD at low temperature (150°C). The deposition conditions of all the i-layers were kept constant while they varied in the n- and p-layer by adding methane during the deposition process. Depending on the methane flux the deposited n- and p-layers present conductivities, σ_d, in the range of 1.9×10^{-12} Ω^{-1}cm^{-1} to 1.8×10^{-5} Ω^{-1} cm^{-1} and optical gaps, E_{op}, between 2.2 eV and 1.8 eV. The i-layer has a dark conductivity of approximately 7×10^{-11} Ω^{-1}cm^{-1} and a photosensitivity higher than 10^4 under AM1.5 (100 mW/ cm^2). Junction properties, carrier transport and photogeneration are investigated from dark and illuminated current-voltage and capacitance-voltage characteristics at room temperature. The collection efficiency is evaluated from spectral response measurements under different applied bias voltages. For the heterojunction cells S-shaped J-V characteristics under different illumination conditions (in the range of 1 mW/ cm^2 to 100 mW/ cm^2) are observed leading to poor fill factors. High serial resistances around 10^5 Ω are also measured. The heterojunctions were compared with the corresponding p-i-n-Si:H homojunctions. At low light intensity they show the normal J-V characteristics, however as the light intensity increases the current starts decreasing around zero bias voltage and the fill factor lowers. In this case the serial resistance depends on the illumination conditions and decreases from 750 Ω to 40 Ω as the light intensity increases. Having as input parameters the experimental data a detailed numerical simulation is presented and gives insight into the internal physical process. Simulated results confirm the experimental findings. Considerations about induced electric field and inversion layers at the interfaces, drift-diffusion transport mechanism and the generation-recombination process are used to explain the device output and the atypical shape of the J-V characteristics under different illumination conditions.

A25.11
CONTROLLING THE LATERAL PHOTOEFFECTS IN a-Si:H P-I-N HETEROJUCTION STRUCTURES: THE INFLUENCE OF THE BAND OFFSET ANYLISED THROUGH A NUMERICAL SIMULATION. A. Fantoni[a,b], P. Louro[a], R. Schwarz[a], M. Vieira[a]; [a]Electronics and Communications Dept., ISEL, R. Conselheiro Emidio Navarro, Lisboa, PORTUGAL; [b]FCT-UNL Quinta da Torre, Caparica, PORTUGAL.

When an a-Si:H p-i-n structure is locally illuminated by a light spot, the non uniformity of light causes the appearance of a gradient in the carriers concentrations between the illuminated and the dark zones. Carriers start to flow in agreement with such gradients, and when equilibrium is reached, the lateral diffusion process is counterbalanced by the appearance of a lateral component of the electric field vector in addition to the usual transverse component. The lateral fields act as a gate for the lateral flow of the free carriers and small lateral currents appears at the transition regions between the illuminated and dark region. Such lateral photo effects depend on the incident light wavelength, light intensity and on the device operation condition (short or open circuit condition). The introduction of carbon in the doped layers modifies the intensity and the extension of these lateral effects through the potential barriers deriving from the band banding at the n-i and the p-i junctions. We have used the 2D numerical simulator ASCA to analyse the behaviour of an a-Si:H p-i-n structure under non-uniform illumination with the goal of observing the appearance of the lateral components of the electric field and the current density vectors in the transition area between the illuminated and dark regions. Different homo and hetero-structures under local illumination have been simulated, outlining how the band offset at the two juctions influences the induced lateral photoeffects and aiming to explain how a correct device design and engineering can, depending on the foreseen application of the device, alternatively enhance or reduce the intensity of such lateral effects.

A25.12
MICROCRYSTALLINE GERMANIUM CARBIDE: A NEW THIN FILM MATERIAL FOR PHOTOVOLTAICS. Vikram L. Dalal, Iowa State University, Dept. of Electrical and Computer Engineering, Ames, IA.

