SYMPOSIUM S

Integrative and Interdisciplinary Aspects of Intermetallics

November 29 - December 1, 2004

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* Invited paper

SESSION S1: Iron and Nickel Aluminides
Chairs: I. Baker and Y. Mishima
Monday Morning, November 29, 2004
Room 208 (Hynes)

8:30 AM *S1.1
Magnetic Interaction and Solid Solution Effects in Ni-Rich NiAl. C. T. Liu, C. L. Fu, M. F. Chisholm, Xun-Li Wang, M. Kvcmar and James R. Thompson; Metals & Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

This paper summarizes our recent research on solute effects in Ni-rich NiAl alloys. As Ni and Co solute atoms occupy the Al sublattice sites in NiAl, normal lattice contraction and solid solution hardening have been observed. On the other hand, as Fe, Mn and Cr solute atoms occupy the Al sublattice sites, experimental studies reveal unusual lattice dilation and resultant solid solution softening in NiAl alloys, all of which can not be explained by the current solid solution theories. To explain these results, the first-principles calculations reveal the development of a large electron spin polarization only when the solute atoms of Fe, Mn and Cr are surrounded by Ni atoms in NiAl lattice. The spin polarization results in a large magnetic moment (e.g., 2.5 μ_B per Fe atom) that dilates the lattice parameter and affects mechanical properties. The calculated magnetic moment is unambiguously supported by electron energy-loss spectroscopy (EELS) and the measurements of magnetic susceptibility as a function of temperature. Effect of magnetic interaction on alloy design of NiAl alloys will be discussed. Research sponsored by the Division of Materials Science and Engineering , Office of Basic Energy Sciences, U.S. Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

9:00 AM S1.2
Microstructures and Mechanical Properties of NiAl-Mo Composites. Hongbin Bei[1,2] and Easo P. George[1,2]; [1]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee.

NiAl-Mo ternary eutectic alloys were directionally solidified in a high-temperature optical floating zone furnace to obtain well-aligned microstructures consisting of NiAl matrix and continuous Mo fibers having a square cross-section. With increasing growth rate, the spacing and size of the Mo fibers decreased, with fibers as small as 400 nm in cross section obtained at a growth rate of 80 mm/h. Electron backscatter diffraction patterns identified the growth directions and Mo/NiAl interface boundaries to be parallel to <100> and {011}, respectively, in both Mo and NiAl. Tensile tests were used to investigate the temperature dependence of the strength and ductility of the composite. Its ductile-to-brittle transition temperature was found to be 675°C, and its yield strength about 1.5 times that of NiAl single crystal at 800°C. * Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U. S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC.

9:15 AM S1.3
Thermal Stress Induced Cracking of NiAl Thin Films Constrained by a Si Substrate. Gerhard Dehm[1], Patrick Wellner[1], Oliver Kraft[2], Janis Andersons[3], Helmut Clemens[4] and Eduard Arzt[1]; [1]Max Planck Institute for Metals Research, Stuttgart, Germany; [2]Institut fuer Materialforschung II, Forschungszentrum Karlsruhe und Institut fuer Zuverlaessigkeit von Bauteilen und Systemen, University of Karlsruhe, Karlsruhe, Germany; [3]Institute of Polymer Mechanics, Riga, Latvia; [4]Physical Metallurgy and Materials Testing, University of Leoben, Leoben, Austria.

It is well established that flow stresses of metallic thin films increase with decreasing film thickness to values significantly exceeding those of the corresponding bulk material. However, it is unclear whether similar size effects are present in the cra cking behavior of brittle thin films constrained by a substrate. Whereas theoretical models are reported in literature, a conclusive experimental picture has not yet been obtained. In the present study we analysed the cracking behavior of intermetallic NiAl films on Si substrates as a function of the Al content (45.0 to 52.4at-percent) and film thickness (400 to 3000nm). The films were thermally cycled to a maximum temperature of 1000K resulting in a thermal strain of up to 0.9percent. Ni-rich NiAl films were found to sustain higher tensile stresses than Al-rich films. Al-rich NiAl films failed by the formation of intergranular cracks, which even extended into the Si substrate. The fracture toughness of the Al-rich films was determined from the fracture stress, substr ate crack depth and film thickness. In contrast to the fracture toughness, the fracture stress was found to increase with decreasing film thickness indicating that the film thickness corresponds to a critical crack length.

9:30 AM S1.4
First-principles Study of Structural and Defect Properties in FeCo Intermetallics. Maja Krcmar, Chong Long Fu and James R. Morris; Oak Ridge National Lab, Oak Ridge, Tennessee.

Using first-principles calculations and statistical mechanic modeling, we investigate magnetism-induced structural stability, defect structure, and order-disorder transition characteristics in FeCo alloys. We find that the ordered B2 structure is stabilized by the presence of magnetism. However, B2 FeCo is only weakly ordered: antistite defects dominate point-defect structure on both sides of stoichiometry, and the presence of lattice vacancies is negligibly small. We then use defect structure analysis to estimate the site-exchange energy and order-disorder transition temperature Tc as a function of alloy compositions near stoichiometry. We find that the stoichiometric FeCo has the highest Tc, and that Tc decreases parabolically with the increase in variation of off-stoichimetric composition from stoichiometry. The anti-phase boundary (APB) energies for <111> slip on the (110) and (112) planes are found to be low, despite the brittle nature of B2 FeCo. Due to the weak ordering, we also find that the structural stability of B2 FeCo is very sensitive to the reduction of dimensionality (3D to 2D), and the state of stress. Finally, we discuss conditions for stress-induced structural phase transformation in FeCo, suggesting the possibility of local structural changes under the internal stress near/at dislocation cores. Work was sponsored by the Division of Materials Sciences and Engineering, the US DOE, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

9:45 AM S1.5
Effect of Heat Treatments on Microstructures of Rapidly Solidified TiCo Ribbons. Kyosuke Yoshimi[1], Akira Yamauchi[1], Nakamura Ryusuke[1], Sadahiro Tsurekawa[2] and Shuji Hanada[1]; [1]Institute for Materials Research, Tohoku University, Sendai, Japan; [2]Nanomechanics, Tohoku University, Sendai, Japan.

Effect of heat treatments (aging or annealing) on microstructures was investigated for rapidly solidified ribbons of near-stoichiometric TiCo. In as-spun ribbons, it was observed by TEM that equiaxed grain structure was developed and its crystal structure had been already B2-ordered, while a small amount of second phase was finely precipitated in grains and along grain boundaries. Some grains were dislocation-free but others contained a certain amount of curved or helical dislocations and loops having the Burgers vector parallel to <100>. There was no significant change in the microstructure of the ribbons aged at 473 K for 100 h. In the ribbons annealed at 973 K for 24 h, grain growth seemed to occur slightly. In addition, the dislocation density in the annealed ribbons was obviously higher than those in the as-spun and aged ribbons. It is considered that the increase of the dislocation density in the annealed ribbons would result from the condensation and/or absorption of supersaturated thermal vacancies. Therefore, the observation results indicate that a large amount of supersaturated thermal vacancies were retained in the TiCo ribbons by the rapid solidification. However, in DSC measurements, any peak did not appear for the TiCo ribbons, whereas relaxation peaks stemming from the condensation of supersaturated thermal vacancies have been often observed in the DSC curves of B2-type aluminides such as FeAl and NiAl. Based on the obtained results, vacancy condensation behavior in B2-type TiCo is discussed.

10:15 AM *S1.6
Complex Intermetallic Compounds: Defects, Disordering, Details. W. Sprengel[1], F. Baier[2], K. Sato[3], X. Y. Zhang[4] and Hans-Eckhardt Schaefer[1]; [1]Institute of Theoretical and Applied Physics, Stuttgart University, Stuttgart, Germany; [2]Physical Metallurgy, Technical University Darmstadt, Darmstadt, Germany; [3]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; [4]Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao, China.

A short overview will be given on the thermodynamics of the formation of thermal defects in intermetallic aluminides. We focus on thermal vacancies [1] studied by the specific techniques of positron annihilation [2] and time-differential dilatometry [3] and discuss the results together with self-diffusion data [4]. We then demonstrate that these techniques can be employed for studying vacancies in compound semiconductors specifically [5]. Furthermore, structural order-disorder phase transitions can be investigated from an atomistic point of view [6] by making use of positron annihilation as shown in the exemplary case of Al-Ni-Co quasicrystals. A few examples for the application of intermetallics will be given in the introductory part. [1] R. Wuerschum et al., PRL 75, 97 (1995); [2] X. Y. Zhang et al., PRL 92, 155502 (2004); [3] H.-E. Schaefer et al., PRL 82, 948 (1999); [4] H.-E. Schaefer et al., Intermetallics 7, 277 (1999); [5] A. A. Rempel et al., PRL 89, 185501 (2002); [6] K. Sato et al., PRL 92, 127403 (2004).

10:45 AM *S1.7
Strengthening of Iron Aluminide Alloys for High-Temperature Applications. Andre Schneider, Martin Palm, Frank Stein and Gerhard Sauthoff; Max-Planck-Institut fur

Eisenforschung GmbH, Dusseldorf, Germany.

An overview of materials developments of ferritic and Fe3Al-based iron aluminium alloys with strengthening precipitate phases is given in view of possible high-temperature applications. A development of high-temperature alloys for structural applications is to be focussed on optimisation of strength, creep and corrosion resistance at high temperatures and sufficient ductility at lower temperatures. This is discussed with respect to recent studies and ongoing work on Fe-Al-based alloys with strengthening precipitates, such as κ-carbide Fe3AlCx, MC-carbides, Laves phase, and the B2-ordered intermetallic phase NiAl. The following alloy systems have been investigated: Fe-Al-C, Fe-Al-Ti, Fe-Al-Ta, Fe-Al-Ti-Nb, Fe-Ni-Al-Cr, and Fe-Al-M-C (M=Ti, V, Nb, Ta). The investigations have been focussed on microstructure, constitution, mechanical properties, and high-temperature corrosion behaviour of such Fe-Al-based alloys with Al contents ranging from 10 to 30 at. %. Mechanisms and problems are discussed and perspectives are outlined.