We report on the growth and electronic and optical properties of materials and devices in microcrystalline Germanium Carbide, a very promising new material sysytem for thin film photovoltaic energy conversion. This material system has a unique band structure in that the indirect L valley appears to be separated by only about 0.25 eV from the direct gap central gamma valley. The bandgap of the material can be varied from 0.7 to about 1.3 eV bychanging the C:Ge ratio. This unique combination of bandgap and favorable band structure makes the optical absorption coefficient near direct gap in the wavelength region of interest for solar energy conversion. The absorption coefficient of (Ge,C) with a bandgap of 1.1 eV is nearly 20 times that of c-Si near the band edge. The electronic properties can be controlled by doping, and p-n junctions can be made. The material was fabricated using reactive plasma beam deposition, using a remote ECR source and mixtures of methane, germane and hydrogen. The paper will describe the various results achieved in materials and dev ices, and the real possibility that even a direct gap material can be produced in this system by using strain engineering.

SESSION A26: POSTER SESSION
TFTs AND SENSORS
Chair: Jun-ichi Hanna
Thursday Evening, April 19, 2001
8:00 PM
Metropolitan Ballroom (Argent)

A26.1
HIGH ELECTRON MOBILITY TFTS OF NANOCRYSTALLINE SILICON DEPOSITED AT 150°C ON PLASTIC FOIL. I-Chun Cheng and Sigurd Wagner, Department of Electrical Engineering, Princeton University, Princeton, NJ.

High performance thin film transistor circuits on plastic are an important need for highly integrated low cost large-area electronic

backplanes. We have made a key step toward a directly deposited high mobility silicon technology on Kapton polyimide foil, by fabricating n-channel thin film transistors (TFTs) of nanocrystalline silicon (nc-Si:H) at a substrate temperature of 150°C. Our results suggest that eventually a complete CMOS technology may be accessible through directly deposited silicon on plastic. We made the n-channel TFTs on both Kapton and glass substrates for comparison. The TFTs have top gate geometry. Both the intrinsic channel layer and the n^+ source/drain layer were deposited at 80 MHz excitation frequency. Small flows of dichlorosilane were added to the silane/hydrogen source gas to obtain near intrinsic conductivities of 10^{-7} to 10^{-6} S·cm^{-1}. The film thicknesses were 300 nm for nc-Si:H, 60 nm for n^+ nc-Si:H, and 300 nm for the plasma deposited gate SiO_2. We used digitally printed masks for standard photolithography. The channel width/length was 180 μm/45 μm. The top gate device technology used in our TFTs requires a plasma etch step for source/drain isolation, which is followed by deposition of the gate SiO_2. These two steps have not yet been optimized, and we obtain "off" currents as high as $\sim 10^{-7}$ A, threshold voltages of $\sim$ 17 V and substantial and widely scattering gate leakage currents. However, when properly evaluated the "on" current is a reliable criterion for field effect mobility. Hence the goal of our initial program reported here was a high "on" current. The n-channel TFTs of 150°C nc-Si:H on Kapton have reached "on" currents of $\sim 3\cdot10^{-4}$ A, a linear electron mobility of $\sim$ 25 cm^{2}V^{-1}s^{-1} and a saturated electron mobility of $\sim$ 30 cm^{2}V^{-1}s^{-1}. These mobility values suggest that directly deposited nc-Si:H is an attractive alternative for a channel material for TFTs made on plastic substrates, when compared to a-Si:H and laser crystallized Si. This work is supported by the DARPA HDS program.

A26.2

DENSITY OF STATES IN a-Si:H FROM SCLC AND ITS APPLICATION IN MODELLING A VERTICAL TFT. Naser Sedghi, William Eccleston, University of Liverpool, Dept of Electrical Engineering and Electronics, Liverpool, UNITED KINGDOM.

Steady-state space-charge limited current (SCLC) measurements are used to investigate the density of states (DOS) in the mobility gap of hydrogenated amorphous silicon (a-Si:H). The density of states found by the SCLC method is used to set the trap densities and energy levels to model a vertical a-Si:H thin-film transistor (TFT) using Medici device simulation package. Simulation on the space-charge limited current was also performed to verify the validity and accuracy of methods of investigating the DOS using SCLC. Nearly all researchers have claimed that a-Si:H has a continuous density of states, however, there are some peaks or maximum points in the DOS distribution that can be treated as discrete trap levels. The density of states was calculated by different methods based on both continuous DOS and discrete trap assumptions. Treating as discrete trap levels is especially useful in simulations using packages like Medici in which a limited number of trap levels can be defined. The effect of various trap densities and trap energy levels in the bulk of the a-Si:H on the characteristics of a vertical TFT is studied by modeling the transistor using Medici. It is shown that the threshold voltage and subthreshold swing is affected by the low energy traps, while the effect of the higher energy traps is just reducing the on-current. The off-current is also increased by the presence of the traps. Variations of the device characteristics by the physical dimensions of the TFT is also studied by transistor modeling.

A26.3

PHOTOCAPACITANCE OF HYDROGENATED AMORPHOUS SILICON PHOTOTRANSISTORS. D. Caputo, G. de Cesare, F. Lemmi, A. Nascetti, F. Palma, University of Rome "La Sapienza", Dept of Electronic Engineering, Rome, ITALY.

Amorphous silicon-based phototransistors are investigated to determine the extent of their applicability to large-area imaging systems. In particular, the non-linear optical gain of the phototransistors is appealing for applications that require a very large dynamic range. Also, the large gain can match the increasing demand for pixel-level amplifiers. In a typical charge storage operation mode in imaging arrays, sensors integrate charge on their capacitance. Data is subsequently read out by charge-sensitive amplifiers. To understand the implications of this operation mode in the case of phototransistor pixels, a study of their capacitance is needed. This paper reports measured capacitance values largely exceeding the geometrical one at low frequencies (down to 100 μHz) of the probe signal, both in the dark and under illumination. In particular, capacitance values in excess of 60 μF/cm^2 are measured under 220 μW/cm^2 illumination at 600 nm. Capacitance increases with the inverse of the frequency and such 1/f dependence is justified by trapping and release processes. The photocapacitance is linear with the illumination intensity, while the dependence of the photocurrent is sub-linear as expected. A difference is also found for the dependence on the bias voltage: while the photocurrent and the gain are strongly bias-dependent, the photocapacitance is not. The physical mechanism for the 1/f law of the photocapacitance is discussed along with its dependence on the bias and illumination intensity. Implications of the results on the operation of large-area imaging systems will be presented.

A26.4

ELECTROMECHANICAL PROPERTIES OF AMORPHOUS AND MICROCRYSTALLINE SILICON MICROMACHINED STRUCTURES. M. Boucinha, J. Gaspar, V. Chu, Instituto de Engenharia de Sistemas e Computadores (INESC), Lisbon, PORTUGAL; J.P. Conde, Department of Materials Engineering, Instituto Superior Técnico (IST), Lisbon, PORTUGAL.

Recently, thin-film 3-D micromachined structures (thin-film MEMS) based on a-Si:H and other thin-film materials have been demonstrated. Devices such as microswitches, air-gap TFTs, and microresonators have been fabricated. Bridge and cantilever structures were fabricated using a low-temperature ($\leq$100°C) surface micromachining process. The structural material in the microstructure is a-Si:H, μc-Si:H, a-C:H or SiN_x, or a bilayer of these materials and Al. A conductive gate is placed under the structure to enable the application of an electrical actuation voltage. DC current-voltage measurements of the pull-in voltage (V_{PI}) are used to estimate the Young's modulus (E) of the thin-film in the bridges and cantilevers. These measurements and the electromechanical modeling show that V_{PI} is not sensitive enough to allow the extraction of an accurate value of E. To measure the electromechanical properties of the thin-film structures, two techniques are used: Optical detection: a laser is focused on the top of the microstructure and reflected onto a position detector, whose signal can be used to monitor the electrically induced deflection. Lock-in detection of the deflection upon application of a quasi-DC voltage allows the precise measurement of the position of the microstructure as a function of the applied voltage. These results are used, together with the electromechanical model, to extract the value of E of the thin-films. The optical detection method can be used to measure the deflection in a wide range of frequencies, namely in the MHz regime where mechanical resonance occurs. AC electrical detection: results for electrical detection of AC electrically actuated thin-film microresonators in the RF frequency regime (using impedance-voltage measurements) will be presented. In addition, electrical detection will open up the possibility of the integration of thin-film micromachined structures with control electronics on a large-area substrate, thus enabling the fabrication of complex microsystems for a wide range of applications.