11:15 AM S1.8
Development of High Temperature Creep Resistance in Fe-Al Alloys. David G. Morris[1], Maria A. Munoz-Morris[1] and Carmen Baudin[2]; [1]Physical Metallurgy, CENIM,CSIC, Madrid, Spain; [2]Instituto de Ceramica y Vidrio, CSIC, Madrid, Spain.

Most of the studies aimed at the development of creep-resisting Fe-Al intermetallics have been oriented at application temperatures of the order of 500-650C, where these materials may compete with conventional stainless steels. The Fe-Al intermetallics are, however, particularly excellent in their oxidation and corrosion resistances at temperatures of the order of 1000C, where Chromium-Nickel steels are no longer able to withstand the aggressive environments. This presentation is part of a study aimed at the development of good creep resistance at such high temperatures. Studies of a variety of cast Fe3Al-base alloys will be reported, which are strengthened by solution or precipitate/dispersoid-forming alloying additions. The alloys studied show good strength from room temperature to about 500C, but thereafter strength falls rapidly as thermally-activated deformation processes become operative. Solution additions are capable of producing good low temperature strength, but do not contribute significantly to creep strength at very high temperatures (above 700C). Precipitation hardening has been examined in Nb-containing alloys, where Fe2Nb Laves precipitates form at intermediate temperatures. These materials show good strength up to about 700C, but at higher temperatures the fine precipitates coarsen excessively. Strengthening in this intermediate temperature range varies depending on whether the solute is precipitated prior to high temperature testing or concurrent with this. Studies with a variety of stable carbide and boride additions show relatively poor strengthening by the coarsely-distributed dispersoids, but excellent thermal stability and good strength retention to very low strain rates. Alloying and structural parameters important for obtaining good high temperature creep strength in cast Fe3Al alloys will be discussed. Aspects such as segregation during solidification, as well as thermal stability of the structures obtained, are seen to be as important in controlling strength of the materials as the mechanisms of creep deformation themselves.

11:30 AM S1.9
Pseudo-Elasticity of $D0_3$ Ordered Monocrystalline Fe_3Al. Saurabh Kabra[1], Hongbin Bei[1], Donald W. Brown[3] and Easo P. George[2,1]; [1]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Knoxville, Tennessee; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Los Alamos National Laboratory, Los Alamos, New Mexico.

Single crystals of Fe_3Al were grown in an optical floating zone furnace and their pseudo-elastic behavior investigated by tension and compression experiments. The stress-strain behavior was studied as a function of orientation, strain rate and environment. The maximum recoverable strain was found to depend on strain rate. In-situ electron backscatter diffraction as well as neutron diffraction were performed as a function of strain to understand the mechanism of deformation and recovery. * Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U. S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. This work benefited from the use of the Los Alamos Neutron Science Center (LANSCE) at the Los Alamos National Laboratory. This facility is funded by the US Department of Energy under Contract W-7405-ENG-36.

11:45 AM S1.10
Effect of Alloying Elements (Ga, Ge, Si) on Pseudoelasticity in Fe_3Al Single Crystals. Hiroyuki Y. Yasuda[1,2], Takashi Kase[2] and Yukichi Umakoshi[2]; [1]Research Center for Ultra-High Voltage Electron Microscopy, Osaka University, Ibaraki, Japan; [2]Materials Science and Engineering, Osaka University, Suita, Japan.

Pseudoelasticity in Fe_3Al single crystals doped with a small amount of Ga, Si and Ge was investigated focusing on the antiphase boundary (APB) energy and the ordered domain structure. Single crystals of Fe-23at%Al and Fe-21at%Al-2at%X (X=Ga, Si, Ge) were grown by a floating zone method. In Fe-23at%Al single crystals, superpartial dislocations with Burgers vector (b) of $\frac{1}{4}$<111> moved dragging APB during loading, while APB pulled back the dislocations during unloading. This resulted in giant pseudoelasticity regardless of martensitic transformation and the recoverable strain was about 5%. Ga addition was found to be effective in increasing the recovery strain compared with Fe-23at%Al. In contrast, both Si and Ge additions decreased the amount of shape recovery. Stress at which the shape recovery started, was increased by Ga, Si and Ge additions. This means the APB energy increased by the additions, since the surface tension of APB pulling back the superpartials increases with increasing the energy. Ordered domains with displacement vector (R) of $\frac{1}{4}$<111> in Fe-23at%Al and Fe-Al-Ga alloys were observed to be small, less than 100nm. In contrast, Si and Ge additions increased the domain size to more than 500nm. The domain boundaries with R=$\frac{1}{4}$<111> played an important role in the individual motion of the superpartials with b=$\frac{1}{4}$<111>. Therefore, the fine domain structure was found to be favorable for giant pseudoelasticity in Fe_3Al single crystals. Ga addition increased the APB energy following the superpartials and kept the domain size small, resulting in the increase of recovery strain.

SESSION S2: Nickel Aluminides and Silicides
Chairs: Diana Farkas and D. P. Pope
Monday Afternoon, November 29, 2004
Room 208 (Hynes)

1:30 PM *S2.1
Specimen Size Effects in Ni_3Al Alloys. Michael D. Uchic[1], Dennis M. Dimiduk[1], Steven J. Polasik[2], Triplicane A. Parthasarathy[3], Michael J. Mills[2] and Hamish L. Fraser[2]; [1]Materials & Manufacturing Directorate, Air Force Research Laboratory, Wright Patterson AFB, Ohio; [2]Department of Materials Science & Engineering, The Ohio State University, Columbus, Ohio; [3]UES, Inc., Dayton, Ohio.

It is now possible using micro-fabrication and testing methodologies to systematically explore specimen-size effects related to mechanical properties, i.e., changes in mechanical response due simply to shrinking the physical size of the deforming volume. Significant size effects have been discovered in the uniaxial compression testing of micron-size single-crystal samples in Ni_3Al alloys containing Ta and Hf, where the flow stress has been observed to increase in proportion to the inverse-square-root of the sample diameter. This behavior results in samples having a 500 nm diameter and a flow stress that is approximately 2 GPa, while the flow stress for bulk samples is smaller by two orders of magnitude. In this talk, we will present these mechanical test results in detail, and also show additional results from the testing of binary Ni3Al and an alloy with high Hf concentration. Collectively, these studies explore the influence of fault energy on the size-affected behavior. Further, there is little connection between observed size effects and the underlying changes to the fundamental deformation mechanisms governing dislocation-mediated flow, primarily because of the challenges in preparing transmission electron microscope (TEM) foils from miniature test specimen. There is considerable evidence that at temperatures in the anomalous flow regime, the mobility of screw-character dislocations is greatly influenced by the lateral motion of large jogs and kinks along the length of the dislocations, i.e., it is likely that dislocation kinetics are strongly influenced by the characteristic active line length of dislocations known to be on the order of a few microns. We will present the results of TEM analysis of deformed microsamples from these alloys, in order to gain a better understanding of the effect that artificially truncating the sample dimensions has on the fundamental micromechanisms of dislocation glide, storage, and multiplication.

2:00 PM S2.2
Evaluating the Yield Stress Anomaly in Ni_3Al Thin Films. T. John Balk, Johannes Gentil and Eduard Arzt; Max-Planck-Institut fuer Metallforschung, Stuttgart, Germany.

Ni_3Al typically exhibits the yield stress anomaly (YSA), by which yield stress increases with increasing temperature. The thermally activated locking of superdislocations creates sessile Kear-Wilsdorf segments that are connected by superkinks, and net forward motion of the entire superdislocation occurs via lateral motion of these superkinks. In an attempt to confine the maximum length of superkinks and thus make them immobile, thin films of Ni_3Al were produced. The film thickness should provide an upper limit on superkink length and should, at a certain length scale, prevent

superkink motion and lead to a change in deformation mechanism for Ni_3Al. To this end, the thermomechanical behavior of Ni_3Al thin films was characterized for film thicknesses between 50 nm and 2 μm. Based on stress-temperature data for the apparent onset of plasticity during repeated thermal cycling, the yield stress was seen to clearly decrease (from 1300 to 500 MPa) with increasing temperature (from 170 to 370°C). Thus, it appears that the Ni_3Al films in this thickness range do not exhibit an anomaly, but rather normal behavior. However, the activation volume, as determined from stress relaxation experiments for various film thicknesses at different temperatures, shows a peak at an intermediate temperature of 600°C. Although higher than was found by Kruml et al. for Hf-doped single crystal Ni_3Al (300°C), the existence of the peak in the current study suggests that a YSA could indeed exist in the thicker films (1 μm and higher). These apparently contradictory results, which nonetheless indicate the lack of a YSA for Ni_3Al films 2 μm and thinner, will be discussed. Additionally, the effect of the thin film geometry on thermomechanical behavior will be presented and compared to that of other thin film systems.

2:15 PM S2.3
Quantitative Analysis of γ Precipitate in Cyclically Deformed Ni_3(Al,Ti) Single Crystals Using Magnetic Technique.
Yukichi Umakoshi[1], Hiroyuki Y. Yasuda[2,1] and Toshifumi Yanai[1]; [1]Materials Science and Engineering, Osaka University, Suita, Japan; [2]Research Center for Ultra-High Voltage Electron Microscopy, Osaka University, Ibaraki, Japan.