A26.5

MICROCRYSTALLINE GERMANIUM DETECTORS. Mathias Krause, Helmut Stiebig, Reinhard Carius, Heribert Wagner, Institut für Photovoltaik, Forschungszentrum Jülich GmbH, Jülich, GERMANY.

Crystalline germanium photodiodes are applied to detect light in the near infrared wavelength region due to the low band gap of germanium. We have investigated μc-Ge:H as an alternative to bulk c-Ge. The μc-Ge:H films were prepared by PECVD at the same conditions as μc-Si:H and μc-SiGe:H alloys (T_S=200°C, P=200mTorr, ν_{ex}=95.7MHz). Crystallinity was evaluated from Raman spectra. To obtain microcrystalline films much lower germane concentrations (GC=[GeH_4]/[H_2]<1%) had to be used. This agrees with the trend observed in μc-SiGe:H alloys where the transition to microcrystalline growth shifts towards higher hydrogen dilution when germane is added. The dark conductivity of μc-Ge:H decreases with increasing GC likely due to a change in the equilibrium carrier concentration. The optical absorption measured by PDS is significantly enhanced below the band edge and similar at higher photon energies when compared with c-Ge.
Next, we employed μc-Ge:H as absorber material in pin detectors which were prepared on glass substrates coated with smooth TCO. The device performance of diodes with a pure μc-Ge:H absorption layer deteriorates when abrupt transitions at the μc-Si:H(p) and a-Si:H(n) layer are prepared. Thus, we introduced 30nm thin band gap gradings in the front and the rear part of the i-layer in addition to the 50nm thin μc-Ge:H bulk. The gradings were achieved by a continuous change of the process gas from silane to germane. The detectors were characterized by I/V measurements in the dark and under AM1.5 illumination and spectral response measurements. The dark current, which is high due to the low band gap, decreases with increasing GC and limits the fill factor (FF). FF shows a maximum for GC=0.5%. The short circuit current drops with increasing GC due to increasing recombination losses. Additionally, temperature dependent measurements demonstrate that the high dark current is the limiting factor of the device performance.

A26.6

AMORPHOUS SILICON SCHOTTKY BARRIER DIODES USING ZnO AS OHMIC CONTACT AND AS GAS SENSOR. Hugo Iguas, Patricia Nunes, Vitor Silva, Elvira Fortunato, Rodrigo Martins, Departamento de Ciencia dos Materiais, Faculdade de Ciencias e

Tecnologia, Universidade Nova de Lisboa, Caparica, PORTUGAL.

Zinc oxide based coatings have recently received much attention because they have advantages over the more commonly used indium and tin-based oxide films namely, a high transparency associated with a high electrical conductivity and its sensitive to several gases. These properties make it possible to the used in photochemical diodes, such as Schottky barrier diodes, namely in a glass/Cr/a-Si:H(n^+)/ a-Si:H(i)/ZnO structure. Here the ZnO forms a Schottky barrier with the a-Si:H(i). In this configuration the ZnO is at the surface of the device, where its resistivity changes by exposition to a gas atmosphere (H_2, CH_4, CO_2) and so it can be used as a gas sensor. Apart from that, amorphous silicon Schottky barrier diodes using ZnO as the ohmic contact are investigated advising its application to linear position sensitive detectors. The first structure consists of glass/ZnO/a-Si:H(n^+)/a-Si:H(i)/Pd, where the ZnO works as transparent conductive oxide, so that the illumination can be made through the glass side of the device. The second structure consists of glass/Pd/a-Si:H(i)/a-Si:H(n^+)/ZnO. In this structure the illumination is made directly on the ZnO. This configuration opens the range of allowed substrates that can be used, since it does not have to be transparent. In this paper we present the performances of the devices developed, where I-V curves as function of the temperature and gas concentration were measured under dark and AM1.5 illumination conditions and with an He-Ne laser (λ=632 nm) which is the light source to be used with the position sensors. We also measure the spectral response of the devices and correlate the results with the layer properties to achieve the devices optimisation and to determine the main characteristics of the set of devices developed.

A26.7

POROUS SILICON UNDOPED THIN FILM GAS SENSOR. I. Ferreira, R. Martins and E. Fortunato, CENIMAT, Department of Materials Science, Faculty of Science and Technology, New University of Lisbon and CEMOP-UNINOVA, Caparica, PORTUGAL.

We present for the first time the performances of nano-crystalline silicon undoped films as gas detector. The films were produced by the hotwire chemical vapour deposition (HW-CVD). These films present a porous like-structure which due to the uncompensated bounds, oxidise easily in the presence of air. This behaviour is a problem when the films are used for solar cells or thin film transistors. In this case the films have to be passivated with hydrogen after the deposition. For other purposes such as gas detector the oxidation is a benefit, since the CO, H_2 or O_2 molecules replace the OH adsorbed group. Here, we report the performances of intrinsic nano-crystalline hydrogenated silicon (i-nc-Si:H) films as ethanol gas detector. We observed a current change on the nano-crystalline porous silicon undooped thin films in the presence of ehtanol, at room temperature. The change in the current value can reach more than three orders of magnitude depending of the film preparation condition. This current behaviour is due to the adsorption of the OH chemical group by the Si uncompensated bounds as can be observed in the infrared spectra. The current is recovered to the initial value when samples are kept in 10^{-2} mbar vacuum condition for few minutes.

SESSION A27: AMORPHOUS-TO-MICROCRYSTALLINE TRANSISTION

Chair: Peter A. Fedders
Friday Morning, April 20, 2001
Metropolitan III (Argent)

8:30 AM *A27.1

PARACRYSTALLINE MEDIUM-RANGE ORDER IN AMORPHOUS SILICON. P.M. Voyles, Bell Labs, Lucent Technologies, Murray Hill, NJ; M.M.J. Treacy, NEC Research Institute, Princeton, NJ; J.M. Gibson, Materials Science Division, Argonne National Laboratory, Argonne, IL; J.E. Gerbi and J.R. Abelson, Dept. of MS&E and Coordinated Science Lab, Univ. of Illinois, Urbana, IL.

Fluctuation electron microscopy measurements have led us to propose a new model for the structure of amorphous silicon called the paracrystalline (PC) model. Fluctuation microscopy is a transmission electron microscopy technique that is sensitive to medium-range order (MRO) in disordered materials at a length scale of ~15 Å; the paracrystalline model is essentially concerned with MRO. A PC structure consists of small (<30 Å in diameter) topologically crystalline grains which may sit in a more disordered matrix. Because the grains are strained, PC structures reproduce the measured structure factor and radial distribution function of amorphous silicon. However, PC structures have more MRO than conventional continuous random network models. This MRO can be measured by fluctuation microscopy. We will discuss the experimental evidence for paracrystallinity in amorphous silicon and hydrogenated amorphous silicon and the ways in which the degree of paracrystalline MRO can be modified. In particular, we observe an increase in MRO in magnetron sputtered amorphous silicon as a function of substrate temperature during deposition, up to the temperature at which identifiable crystals begin to appear in the film. In the context of the paracrystalline model, this indicates that there is no first-order phase transition between amorphous and polycrystalline silicon deposition.

9:00 AM A27.2

HYDROGEN DIFFUSION DURING AMORPHOUS SILICON GROWTH AND ITS APPLICATION TO THE TRANSITION TO MICROCRYSTALLINE GROWTH. Jack Thiesen, Technology Applications, Boulder, CO; Richard S. Crandall, National Renewable Energy Laboratory, Golden, CO.

We obtain the first closed-form, time-dependent solution to the partial differential equation representing hydrogen diffusion in the frame of a growing hydrogenated amorphous silicon (a-Si:H) film. This solution gives us considerable insight into processes controlled by hydrogen in silicon. Using only three parameters, all of which can be measured, we obtain the time-dependant hydrogen profile in the growing film. The fundamental parameters are: the hydrogen diffusion coefficient (D), the film growth velocity (V) and the flux of hydrogen (F) at the growing surface. As the film grows the surface and bulk concentrations hydrogen increase. What is presumably important for microcrystalline growth is a sufficiently high density of H in the growing surface to insure etching and re-growth to a more ordered surface region. The time to reach this concentration is proportional to D and inversely proportional to the square of F. This simple relation shows, in agreement with experiment, that the higher the hydrogen flux and the lower the temperature the quicker the transition to microcrystalline growth. For normal a-Si:H growth we demonstrate why a lower temperature results in a larger H concentration in the film. In this presentation we will describe H concentrations in growing films of a-Si:H as well as show how this theory gave the first quantitative explanation, with no adjustable parameters, for the well known breakdown of silicon epitaxy.[1]