Ni_3Al with the $L1_2$ structure has been used as a main component of Ni-based superalloys because of an anomalous increase in yield stress at high temperatures. Control of duplex structure composed of ordered γ' and disordered γ phases is important to improve mechanical properties of the superalloys. Since observation of small precipitates and the interaction between the precipitates and dislocations is very difficult in strongly deformed superalloys, transmission electron microscopy and magnetic technique were applied for it. γ phase shows ferromagnetism. Therefore, changes in size and shape of γ precipitates were observed in aged and cyclically deformed Ni_3(Al,Ti) single crystals using magnetic technique and deformation mechanism of the fatigued crystals was examined. Single crystals were grown from the arc melted Ni-18at%Al-4at%Ti ingots by a floating zone method and were homogenized at 1423K for 168h. After solution treatment at 1423K, γ phase was precipitated at 1073K. Specimens with a loading axis of <149> for fatigue test were prepared and the plastic-strain-controlled fatigue test was performed at $\Delta\epsilon$=±0.2% at room temperature. Magnetization process of aged and fatigued specimens was measured by a vibrating sample magnetometer at temperatures between 77 and 273K. Spontaneous magnetization spontaneously increased with increasing volume fraction and size of γ precipitates during aging, while coercive force rapidly increased after a gradual increase. Change in the coercive force exhibits that γ precipitates change from spherical to plate-like shape. Spontaneous magnetization of specimens aged for 3h or 100h rapidly decreased with increasing number of cycles. The decrease in spontaneous magnetization corresponds to decrease in size of γ precipitates due to cutting by dislocations during fatigue deformation because small γ precipitates with nano scale show superparamagnetism. Changes in size, shape and their distribution of γ precipitates in Ni_3(Al,Ti) single crystals during fatigue will be quantitatively analyzed from magnetic properties and the deformation mechanism will be discussed.

2:30 PM S2.4
Shearing Mechanisms of the γ' Phase in Superalloys at Intermediate Temperatures.
Michael John Mills[1], Gopal B. Viswanathan[1], Peter Sarosi[1], Raymond Unocic[1] and Deborah Whitis[2]; [1]Materials Science and Engineering, The Ohio State University, Columbus, Ohio; [2]Materials and Processes Engineering Department (MPED), GE Aircraft Engines, Cincinatti, Ohio.

The deformation mechanisms in single phase Ni_3Al and related $L1_2$ intermetallics have been extensively studied. One motivation for these studies has been as a means to understand the behavior of the strengthening phase in the technologically important superalloys. In fact, the principal γ' shearing mechanism in superalloys at lower temperatures is via APB-coupled a/2<110> dislocations, similar to the process observed in single phase Ni_3Al. However, at intermediate temperatures (in the range from 873-1073K), it is now abundantly clear that the γ' shearing mechanisms in superalloys are quite different from those in single phase γ'. Studies of substructures following creep of the superalloys Rene 88DT and ME3 in the supersolvus condition with bimodal γ' size distributions reveals at least two distinct shearing processes. In coarser γ' microstructures, and higher stress levels, γ' particles are sheared via the formation of superlattice extrinsic stacking faults, with isolated a/2<110> dislocations in the matrix. In finer microstructures and lower stresses, deformation twinning is the dominant mechanism. Our TEM observations support a twinning process similar to that proposed recently by Kolbe in which 1/6<112> Shockley partials cooperatively shear both matrix and γ' particles. Atomic rearrangements in the wake of these twinning partials enable the γ' particles to retain the L12 structures, and it is proposed that these atomic rearrangements correspond to the rate limiting, thermally activated process under these conditions. The implications of these results for modeling creep in superalloys will be discussed.

2:45 PM S2.5
Microstructures and Mechanical Properties in Ni_3Si-Ni_3Ti-Ni_3Nb-Based Multi-Intermetallic Alloys.
Takayuki Takasugi, Koji Ohira and Yasuyuki Kaneno; Department of Metallurgy and Materials Science, Osaka Prefecture University, Sakai, Osaka, Japan.

The phase relation, microstructures, high-temperature deformation, and oxidation and corrosion behavior of intermetallic alloys based on Ni_3Si-Ni_3Ti-Ni_3Nb pseudo-ternary alloy system were investigated. As the constituent intermetallic phases, $L1_2$(Ni_3Si), $D0_{24}$(Ni_3Ti), D0a(Ni_3Nb) and $D0_{19}$($Ni_3Ti_{0.7}Nb_{0.3}$) were identified and then their phase fields were discussed based on the electrical and geometrical factors of constituent atoms. Among four intermetallic phases, five kinds of two-phase relations and two kinds of three-phase relations were found to exist. The prepared alloys exhibited widely different microstructures, depending on the number and kinds of the constituent intermetallic phases. Three-phase microstructures composed of $L1_2$(Ni_3Si), $D0_{24}$(Ni_3Ti) and D0a(Ni_3Nb) showed superior tensile strength and ductility in a wide range of temperatures. Also, the mechanical and chemical properties obtained in the present alloy system were compared with those reported in Ni_3Al-Ni_3Ti-Ni_3Nb and Ni_3Al-Ni_3Ti-Ni_3V-based multi-intermetallic alloys.

3:15 PM *S2.6
Atomistic Modeling of Advanced Intermetallic Alloys.
Yuri Mishin, School of Computational Sceinces, George Mason University, Fairfax, Virginia.

This talk gives an overview of our recent work on atomistic computer modeling of ordered intermetallic compounds of the Ni-Al and Ti-Al systems. Atomic interactions in these systems are modeled by semi-empirical potentials fit to both experimental and first-principles data. The methodology includes a large variety of techniques ranging from harmonic lattice dynamics to molecular dynamics and Monte Carlo simulations. The properties studied include lattice characteristics (elastic constants,phonons, thermal expansion), point-defect properties, atomic diffusion, generalized stacking faults, dislocations, surfaces, grain boundaries, interphase boundaries, and phase diagram calculations. The talk emphasizes the recent progress in the understanding of diffusion mechanisms in NiAl and Ni3Al, calculation of stacking fault energies in Ni3Al in relation to dislocation behavior, and calculation of gamma/gamma' interface boundaries in Ni-Al alloys. Preliminary simulation results for nucleation of gamma' particles in the gamma matrix will be discussed.

3:45 PM S2.7
Dislocation Structure, Phase Stability and Yield Stress Behavior of Ultra-High Temperature $L1_2$ Intermetallics: Combined First Principles-Peierls-Nabarro Approach.
Oleg Kontsevoi, Yuri Gornostyrev and Arthur J. Freeman; Physics & Astronomy, Northwestern University, Evanston, Illinois.

The microscopic mechanisms governing the deformation and fracture behavior and anomalous mechanical response of intermetallic alloys are still far from being well understood and remain the challenge for theoretical explanation. Progress in this complex area requires understanding such key phenomena as dislocation structure and mobility: while they have been characterized by mesoscopic length and energy scales, they are determined on the microscopic level by the electronic structure. To reach the goal of connecting the microscopic and mesoscopic scales in the analysis of dislocation structure and mobility, we employ a combined approach based on highly accurate first-principles calculations of the cleavage/shear energetics and the modified semi-discrete 2D Peierls-Nabarro (PN) model with an ab-initio parameterization of the restoring forces. We present the results of fundamental comparative studies of the dislocation properties and the mechanical behavior for a new class of intermetallic alloys based on platinum group metals (PGM) which are being developed for ultra-high temperature applications. These alloys, which include Ir_3X, Rh_3X (X = Ti, Zr, Hf, V, Nb, Ta) and Pt_3X (X = Al, In, Ga), possess very high melting temperatures and superior environmental properties. The two-phase PGM-based superalloys are considered as a replacement for Ni-based superalloys for ultra-high temperatures. Further progress in the development of these alloys relies on understanding the fundamental factors that control their mechanical properties. Using our combined approach, we analyze the dislocation properties, structure and mobilities in PGM-based intermetallics and, based on our analysis, provide an explanation of

the observed unusual features of the mechanical behavior of these alloys, and provide predictions of their high temperature yield stress behavior. We establish the connection of the mechanical behavior of PGM alloys with features of their electronic structure, and demonstrate that the peculiarities of their behavior are directly connected with structural stabilities, namely $L1_2 \rightarrow D0_{19}$ for $Ir(Rh)_3X$ alloys or $L1_2 \rightarrow D0'_c$ for Pt_3X. Supported by the AFOSR (grant No. F49620-01-1-0166).

4:00 PM S2.8
A Bond-Order Potential Incorporating Analytic Screening Functions for the Molybdenum Silicides. Marc J. Cawkwell[1], Matous Mrovec[2], Duc Nguyen-Manh[3], David G. Pettifor[4] and Vaclav Vitek[1]; [1]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania; [2]Fraunhofer IWM, Freiburg, Germany; [3]UKAEA Fusion, Culham Science Centre, Abingdon, United Kingdom; [4]Department of Materials, University of Oxford, Oxford, United Kingdom.

The intermetallic compound $MoSi_2$, which adopts the $C11_b$ crystal structure, and related alloys exhibit an excellent corrosion resistance at high temperatures but tend to be brittle at room and even relatively high temperatures. The limited ductility of $MoSi_2$ in ambient conditions along with the anomalous temperature dependence of the CRSS of the (110)<111], (011)<100] and (010)<100] slip systems and departure from Schmid law behavior of the (013)<331] slip system can all be attributed to complex dislocation core structures. We have therefore developed a Bond-Order Potential (BOP) for $MoSi_2$ for use in the atomistic simulation of dislocations and other extended defects. BOPs are a real-space, $O(N)$, two-center orthogonal tight-binding formalism that are naturally able to describe systems which exhibit mixed metallic and covalent bonding, such as $MoSi_2$. In this development novel analytic screening functions have been adopted to properly describe the environmental dependence of bond integrals in the open, bcc-based $C11_b$ crystal structure. A many-body repulsive term is included in the model that allows us to fit the elastic constants and negative Cauchy pressures of $MoSi_2$ exactly. For the first time we report an analytic screening function for this term fitted to force-constants calculated *abinitio*. The purpose of this screening is to include repulsive interactions due to the non-orthogonality of orbitals in our orthogonal TB model. The BOP is found to be an excellent description of cohesion in $C11_b$ $MoSi_2$ and we have carefully assessed its transferability to other crystal structures and stoichiometries, notably $C40$, $C49$ and $C54$ $MoSi_2$, $A15$ and $D0_3$ Mo_3Si and $D8_m$ Mo_5Si_3 by comparing with *abinitio* structural optimizations. Furthermore, we have studied the ideal tensile strength of $C11_b$ $MoSi_2$ and compared the predictions with *abinitio* calculations. Finally, we report γ-surfaces for the (110), (011), (010) and (013) planes and use these to guide subsequent atomistic simulations of dislocation core structures. This research was supported by the U.S. Department of Energy, BES Grant no. DE-PG02-98ER45702 and the United Kingdom EPSRC.

4:15 PM S2.9
Role of Microstructure in Promoting Fracture and Fatigue Resistance in Mo-Si-B Alloys. Jamie Kruzic[4], Joachim Schneibel[3] and Robert Ritchie[1,2]; [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California; [2]Department of Materials Science and Engineering, University of California, Berkeley, California; [3]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Department of Mechanical Engineering, Oregon State University, Corvallis, Oregon.

Intermetallic based Mo-Si-B alloys consisting of α-Mo, Mo_3Si, and Mo_5SiB_2 (T2) phases have been targeted for high temperature turbine engine applications. To reach this goal, adequate resistance to oxidation, creep, fracture, and fatigue, must be achieved. However, microstructural features which promote improvements in one property are often detrimental to others. Accordingly, a thorough understanding of how microstructure affects each property is needed so that appropriate trade-offs can be made in the optimization of these alloys. To further this goal, an investigation of how microstructural features affect the fracture and fatigue properties at ambient to high temperature is presented. Specifically, the fracture toughness and fatigue-crack growth resistance have been investigated from 25 to 1300C for several Mo-Si-B alloys with both intermetallic and α-Mo matrix microstructures. These alloys were produced by both ingot and powder metallurgy processing routes with compositions nominally as Mo (bal.), 12-20 at.% Si, 8-10 at.% B. The role of microstructural variables, including volume fraction of α-Mo, its ductility, and the morphology and coarseness of the microstructure are considered in terms of how each variable influences the observed toughening mechanisms, identified to include crack trapping, crack bridging, and in some cases microcrack toughening. Additionally, fatigue-crack growth behavior, and associated mechanisms, are assessed, again in terms of microstructural variables. Work supported by the Department of Energy, through the Office of Science (Basic Energy Sciences) under Contract No. DE-AC03-76SF00098, and the Office of Fossil Energy (Advanced Research Materials) under Contract No. DE-AC05-00OR22725.

4:30 PM S2.10
The Effects of Substitutional Additions on Tensile Behavior of Nb-Silicide Based Composites. Laurent Cretegny, Bernard P. Bewlay, Melvin Jackson and Ann Ritter; General Electric Global Research, Schenectady, New York.

Nb-silicide based in-situ composites consist of a ductile Nb-based solid solution with high-strength silicides, and they show excellent promise for aircraft engine applications. The Nb-silicide controls the high-temperature tensile behavior of the composite, and the Nb solid solution controls the low and intermediate temperature capability. The aim of the present study is to understand the effects of substitutional elements on the constitutive properties of the phases. These data are then used to understand the effects of the scale of the phases and their volume fractions, on the tensile behavior of Nb-silicide based composites. To pursue this goal alloys with a range of compositions were prepared and the tensile behavior was investigated from room temperature to 1200oC. The experimental measurements will be compared with predictions for the Nb-Si composite strength.

4:45 PM S2.11
Microsturctural Relationship to Mechanical Properties of LENS Deposited Nb-Si Alloys. Ryan R. Dehoff, Peter Collins, Peter Sarosi, Hamish L. Fraser and Michael J. Mills; Materials Science and Engineering, The Ohio State University, Columbus, Ohio.

Nb-Si "in-situ" metal matrix composites consist of Nb_3 and Nb_5Si_3 intermetallic phases in a body centered cubic Nb solid solution, and show promising potential for elevated temperature structural applications. Cr and Ti have been shown to increase the oxidation resistance and metal loss rate at elevated temperatures compared to the binary Nb-Si system. In this study, the LENS^{TM} (Laser Engineered Net Shaping) process is being implemented to construct the Nb-Ti-Cr-Si alloy system from elemental powder blends. Fast cooling rates associated with LENS^{TM} processing yield a reduction in microstructural scale over conventional alloy processes such as directional solidification. Other advantages of LENS^{TM} processing include the ability to produce near net shaped components with graded compositions as well as a more uniform microstructure resulting from the negative enthalpy of mixing associated with the silicide phases. Processing parameters can also be varied, resulting in distinct microstructural differences. Deposits were made with varying compositions of Nb, Ti, Cr and Si. The as-deposited as well as heat treated microstructures were examined using SEM and TEM techniques. The influence of composition and subsequent heat treatment on microstructure and mechanical properties such as microhardness and microtensile testing will also be discussed.

SESSION S3: Functional Intermetallics I
Chairs: T. J. Balk and G. Dehm
Tuesday Morning, November 30, 2004
Room 208 (Hynes)

8:30 AM *S3.1
Microstructure and Mechanical Properties of Shape Memory Thin Films Formed by Sputtering. Akira Ishida, National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

Shape memory thin films formed by sputtering have been attracting great interest as powerful actuators in microelectromechanical systems(MEMS) such as microvalves, microfluid pumps, and micromanipulators. Their shape memory effect and mechanical properties were evaluated quantitatively with a small tensile tester and it was established that sputter-deposited thin films have mechanical properties superior to those of bulk alloys. The improvements in tensile strength, elongation and shape memory effect of thin films were achieved owing to very fine structure of unstable phases resulting from the crystallization of amorphous films. While Ti-rich Ti-Ni bulk alloys show only blocky Ti_2Ni particles along the grain boundaries irrespective of heat-treatment, thin films show a peculiar structure evolution of (1)GP zones, (2)GP zones and Ti_2Ni precipitates within the grains, (3)Ti_2Ni precipitates within the grains, and (4)Ti_2Ni precipitates along the grain boundaries with increasing heat-treatment temperature and time. These fine precipitates brought about an excellent combination of a large transformation strain and a small plastic strain. According to the high-resolution transmission electron microscopy observation of a deformed sample, the coherent interfaces of GP zones are effective to prevent dislocation movement, but allow twinning to pass through the GP zones. Another improvement of mechanical properties due to fine structures was observed in ternary alloy films. Extremely small grain size in Ti-Ni-Zr

thin films realized tensile tests, while bulk alloys are so brittle that they have not been tensile-tested. The addition of a third element such as Cu and Pd was found to improve the shape memory behavior similarly to in bulk alloys. As a special issue in thin films, the thickness effect of mechanical properties was also investigated, focusing on the effects of surface oxidation and thickness-to-grain size ratio. Finally, some applications of shape memory thin films such as a microgripper, a microconveyer, and a microrobot are demonstrated.

9:00 AM S3.2
Mechanical Properties of TiNiPt Melt Spun Rribbons with Various Heat Treatments. Tomonari Inamura[1], Yohei Takahashi[1], Hideki Hosoda[1], Kenji Wakashima[1], Takeshi Nagase[2], Takayoshi Nakano[2], Yukichi Umakoshi[2] and Shuichi Miyazaki[3]; [1]Precision and Intelligence Laboratory, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan; [2]Department of Materials Science & Engineering, Graduate School of Engineering, Osaka University, Suita, Osaka, Japan; [3]Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki, Japan.

Mechanical properties of TiNi containing 10mol%Pt melt-spun ribbons were investigated where the heat treatment temperature was systematically changed from 473K to 773K. A hot-forged bulk TiNiPt material with the similar chemical composition was also tested as a comparison. It was revealed by differential scanning calorimetry (DSC) that martensitic transformation temperature of the TiNiPt melt-spun ribbons is 60K higher than that of the hot-forged bulk material, and that the martensitic transformation temperature decreases with increasing heat treatment temperature. It was also revealed by XRD theta-2theta analysis that the apparent phase at room temperature is B19' martensite for the melt-spun ribbons instead of B2 parent phase for the hot-forged bulk material. By mechanical tests at temperatures from room temperature to 373K, superior superelasticity around 5% was confirmed for the melt-spun ribbons when the test temperature is above the reverse martensitic transformation finish temperature. The stress for inducing martensitic transformation is discussed in terms of heat treatment condition. Microstructures of the TiNiPt melt-spun ribbons observed by transmission electron microscopy are also presented.

9:15 AM S3.3
Laser Annealing of Shape Memory Alloy Thin Films: Microstructure Investigation. Xi Wang[1], Joost J. Vlassak[1], Fadila Khelfaoui[2] and Yves Bellouard[3]; [1]Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts; [2]DTSI/LIST, CEA, Fontenay-aux-Roses, France; [3]Center for Automation Technologies, Rensselaer Polytechnic Institute, Troy, New York.

For a decade, shape memory alloys thin films have been considered for application as actuators in numerous MEMS devices. However, the lack of intrinsic shape change reversibility has plagued their broader acceptance. Laser Annealing of Shape Memory Alloy (LASMA) amorphous thin films has recently emerged as a powerful method to bypass this limitation. Instead of doing a high-temperature deposition or a post-deposition anneal in a vacuum furnace, the Laser Annealing process consists of using a continuous laser beam to selectively crystallize an amorphous film in specific zones where shape memory properties are desired. In order to fully comprehend the role of interfaces between amorphous and crystallized zones as a mean to introduce a TWSME, it is essential to investigate the microstructure of laser-annealed films. In this paper, we present a microstructure investigation of Ti-rich Ni-Ti laser annealed thin films. Amorphous, 1.5 micron thick films were deposited on fused quartz substrates by means of UHV sputtering. Optical microscopy and X-ray diffraction were used to determine whether the films were crystallized and to establish the useful parameter space in terms of power density and scan speed. The microstructure of the crystallized regions of the films was characterized using transmission electron microscopy (TEM) in order to investigate the effects of power density and scan speed.

9:30 AM S3.4
Factors to Control the Martensitic Transformation Temperature of TiNi Shape Memory Alloy Containing Ternary Elements. Hideki Hosoda[1], Kenji Wakashima[1], Shuichi Miyazaki[2] and Kanryu Inoue[3]; [1]Precision and Intelligence Laboratory, Tokyo Institute of Technology, Yokohama, Kanagawa, Japan; [2]Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki, Japan; [3]Department of Materials Science and Engineering, University of Washington, Seattle, Washington.