1 Thiesen, J., H.M. Branz, and R.S. Crandall, Appl Phys Lett, to be published 11/2000

9:15 AM A27.3

CONTROL OF MEDIUM RANGE ORDER IN AMORPHOUS SILICON VIA ENERGETIC PARTICLE BOMBARDMENT DURING GROWTH. Jennifer E. Gerbi, John R. Abelson, Department of Materials Science and Engineering and Coordinated Science Laboratory, University of Illinois at Urbana-Champaign, Urbana, IL; Paul M. Voyles, NEC Research Institute and the University of Illinois at Urbana-Champaign, Urbana, IL; Michael M.J. Treacy, NEC Research Institute, Princeton, NY; J. Murray Gibson, Argonne National Laboratory, Argonne, IL.

The fluctuation microscopy TEM method has recently revealed that amorphous silicon films deposited by various methods all contain medium range structural order (MRO) on a length scale of 1-2 nm. The data are consistent with the paracrystalline model, which is essentially a fine-grained nanocrystalline structure in which strain fields penetrate throughout the network, shifting the atoms slightly from their crystalline positions, rendering the crystalline order invisible to standard diffraction techniques. MRO decreases both with light soaking and thermal annealing, suggesting that the paracrystalline state is metastable and possibly related to electronic metastability. The paracrystalline state has been hypothesized to develop as the result of frustrated nanocrystallinity: nuclei form on the growth surface at a high rate, but are buried by other grains before reaching a size which is energetically stable. The formation of paracrystals should therefore be sensitive to processes which either promote crystalline order or structural relaxation. For the first time, we demonstrate specific control of MRO during growth by reactive magnetron sputtering using energetic particle bombardment to transfer momentum, and thus promote Si-Si bond-switching events, during film deposition. We increase the flux of relatively low energy (~27 eV) Ar ions impinging on the substrate to modify the film surface, increasing the MRO. Alternately, we inject H2 or D2 into the Ar plasma. Ion reflection at the Si target surface produces a large flux of fast (~100 eV) H or D neutrals which implant to a depth of ~5nm in the growing film. Binary collision (TRIM) simulations indicate that D transfers twice as much momentum to Si in the sub-surface. Correspondingly, the D flux is much more effective at reducing MRO. We compare the fluctuation microscopy data with Raman scattering, spectroscopic ellipsometry, and SAXS, and discuss our current understanding of the formation of MRO in light of these results.

9:30 AM *A27.4

PROTON NMR AND MAGNETIC SUSCEPTIBILITY IN a-Si:H. Jonathan Baugh, Daxing Han, Alfred Kleinhammes, Yue Wu, Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC.

The magnetic susceptibility χ is enhanced by a factor of 4.5 when crystalline silicon is made amorphous. Theory shows that the increased short- and medium-range disorder inherent to the amorphous phase leads to such enhancement of χ. Thus, precise measurement of χ could provide information on differences in structural order between a-Si:H films produced under different conditions. The measurement of χ in device quality a-Si:H is difficult because of the small amount of sample available. Here we describe an NMR technique for the precise measurement of χ in a-Si:H by carrying out proton NMR on a single a-Si:H film on quartz substrate. The orientation dependence of the spectral shift provides the information needed to calculate the bulk magnetic susceptibility. In this work, device-quality PECVD, HWCVD and H-dilution PECVD films were compared and differences in χ were detected. Such differences indicate better structural ordering in HWCVD and H-dilution PECVD films. Because of the removal of susceptibility broadening, the proton spectrum also contains more structural information. The proton spectra reveal in HWCVD and H-dilution PECVD films some new microstructures that are absent in conventional PECVD films. In addition, using the orientation dependence of the spectral shift, microstructural anisotropy was detected in some of these films.