Ternary alloying elements are generally added to TiNi shape memory alloys in order to control the martensitic transformation behavior. It is believed that the martensitic transformation temperature of TiNi is influenced by the electron atom ratio (e/a). However, other factors such as atomic size and electron hole number are not systematically considered. In this paper, we have systematically investigated the transformation behavior of ternary TiNi with a similar heat treatment condition, and the change of martensitic transformation temperature is analyzed by several factors such as the number of electrons (s, s+d and so on), atomic size, atomic volume and electron hole number. On the analysis, substitution behavior of ternary elements is taken into account. It is revealed that martensitic transformation temperature of TiNi is mainly correlated with the electron hole number of ternary elements, and also martensitic transformation temperature shows a tendency to increase with increasing the atomic volume of ternary elements. Other shape memory alloys such as TiPd are also discussed similarly.

9:45 AM S3.5
Creep Formation of Super-Elastic Porous NiTi for Biomedical Applications. Scott M. Oppenheimer[1], Christian Greiner[1] and David C. Dunand[2]; [1]Mat. Sci., Northwestern Univ., Evanston, Illinois; [2]Institut fuer Metallkunde, Universitaet Stuttgart, Stuttgart, Germany.

Argon gas was trapped within a NiTi matrix during hot consolidating of NiTi powders. Upon subsequent heating to 1200 °C, creep of the surrounding NiTi matrix allows the Ar-filled pores to grow up to an average size of 20.9 μm, resulting in porous NiTi with a total porosity of 20.5%. This foaming process is modeled by axisymmetric and three-dimensional finite element models. Porous NiTi specimens were mechanically tested and found to be superelastic at room temperature. Possible applications for porous NiTi include bone-replacement implants and energy-absorbing, "smart" sandwich structures.

10:15 AM *S3.6
Advanced TEM Investigations on Ni-Ti Shape Memory Material. Dominique Schryvers, Wim Tirry and Zhiqing Yang; EMAT, Physics, University of Antwerp, Antwerp, Belgium.

The fundamental aspects of the shape memory behaviour of Ni-Ti material are still not completely understood. In the present talk we will highlight some of the recent results that we have obtained when investigating this material with advanced transmission electron microscopy (TEM) techniques. The atomic structure and internal lattice defects of the precipitates are documented by High resolution TEM (HRTEM) and the atomic positions are refined by the multi-slice least-squares (MSLS) technique based on the intensities of superreflections measured on CCD. The results are compared to density functional theory (DFT) calculations. HRTEM combined with image processing techniques was also used to measure the strain fields in the austenitic Ni51Ti49 matrix surrou nding coherent lens-shaped Ni4Ti3 precipitates. Atomic lattice images were obtained in the [11-1]B2 and the [10-1]B2 zones and the interplanar distances of the {110}B2 planes are used to determine the strain. These measurements were done for small precip i tates with a diameter around 50nm and for larger ones with a diameter of 300nm. From these observations the amplitude and location of the maximum strain in the surrounding matrix could be determined and whether it is compressive or tensile. Also the int eraction between strain fields from different precipitates is investigated. A simple model for the strain based on the observations is proposed, in which the maximum strain is not localised at the matrix-precipitate interface but at a distance from it. Th e measurements and model are compared to the analytical solution based on the Eshelby approach. In parallel with the structural investigations the existence of concentration gradients in the B2 matrix surrounding Ni4Ti3 precipitates or close to a grain bo undary is investigated with energy dispersive X-ray analysis (EDX), electron energy loss spectroscopy (EELS) and energy filtered TEM (EFTEM). In some cases very small concentration deviations from the nominal values can be measured, but such deviations, if existing, often fall under the detection limit of all three techniques applied. Both matrix deformations and concentration gradients will influence the nucleation and growth of martensite plates and variants active during the shape memory behaviour.p

10:45 AM S3.7
Variation in Ferroelastic Transition of Shock-Compressed NiTi. Takamitsu Kurita, Hitoshi Matsumoto, Kentaro Motoki, Kozo Ojima and Hiroshi Abe; Materials Science And Engineering, National Defence Academy, Yokosuka, Japan.

On impact of the flyer plate at a high velocity, a high shock pressure with a duration time of 10-6 second is generated by using a powder gun. We applied this high pressure to a NiTi alloy, which is well known to show an excellent shape memory effect. Then, the effects due to the propagation of a shock wave was investigated on the phase transition in NiTi, because the shock compression is expected as a new processing for synthesis of materials and modification of micro-structure, etc. In this work, the maximum shock pressure was about 20Gpa, as the projectile was impinged on NiTi plate at the velocity of about 1km sec-1. The differential scanning calorimeter revealed that in the NiTi shock treated the temperature region of the

phase transition was expanded and the thermal hysteresis between the high temperature phase and the low temperature phase was narrow, in comparison with those of non-treated. X-ray diffraction measurements and transmission electron microscopy were performed to characterize the micro-structure in each phases. The phase transition depends on defects induced during the propagation of a shock wave.

11:00 AM S3.8
Shape memory effect through $L1_0$-fcc order-disorder transition. Katsushi Tanaka, Advanced Materials Science, Kagawa University, Takamatsu, Kagawa, Japan.

Shape memory effect not associated with martensitic transformation but with order-disorder transition has been examined in the compounds AuCu, CoPt and FePd. For single crystal specimens, a reversible shape change (reduction and elongation in edge length) is observed at the trasition temperature by cooling and heating under a uniaxial compressive stress along the [001] direction. The magnitude of the shape change agrees with the change in the lattice parameters at the transition; a mono-variant ordered specimen has formed under a compressive stress. For poly crystal specimens, similar but small shape change have been observed. As an application of the compounds, a trial actuator consisting of a FePd wire and conventional inconel wire has been constructed. The actuator has properly functioned with heat cycles.

11:15 AM S3.9
Coarsening Behavior and Coercivity in L1o-ordered Intermetallic Iron-palladium Ferromagnets with Equiaxed Grain Morphology. Jorg M.K. Wiezorek and Anirudha Rajendra Deshpande; MSE, University of Pittsburgh, Pittsburgh, Pennsylvania.

The L1o-ordered intermetallic phase FePd can be established in the vicinity of the equiatomic composition for temperatures below about 925K and is a member of a class of uniaxial ferromagnetic intermetallics that exhibit large magnetocrystalline anisotropy and includes also FePt, MnAl and CoPt. Permanent magnet alloys based on these anisotropic ferromagnetic intermetallics are currently of interest for novel and advanced applications in the information technology sector. The technologically relevant properties depend very strongly on the morphology and scale of the microstructure and the defect structures produced during solid-state processing. Here the equiatomic FePd alloys are used as model systems to investigate aspects of the processing-structure-property relationships in this class of L1o-orderd ferromagnets during the latter stages of order annealing after cold-deformation. Depending on the details of the processing parameters employed during the combinations of cold-deformation and annealing treatments a number of morphologically different microstructures with relevant average scale (e.g. grain size) ranging from the nanometer to the conventional micron range can be established. Combinations of property measurements using a vibrating sample magnetometer and microstructural studies by scanning and transmission electron microscopy, including dynamic in-situ heating observations, have been performed on the deformation processed FePd with equiaxed morphology during annealing. Mechanisms for defect-interactions and defect genesis during the grain growth stage have been identified. Activation energies for the dominant elementary diffusional processes during grain coarsening have been determined. A 'Hall-Petch'-type relationship has been established between the coercivity and the average grain size of the equiaxed L1o-FeP intermetallics. Implications for bulk-processing of FePd-based and other L1o-ordered intermetallic ferromagnets are discussed. Support from the National Science Foundation (DMR) is gratefully acknowledged.

11:30 AM S3.10
Comparison of Temperature Driven Ordering and its Influence on the Magnetic Behaviour in Bulk and Thin Film $L1_0$ Ordered FePd. Wolfgang Pfeiler[1], Chaisak Issro[1], Wolfgang Pueschl[1], Peter Franz Rogl[2], William A. Soffa[3], Rafal Kozubski[4], Guy Schmerber[5] and Veronique Pierron-Bohnes[5]; [1]Materialphysik, University of Vienna, Vienna, Austria; [2]Physikalische Chemie, University of Vienna, Vienna, Austria; [3]Materials Science and Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania; [4]M. Smoluchovski Institute of Physics, Jagellonian University, Cracow, Poland; [5]IPCMS-GEMME, CNRS-ULP, Strasbourg, France.

$L1_0$-ordered intermetallics are promising high density magnetic recording materials. The reason is the high magnetic anisotropy with the the c-axis of the tetragonal structure as the easy axis of magnetization. We present preliminary results on FePd films (thickness 50 nm) sputtered on Si and epitaxially co-deposited on MgO substrates and compare them with FePd bulk material (thin foil, $<10\mu$m). Results from X-ray diffraction, electrical resistivity (in-plane) and magnetization (in-plane and out-of-plane) are presented. The cold-rolled thin foil is initially disordered and orders during a subsequent isochronal annealing procedure which is monitored by X-ray diffraction, electrical resistivity and magnetization behaviour. FePd film as-sputtered on Si substrate is fine grained (grain size 15nm) and completely disordered. During annealing the grain size grows (final grain size 30nm) and the film orders $L1_0$ with an increase in all variants of ordered domains. FePd film epitaxially grown on MgO(001) is already highly ordered in the as-prepared state and shows a nearly single-crystalline structure (c-axis perpendicular to sample surface). During isochronal annealing the degree of order further increases and above 650K starts to decrease again. The magnetization curves reflect the initially high magnetic anisotropy (easy axis along c-axis perpendicular to film surface). Starting with annealing at 500K an ever increasing number of ordered domains re-orient their c-axis into the film plane. This surprising effect is in correpondence with recent Monte-Carlo simulations of ordering kinetics in $L1_0$-ordered nano-layers.

11:45 AM S3.11
Strain-Induced Ferromagnetism in Single Crystal Intermetallic Compounds. Ian Baker[1], Dongmei Wu[1], Markus W. Wittmann[1] and Paul R. Munroe[2]; [1]Thayer School of Engineering, Dartmouth College, Hanover, New Hampshire; [2]Electron Microscope Unit, University of New South Wales, Sydney, New South Wales, Australia.

Recent research has indicated that the strain-induced paramagnetic to ferromagnetism transition in FeAl arises mostly from the generation of APB tubes, where Fe atoms can have $\geq$3 like nearest neighbors. The resulting saturation magnetization, M_s, depends on both the Fe:Al ratio and the degree of deformation. A quantitative model will be presented that describes the effects of both of these parameters in terms of the local environment theory applied to the atoms in APB tubes. The behavior of both ternary FeAl-based alloys and of the $L2_1$-structured intermetallic compound Fe_2AlMn will be explained by considering the site preferences of ternary atoms on the Fe and Al sublattices. TEM observations of APB tubes in lightly-strained single crystals of FeAl and Fe_2AlMn will be presented, and the annealing out of APB tubes and the associated activation energy will be discussed. The effects of plastic strain on the magnetic properties of some strongly-ordered $L1_2$ intermetallics are also outlined. Research sponsored by NSF grant DMR 9973977 and NIST grant 60NANB2D0120.

SESSION S4: Functional Intermetallics II
Chairs: E. P. George and Y. Umakoshi
Tuesday Afternoon, November 30, 2004
Room 208 (Hynes)

1:30 PM *S4.1
Sub-nano and Nano-structures of Hydrides of $LaNi_5$ and its related Intermetallics. Etsuo Akiba, Kouji Sakaki and Yumiko Nakamura; Energy Electronics RI, AIST, Tsukuba, Ibaraki, Japan.

Sub-nano and nano-structures of intermetallics such as $LaNi_5$ and its related alloys were studied by in-situ X-ray and neutron diffraction methods. From the profile shape analysis, changes in lattice strain and crystalline size during hydrogenation/dehydrogenation were estimated, while the crystal (sub-nano) structures were refined by the Rietveld method using diffraction patterns. We also measured defects formation during hydrogenation especially at the first hydrogenation using positron annihilation technique. It was found formation of remarkably dense dislocations and vacancies in the lattice of intermetallics and their hydrides. However, the crystallite size of the alloys studied did not change during hydrogenation and dehydrogenation.

2:00 PM S4.2
Characterization and Catalytic Properties of Ni_3Al for Hydrogen Production from Methanol. Ya Xu, Satoshi Kameoka, Kyosuke Kishida, Masahiko Demura, An-pong Tsai and Toshiyuki Hirano; Materials Engineering Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

Ni3Al intermetallic compound has attractive high temperature properties, such as high strength and good oxidation/corrosion resistance, and is possible to be used for high temperature chemical processing and manufacture. Until now, the catalytic properties of Ni3Al were rarely investigated since the leaching of aluminum from Ni3Al is difficult to obtain a porous Raney-Ni compared to NiAl3 and Ni2Al3. In the present work, the surface and catalytic properties of Ni3Al were studied by X-ray diffraction, inductively coupled plasma (ICP) analysis, SEM observation, surface area measurement, and hydrogen production reactions from methanol. It was found that Ni3Al without alkali leaching showed a limited catalytic activity for the methanol decomposition (CH3OH -> 2H2+CO), and no activity for the steam reforming of methanol (CH3OH +H2O -> 3H2+CO2)

in the temperature range of 513-633 K. The activity of Ni3Al for the methanol decomposition was improved significantly by alkali leaching. The alkali-leached Ni3Al showed a higher catalytic activity for the methanol decomposition than nickel catalyst above 573 K. Furthermore, Ni3Al catalyst suppressed the formation of methane, i.e. it showed higher selectivity for the methanol decomposition reaction than nickel catalyst. These results indicate a possibility for Ni3Al used as a catalyst for hydrogen production reaction.

2:15 PM S4.3
Ultra-Strong and Ductile Hypereutectic Ti-based Bulk Alloys. Dmitri V. Louzguine[1], Larissa V. Louzguina[2], Hidemi Kato[1] and Akihisa Inoue[1]; [1]Institute for Materials Research, Tohoku University, Sendai, Japan; [2]Research and Development Project, CREST, Japan Science and Technology Agency, Sendai, Japan.

Typical commercial Ti-based alloys have an ultimate tensile strength slightly exceeding 1 GPa which taking into account relatively low density of Ti (4.5 Mg/m3) implies their high strength/density ratio. Moreover, Ti alloys exhibit capability for further strengthening. For example, mould casting technique allows to produce Ti-based bulk glassy alloys having a high strength of about 2 GPa which, however, suffer from the lack of ductility. In the present work we study a number of binary Ti-TM (TM-other transition metals) and ternary Ti-Fe-TM as well as Ti-Fe-RE (RE-rare-earth) alloys and report on the formation of the high-strength and ductile hypereutectic Ti-Fe, Ti-Fe-Cu and Ti-Fe-Nd alloys. The alloys were produced in the form of the arc-melted ingots 20-30 mm diameter and 10-15 mm height. The structure of the high-strength and ductile hypereutectic alloys studied by X-ray diffractometry and scanning electron microscopy is found to consist of the primary cubic Pm3m intermetallic compound (TiFe-phase or a solid solution on its base) and a dispersed eutectic consisting of this Pm3m intermetallic compound + BCC Im3m β-Ti supersaturated solid solution phase. The mechanical properties of the samples cut from the central part of the arc-melted ingots were tested by an Instron-type machine. The Ti65Fe35 alloy having hypereutectic structure consisting of the primary TiFe phase and submicron-size eutectic (TiFe + β-Ti) structure showed excellent mechanical properties: a Young's modulus of 149 GPa, a high compressive fracture strength of 2.2 GPa, a 0.2 % yield strength of 1.8 GPa and 6.7 % ductility. The addition of Cu improves ductility of the alloy, while the addition of Nd improves both strength and ductility. Ni and Mn additions caused embrittlement owing to the formation of the alternative intermetallic compounds. The mechanical properties of the arc-melted Ti70Fe15Cu15 and Ti62Fe33Nd5 alloys are: a Young's modulus of 120 and 160 GPa, a high mechanical fracture strength of 1.78 and 2.49 GPa, a 0.2 % yield strength of 1.53 and 1.5 GPa as well as 8 and 10 % ductility, respectively. The hard round-shaped Pm3m intermetallic TiFe (or Ti(Fe,Cu)) phase, the supersaturated Im3m β-Ti solid solution and the disperse eutectic structure obtained result in a high strength of the Ti-Fe, Ti-Fe-Cu and Ti-Fe-Nd alloys which in addition to that exhibit significantly better ductility compared to that of bulk glassy alloys because the ductile β-Ti solid solution phase enables plastic deformation of the sample. The deformation behaviour and the fractography of the Ti-based alloys are studied in details. The reasons for the high strength and good ductility of the hypereutectic alloys are discussed. The Ti-based alloys are characterized by low cost of the alloying elements and do not require an additional injection mould casting procedure.

2:30 PM S4.4
In-situ Observation of Surface Relief Formation and Dissipation during Order-Disorder Transition of Equi-atomic CuAu alloy using Laser Scanning Confocal Spectroscopy. Seiji Miura, Hiroyuki Okuno, Kenji Ohkubo and Tetsuo Mohri; Mat. Sci. and Eng., Hokkaido Univ., Sapporo, Japan.

In-situ observation of the surface relief formation and dissipation associated with the twinning during the order-disorder transitions among CuAu-I (L10), CuAu-II (PAP) and disordered fcc phases was conducted using Confocal Scanning Laser Microscopy equipped with an image furnace. Retro effect was confirmed in poly-crystalline samples, however no evidence was found in single crystal samples. Also it is observed in poly-crystalline samples that the disordering temperature detected by the change of relieves is different from grain to grain, which is relevant to grain boundary crackings during transitions. The crystallographic orientation relationship among grains investigated by FESEM/EBSD was taken into account to explain the phenomena.

3:15 PM *S4.5
Progress in New Thermoelectric Materials. Brian Sales, Condensed Matter Sciences, Oak Ridge National Lab, Oak Ridge, Tennessee.

A brief overview of the current state of thermoelectric materials research will be presented. Thermoelectric devices can be used for the conversion of heat into electricity or for solid-state refrigeration where the only moving parts are electrons and holes. The poor efficiency of thermoelectric devices has restricted their use to niche applications such as the spot cooling of electronics or the generation of electrical power for NASA's deep space probes. To improve the efficiency of thermoelectric devices requires developing materials with larger values of ZT, where T is average operating temperature for the device and Z = S^2 *sigma /kappa , where S is the thermopower (Seebeck coefficient), kappa is the thermal conductivity and sigma is the electrical conductivity. A variety of new approaches and materials have been proposed over the past 15 years and the merits of several of these ideas will be discussed. Classes of materials that will be covered include: mixed-valence intermetallic compounds, Kondo insulators, skutterudites, clathrates, half-heusler alloys, thin film superlattice structures with and without quantum confinement, superlattices with nanodot crystals, and bulk materials with nanocrystal inclusions.

3:45 PM S4.6
Thermoelectric Performance of Ru_2Si_3 and Re-doped $Ru_{1-x}Re_xSi_{1.5}$ Alloys. Benjamin Andrew Simkin and Haruyuki Inui; Materials Science and Engineering, Kyoto University, Kyoto, Kyoto, Japan.