SESSION A28: RELAXATION AND DIFFUSION

Chair: Wolfhard Beyer
Friday Morning, April 20, 2001
Metropolitan III (Argent)

10:30 AM *A28.1
BASIC MECHANISMS OF STRUCTURAL RELAXATION AND DIFFUSION IN AMORPHOUS SILICON. Gerard Barkema, Theoretical Physics, Utrecht University, THE NETHERLANDS.

At low temperatures, dynamics in amorphous silicon occurs through a sequence of discrete activated events that locally reorganize the topological network. Using the activation-relaxation technique, we create more than 8000 events, providing an extensive database of relaxation and diffusion mechanisms. The generic properties of these events – size, number of atoms involved, activation energy, volume expansion/contraction, etc. – are discussed and found to be compatible with experimental data. With a unique classification scheme, we also study the topological properties of these events. In the absence of coordination defects, we identify three dominant mechanisms. If coordination defects are present, there is a much richer diversity. In both cases, the bond transposition mechanism proposed by Wooten, Winer and Weaire is found to play an important role. We next exploit this knowledge of the topological mechanisms that dominate the dynamics, in the spirit of Wooten, Winer and Weaire, to obtain well-relaxed sample configurations. Our computational approach as well as the structural and electronic properties of our samples will be discussed.

11:00 AM A28.2
DETERMINING THE CHARGE STATE OF DIFFUSING HYDROGEN IN HYDROGENATED AMORPHOUS SILICON. Brent P. Nelson, A. Harv Mahan, Richard S. Crandall, Robert Reedy, Yueqin Xu, and Howard M. Branz, National Renewable Energy Laboratory, Golden, CO.

To determine the charge state of diffusing hydrogen (H) we made device structures with high built-in fields across a thin layer that has a deuterium (D) concentration thirty times higher than the background D concentration within the device. We annealed these devices at 230°C for up to 840 hours and measured the changes in the depth distribution of D by secondary ion mass spectrometry. Using AMPS modeling, we calculate the electric field across the D-tracer layer to be 0.5 MV/cm at the annealing temperature. Without an electric field, annealing would cause D-tracer layers to broaden equally toward the top and bottom of the device. Similarly, if D is diffusing in a neutral charge state, the built-in fields should have no influence on the mobile D atoms and the depth distribution of D would be identical those observed in structures without electric fields. However, the built-in fields in these devices are sufficiently strong that if mobile D is charged, the depth distribution of D should be asymmetric relative to the charge state on the D. Our preliminary observation is that most of the D is diffusing in a positive charge state, while a minority may diffuse as neutral D. We have separate devices with electric fields aligned in opposite directions across the D-tracer layers. We observe asymmetric D diffusion consistent with the direction of the electric fields, and D diffusing in a positive charge state, in each case. We also report on D-tracer experiments in similar structures that allow us to compensate for differences in H-solubility among the various doped layers in these devices. The charge state of diffusing H is likely to have significant implications for Staebler-Wronski degradation of amorphous silicon and for the distribution and elimination of H during material and device fabrication.

11:15 AM A28.3
METASTABLE CHANGES OF THE ELECTRICAL CONDUCTIVITY IN MICROCRYSTALLINE SILICON. N.H. Nickel and M. Rakel, Hahn-Meitner-Institut Berlin, Berlin, GERMANY.

Metastability is a well known phenomenon in amorphous and polycrystalline silicon that manifests itself as a change of the electronic transport properties due to the generation of defects. To overcome this drawback a lot of reseach is devoted to microcrystalline silicon (μc-Si) in the past years since it is widely believed that this material does not suffer from metastability. In fact, to our knowledge metastable defect generation in μc-Si has not been observed so far. In this paper, we present the first observation of a cooling-rate dependent change of the electrical dark-conductivity, σ_D. Microcrystalline silicon samples were prepared by rf-glow discharge of silane-hydrogen gas mixtures. According to Raman backscattering measurements the samples showed a crystalline fraction of 55 % and more. The specimens were characterized by measuring the temperature dependence of σ_D. Rapid thermal quenching from 470 K produced an increase of σ_D by about two orders of magnitude below room temperature. This frozen-in state is metastable: Annealing and a slow cool restores the temperature of the relaxed state. The time and temperature dependence of the relaxation suggests that the origin of the quenching-induced enhancement of σ_D is similar to that reported for polycrystalline silicon, namely the formation of bond-centered H complexes.