Ruthenium sesquisilicide (Ru_2Si_3) has received extensive attention in recent years as a high-temperature thermoelectric compound due to an attractive combination of large Seebeck coefficients and low thermal conductivities at elevated temperatures. The principal limitation to Ru_2Si_3 as a thermoelectric has been the poor electrical resistivity shown by this compound. The poor observed electrical resistivities have been attributed to an number of factors, including the presence of grain boundaries, and internal cracking of polycrystalline and single crystal samples. Attempts to improve conductivity through the growth of single crystals has yielded only marginal property improvements. A recent study has shown that the high temperature tetragonal $\rightarrow$ low temperature orthorhombic phase change in Ru_2Si_3 induces a [100]—[001] 90 degree rotational domain structure in Ru_2Si_3 that is inherent to the compound, and tends to limit the attainable crystal perfection. However, the [010] direction common to both domain orientations has also been shown to posses superior thermoelectric properties to the [100]/[001] orientation, principally due to the higher thermopower along this orientation. Because this phase change appears to be inherent to the compound and not diffusionally driven, it is expected that further structural enhancements to conductivity will be difficult without alteration of the composition. Initial studies of the compound Re_4Si_7 have suggested an extensive solubility range for Re in the Ru_2Si_3 structure, opening the possibility for significant conductivity improvements to Ru_2Si_3 through substitutional doping of Re for Ru. Arc-melted samples of $Ru_{1-x}Re_xSi_{1.5}$ show a tendency toward increasing n-type conductivity, with simultaneous improvements in conductivity. Additionally, Re additions appear to cause ordering of the low temperature orthorhombic Ru_2Si_3 structure into a tetragonal $(Ru\text{-}Re)_2Si_{\sim 3}$ superstructure with a$\approx$22.5$\AA$ and c$\approx$8.9$\AA$.

4:00 PM S4.7
Mechanical Aspects of Structural Optimization in a Bi-Te Thermoelectric Module for Power Generation. Yujiro Nakatani, Reki Takaku, Takehisa Hino, Takahiko Shindo and Yoshiyasu Itoh; Power and Industrial Systems R&D Center, Toshiba Corporation, Yokohama, Japan.

We are currently developing a low-cost and high-efficiency Bi-Te thermoelectric module for power generation. This module aims at heat recovery at temperatures of 150 degrees C or less. Though the total amount of waste heat energy below 150 degrees C is considerably large, it has not been utilized because the density of energy is low. In addition, the utilization of such low-density energy has been considered economically uncompetitive. Therefore, our objective is to enhance the thermoelectric efficiency and to improve the cost performance of the module. One of the methods to improve the cost performance of the module is to achieve a long-range run without maintenance, based on the enhanced reliability of the module. Our module consists of the Bi-Te thermoelements and electrodes of Mo and Al formed by atmospheric plasma spraying. In such multilayer coating structures, the thermal stress and/or strain is induced by the differences between the thermal expansion coefficients of each material, and this can decrease the long-term reliability. This paper describes the analytical studies on evaluation and improvement of the interface integrity of the Bi-Te thermoelements and the coatings caused by the thermal strain. To estimate the strain state on the interface, the three dimensional elastic-plastic finite element method (FEM) was performed. The analysis revealed that compressive plastic strain rose at the coating layer near the interface and this caused tensile residual strain on the interface when cyclic heat was loaded. Then, a statistical optimization analysis based on the FEM and design of experiment (DoE) method was conducted, and the optimum shape and dimensions of the Bi-Te thermoelement and the coating

thickness required for decreasing the thermal strain were obtained. We have participated in "The Japanese National Project on Development for Advanced Thermoelectric Conversion Systems" supported by the New Energy and Industrial Technology Development Organization (NEDO).

4:15 PM S4.8
Effects of Ga- and In-Doping on the Thermoelectric Properties in Ba-Ge Clathrate Compounds.
Norihiko L. Okamoto and Haruyuki Inui; Materials Science and Engineering, Kyoto University, Kyoto, Japan.

There has been great interest in inorganic clathrate compounds in hopes of producing more efficient thermoelectric devices because they have very low thermal conductivity and relatively high electric conductivity. Clathrate compounds possess polyhedral cages encapsulating guest atoms. Although the low thermal conductivity in clathrate compounds is believed to result from the rattling motion of the guest atoms in the cages, the relationships between cage structures and thermoelectric properties have not well known yet. In our research of the thermoelectric properties for the ternary type I clathrate compounds in the Ba-Ge-Ga system, we have found that $Ba_8Ga_{16}Ge_{30}$ exhibits a value of Seebeck coefficient as high as -200 μV/K and the largest thermoelectric figure of merit in the ternary system. In $Ba_8Ga_{16}Ge_{30}$, Ga and Ge atoms constitute the cage structure and they are randomly distributed in the cage structure. Upon substituting Ga atoms in $Ba_8Ga_{16}Ge_{30}$ by In atoms, the thermoelectric power factor increases while the lattice thermal conductivity decreases, leading to a much higher thermoelectric figure of merit (ZT=1).

4:30 PM S4.9
Magnetic Properties of $E2_1$-Base Co_3AlC and the Correlation with the Ordering of Carbon Atoms and Vacancies.
Yoshisato Kimura[1], Fu-Gao Wei[2], Hideyuki Ohtsuka[2] and Yoshinao Mishima[1]; [1]Materials Science and Engineering, Tokyo Institute of Technology, Yokohama, Japan; [2]National Research Institute for Materials Science, Tsukuba, Japan.

The $E2_1$ type intermetallic compound Co_3AlC is a quite hopeful strengthener for a new class of Co-base heat resistant alloys since its ordered crystal structure is almost the same as that of $L1_2$ Ni_3Al. The difference between $E2_1$ and $L1_2$ is distinguished by a carbon atom occupying the octahedral interstice at the body center. It is believed that Co_3AlC and Ni_3AlC form continuous solid solution in Co-Ni-Al-C quaternary system. Our group have reported that the extra ordering of carbon atoms and vacancies is observed in Co_3AlC and $(Co,Ni)_3AlC$ most likely due to minimizing the elastic strain energy. Half of carbon atoms are replaced by vacancies at every other body center site as if $E2_1$ and $L1_2$ were arranged alternatively in every other unit cell. Thus it should be denoted as $E2_1$' $Co_3AlC_{0.5}$ though it remains still controversial that whether the ordering is long range or short range. We also have reported that Co_3AlC phase exhibits weak ferromagnetism while Curie temperature above 1100 K is unusually too high comparing with its small magnetization. In the present work, the relationship between the anti-phase boundary (APB) and the ferromagnetism is evaluated using TEM and VSM for considering the phase stability of Co_3AlC with its ordered crystal structure. We believe that the unusual ferromagnetism of $E2_1$-base Co_3AlC must be correlated with its ordered crystal structure and should be strongly affected by the extra ordering of carbon atoms and vacancies. The anti-phase domain (APD) size, i.e. the total amount area of APB, was controlled by heat treatment conditions. Magnetization measurements at room temperature and 4.5 K have revealed that the magnetization behavior is clearly affected by APD size. Moreover, effects of the Ni addition were investigated on the magnetic properties and the phase stability of $E2_1$ Co_3AlC against $E2_1$ Ni_3AlC and/or $L1_2$ Ni_3Al. It is quite beneficial to investigate the phase stability of $(Co, Ni)_3AlC$ in Co-Ni-Al-C quaternary system for designing attractive heat resistant alloys based on $(Co, Ni)_3AlC$.

4:45 PM S4.10
Atomic, Electronic, and Magnetic Structure of Iron-Based Sigma-Phases. Pavel Korzhavyi[1], Bo Sundman[1], Malin Selleby[1] and Borje Johansson[1,2]; [1]Dept. of Materials Science and Engineering, Royal Inst. of Technology, Stockholm, Sweden; [2]Dept. of Physics, Uppsala University, Uppsala, Sweden.

Sigma-phases are complex tetragonal structures that form in transition metal alloys having the average number of s+d electrons in the interval 6.5 - 7.4. These phases, which may form during solidification or heat treatment, usually cause embrittlement of the alloys. A well known example is the FeCr sigma-phase, whose formation has a deleterious effect on the mechanical properties of stainless steels. Like other sigma-phases, the FeCr and other iron-based sigma-phases possesse high degrees of chemical disorder among the five crystallographically inequivalent sublattices. We perform a theoretical study of the thermodynamic properties of several binary sigma-phase alloys (Fe-V, Fe-Cr, and Fe-Mo) using ab initio total energy calculations combined with the compound energy formalism developed in CALPHAD. We show that a proper thermodynamic description of these systems can only be achieved on the basis of spin-polarized calculations (the paramagnetic state of these alloys can be described by the disordered local moment model). The local spin moments on the iron atoms occupying the high-coordination sites in the sigma-phase structure are found to reach high values of about 2 Bohr magnetons. Using the calculated total energies we were able to reproduce the experimentally observed site occupancies in the iron-based sigma-phases. The calculated electronic structure and thermodynamic properties are discussed and compared with results of previous studies.

SESSION S5: Poster Session
Chairs: B. P. Bewlay, A. Couret, T. Hirano and D.R. Johnson
Tuesday Evening, November 30, 2004
8:00 PM
Exhibition Hall D (Hynes)

S5.1
Effect of Heat Treatment Conditions on Multistage Martensitic Transformation in Aged Ni-rich Ti-Ni Alloys.
Minoru Nishida[1], Toru Hara[2], Yasuhiro Morizono[1], Mitsuhiro Matsuda[1] and Kousuke Fujishima[1]; [1]Materials Science and Engineering, Kumamoto University, Kumamoto, Japan; [2]National Institute of Materials Science, Tsukuba, Japan.

It has been demonstrated with systematic experiments that the appearance and disappearance of multistage martensitic transformation(MMT) in aged Ni-rich Ti-Ni alloys depend on the heat treatment conditions. No multistage transformation occurs when the evaporation of Ti and Ni and/or the preferential oxidation of Ti in the specimen are prevented and the purification of heat treatment atmosphere in an evacuated quartz tube is achieved. The heterogeneity in precipitation morphology of Ti3Ni4 phase which is responsible for the multistage transformation can be suppressed with the regulation of heat treatment atmosphere as mentioned above. We have concluded that the multistage martensitic transformation in aged Ni-rich Ti-Ni alloys is an extrinsic nature, i.e., a kind of artifact during the heat treatment. Effect of alloy composition and specimen size on MMT is also discussed.