11:30 AM A28.4
SURFACE TRANSPORT KINETICS DURING AMORPHOUS SILICON DEPOSITION. K.R. Bray, A. Gupta and G.N. Parsons Department of Chemical Engineering, North Carolina State University, Raleigh, NC.

The dynamic scaling concept was developed to help understand the role of kinetic phenomena that occur on surfaces during non-equilibrium processes (such as film deposition). Plasma deposition of a-Si:H is interesting because it is well known that over a wide temperature range, kinetic growth process results in very smooth (non-random) surface texture indicating significant surface species transport, but the growth rate is not thermally activated. We have used rf plasma deposition to form a-Si:H films from silane diluted with He, Ar, and H_2, and used dimensional and frequency analyses to examine surface topography obtained from AFM images. Surface fractal scaling parameters, including static (α) and dynamic (β) scaling coefficients, Fourier index (i), saturation roughness, and lateral correlation length (Lc), were determined as a function of film thickness and temperature. For films deposited with only He dilution, after film coalescence the scaling coefficients are consistent with the surface topology being described as a self-similar structure: the static scaling coefficient is constant with growth time and is ~1.0, the Fourier index is ~4.0 and the saturation roughness value increases exponentially with time as t^{β}. With the addition of hydrogen, α decreases to ~0.7 and i increases ~5.0, consistent with self-affine geometry, indicating a shift from a linear to a nonlinear continuum model for describing surface topography. Based on models of surface transport, the scaling coefficient values are consistent with surface smoothening driven by diffusion. In this picture, the lateral correlation length can be equated with the surface diffusion length. We find that without hydrogen, Lc ranges from ~50 to 150nm, and is thermally activated, corresponding to a diffusion activation energy of ~0.20eV. With hydrogen addition, the lateral correlation length increases from ~150 to 250nm at 150°C, and the diffusion activation energy decreases to ~0.14eV. This result is consistent with previous models that presume hydrogen surface interactions enhance silicon surface diffusion.

11:45 AM A28.5
EVIDENCE FOR LONG-RANGE HYDROGEN MOTION IN HYDROGENATED AMORPHOUS SILICON UNDER ROOM-TEMPERATURE ILLUMINATION USING RAMAN SCATTERING OF AMORPHOUS TUNGSTEN OXIDE OVERLAYER. Hyeonsik M. Cheong, National Renewable Energy Laboratory, Golden, CO, and Department of Physics, Sogang University, Seoul, KOREA; Se-Hee Lee, Brent Nelson, Angelo Mascarenhas, and Sayten K. Deb, National Renewable Energy Laboratory, Golden, CO.

We demonstrate that one can detect minuscule amounts of hydrogen diffusion out of a-Si:H under illumination at room temperature, by monitoring the changes in the Raman spectrum of amorphous tungsten oxide as a function of illumination. The Staebler-Wronski effect, the light-induce creation of metastable defects in hydrogenated amorphous silicon (a-Si:H), has been one of the major problems that has limited the performance of such devices as solar cells. Recently, Branz suggested the "hydrogen collision model" that can explain many aspects of the Staebler-Wronski effect [1]. One of the main predictions of this model is that the photogenerated mobile hydrogen

atoms can move a long distance at room temperature. However, light-induced hydrogen motion in a-Si:H has not been experimentally observed at room temperature. We utilize the high sensitivity of the Raman spectrum of electrochromic amorphous tungsten oxide to hydrogen insertion as a detection scheme for the long-range motion of hydrogen at room temperature. We observe that illumination causes hydrogen to diffuse out of the a-Si:H layer into the amorphous tungsten oxide layer. This hydrogen motion is observed to saturate after about 30 minutes when the a-Si:H is illuminated with 15 W/cm^2 of the 514.5-nm laser line at room temperature. By comparing the Raman signal changes with those for control experiments where hydrogen is electrochemically inserted into amorphous tungsten oxide, we can estimate semiquantitatively the amount of hydrogen that diffuses out of the a-Si:H layer. This result supports the recently proposed "hydrogen collision model" for the Staebler-Wronski effect.
[1] H.M. Branz, Phys. Rev. B, 59, 5498 (1999).