S5.2
Application of CSL Model to Deformation Twin Boundary in B2 Type TiNi Compound. Minoru Nishida[1], Mitsuhiro Matsuda[1], Yasuhiro Morizono[1], Towako Fujimoto[1] and Hideharu Nakashima[2]; [1]Materials Science and Engineering, Kumamoto University, Kumamoto, Japan; [2]Department of Molecular and Material Sciences, Interdisciplinary Graduate School of Engineering Science, Kyushu University, Fukuoka, Japan.

Near-equiatomic TiNi compound exhibits superior shape memory and superelastic properties. The other peculiar property is anomalous ductility at wide temperature range in comparison to another martensite memory compound such as NiAl. In the present study we have focused on the deformation structure of B2 parent phase around 573 K, since interesting interactions of planer defects have been found. The specimen used is Ti50Ni48Fe2 (Ms = 235 K) in which there is no decomposition of secondary phase during tensile test at elevated temperature and no martensitic transformation during cooling after the test. Serrations are seen in stress-strain curve obtained around 573 K, which corresponds to the formation of various planer defects with twin relation. The dominant planer defect found in the specimens showing serration is {114} compound twin. The other defects are in mirror symmetry with respect to {113}, {115}, {447} planes and so on, which have been confirmed by electron diffraction experiments. These defects are considered to be <110> symmetric tilt boundaries in bcc structure by ignoring the atomic arrangement of B2 structure and are characterized with Σ value based on coincide site lattice (CSL) model. For instance, the Σ value of {114}, {113}, {115} and {447} boundaries are Σ 9, Σ11, Σ27 and Σ81, respectively. Lots of (1-14) defect initially form at grain boundary and grow into grain interior. Some of those deflect to (-114) defect. In such case (4-47) or (-447) Σ81 defect is always observed at the interface of (1-14), Σ 9 and (-114)Σ 9 defects. This fact indicates that sigma combination rule of CSL model can be applied to the triple junction of defects. Similarly, {7710}Σ 99 boundary forms at the interface of {114}Σ9 and {113}Σ11 defects. It can be concluded that the ductility of B2-type TiNi compound is attribute to the formation of various planer defect with large shear strain and the increment of independent slip system due to the formation of planer defects. The interfacial microstructure of planer defects will be

discussed on the basis of CTEM and HREM observations.

S5.3

Structure and Physical Properties of Cu_2MnAl Alloy Films with Significantly Different Atomic Orders. BumJoong Kim[1], Nina Lee[1], Meidong Huang[1], Kiwon Kim[2], Yurij V. Kudryavtsev[3] and YoungPak Lee[1]; [1]q-Psi & Dept. of Physics, Hanyang University, Seoul, South Korea; [2]Dept. of Physics, Sunmoon University, Asan, South Korea; [3]Institute of Metal Physics, Kiev, Ukraine.

Rapidly evolving field of spintronics stimulates a deep interest in ferromagnetic metals with full spin polarization at the Fermi level E_F. These so-called half-metallic ferromagnets are favorable candidates for application as electrodes for spin-polarized current injection into semiconductors. A significant number of intermetallic semi-Heusler and true Heusler alloys (HA) have been predicted theoretically to be half-metals and their films might be used as spin-injectors in such devices. True HA have a formula of X_2YZ, where X and Y are transition metals and Z is a s-p element, and a crystalline structure of $L2_1$. However, recent experiments indicate a limited success in the carrier injection with a high spin polarization from ferromagnet into semiconductor. It is thought to be related to poor interfacial properties (both electrical and magnetic) due to the insufficient spin polarization at E_F, caused by site disorder. Hence, it is important to understand the effect of structural disorder on the physical properties of these alloy films. In this study, the structure and the physical properties of Cu_2MnAl Heusler alloy films with significantly different atomic orders were investigated. The bulk alloy was prepared by melting Cu, Mn and Al pieces together in an arc furnace with a water-cooled Cu hearth. The x-ray fluorescence analysis revealed a alloy composition of $Cu_{0.521}Mn_{0.244}Al_{0.285}$ (hereafter, Cu_2MnAl). The structural homogeneity of bulk alloy was proven to be a single $L2_1$ phase with a lattice parameter of 0.597 nm. The thin films, 74 - 185 nm thick, were deposited by using flash evaporation of the crushed alloy powders onto glass substrates. Several substrate temperatures were chosen from 150 to 750 K to prepare the alloy films with significantly different atomic orders. The structural properties of films were analyzed by x-ray diffraction and transmission electron microscopy. It was found that the most ordered films (among the fabricated) exhibit the $B2$-type crystalline structure with a slightly larger lattice constant than the bulk. Vapor quenching deposition onto substrates, cooled by liquid nitrogen, has led to formation of amorphous phase. The temperature dependence of magnetization of bulk and thin films were investigated in a temperature range from 300 to 700 K by using a vibrating sample magnetometer. While the ordered film shows nearly the same ferromagnetic behavior as the bulk Cu_2MnAl alloy, the disordered film turns out to be nonmagnetic. The transport properties of thin films were measured in a temperature range from 5 to 300 K by employing a four-point method, and the results were analyzed in connection with the structure and the magnetic properties.

S5.4

Laser Annealing of Shape Memory Alloys Thin Films: Oxide Growth Study. Fadila Khelfaoui[2,1], Yves Bellouard[1], Xi Wang[3], Joost Vlassak[3] and Thomas Gessmann[4]; [1]CAT, Rensselaer Polytechnic Institute, Troy, New York; [2]DTSI/LIST, Commissariat a l Energie Atomique (CEA), Fontenay-aux-Roses, France; [3]DEAS, Harvard University, Cambridge, Massachusetts; [4]ECSE, Rensselaer Polytechnic Institute, Troy, New York.

Laser Annealing of Shape Memory Alloy (LASMA) has recently emerged as a powerful method to selectively introduce shape memory properties in amorphous thin films. In particular, the combination of annealed and non-annealed zones in a same substrate can be used to create an intrinsic Two-Way Shape Memory Effect (TWSME), which is otherwise difficult to obtain in thin films. During the anneal, the film is locally exposed to an intense continuous mid-infrared laser beam that is scanned over the specimen to form a given pattern. As the temperature rises, the amorphous film locally crystallizes and an oxide layer grows on the surface of the film as a result of the chemical interaction between the material and the surrounding atmosphere. Although annealing times are short, the oxide layer can significantly alter the film properties and even replace the original material. In this paper, we present a systematic experimental analysis of the oxide growth for three different Ni-Ti thin film compositions. Oxide thicknesses were calculated from measured reflectivity curves using refractive index data obtained by ellipsometry. Specimens were annealed using various laser-scan speeds and power densities. To compare oxide growth behaviors, similar experiments were done on specimens annealed in a furnace for various times and temperatures. For laser annealed thin films - unlike furnace-annealed ones - it is found that the oxide thickness is little affected by the film composition. Discontinuities in oxide growth curves in both furnace- and laser- annealed films were also observed under particular experimental conditions.

S5.5

Structural Properties and Magnetic Behavior in the Pseudobinary Alloys CoFe-CoAl. Nobutoshi Tadachi, Hiroki Ishibashi and Mineo Kogachi; Department of Materials Science, Osaka Prefecture University, Sakai, Osaka, Japan.

Structural properties and magnetic behavior are studied for pseudobinary alloys $CoFe_{1-x}Al_x$ as functions of composition (x = 0-0.7) and quenching temperature (723-1173 K). Both terminal alloys, CoFe ($x = 0$) and CoAl ($x = 1$), form a B2-type ordered structure, which is stable up to 1002 K for CoFe and the melting temperature (1921 K) for CoAl. The former is ferromagnetic while the latter is paramagnetic. From X-ray diffraction measurements for the samples slow-cooled from 1173 K, B2-phase is found to exist stably in a whole composition region. The lattice constant increases with composition x, much rapidly from $x = 0$ to about $x = 0.4$ and then gradually up to $x = 0.7$, indicating a large deviation from Vegard's law. A similar trend is observed for the samples quenched from 1173 K, except for $x < 0.2$ where the two-phase separation of B2 and disordered A2 occurs. In the region of $x < 0.4$, the lattice constant becomes appreciably smaller than that for the slow-cooled sample. This situation suggests a strong correlation with the long-range order (LRO) and further with the magnetism, as was previously confirmed in B2 Co-Fe alloys. $L2_1$ (Heusler)-type ordered structure is observed in Co_2FeAl ($x = 0.5$) alloy by annealing at 873 K for long time after quenched from 1373 K. The mean magnetic moment measured at 4.2 K by using SQUID magnetometer gives 5.16 μ_B in formula unit. This is comparable with the value of 5 μ_B, which is predicted from the relation [(a)] proposed for various ferromagnetic Heusler alloys X_2YZ with a half metallic character. The magnetic behavior is discussed through a correlation with the LRO. (a) I. Galanakis, P.H. Dederichs and N. Papanikolaou: Phys. Rev. B66, 174429 (2002).

S5.6

Formation of Defect Structures During Annealing of Cold-deformed L1o Ordered Equiatomic FePd Intermetallics. Anirudha Rajendra Deshpande and Jorg M.K. Wiezorek; MSE, University of Pittsburgh, Pittsburgh, Pennsylvania.

Equiatomic L1o ordered FePd intermetallics form a good model system for investigation of effects of microstructure on hard magnetic properties in the class of ferromagnetic L1o intermetallics, such as FePt, CoPt, MnAl. These ferromagnetic L1o ordered intermetallics are currently of interest for applications in information technology. The FCC to L1o ordering process in FePd intermetallics leads to a polytwin lamellar microstructural morphology that has been deemed detrimental for hard magnetic behavior of these intermetallics. Alternative thermomechanical processing routes have been employed to avoid the polytwin structure. These thermomechanical strategies employ a combined reaction of annealing of cold deformed metastable FCC phase concomitant with the ordering process and produce microstructures consisting of recrystallized, L1o ordered grains. Various planar defect structures, such as grain boundaries, stacking faults, microtwins, anti-phase structural domain boundaries, evolve in the recrystallized L1o phase grains. The scale, morphology and distribution of these defects are important in determining the hard magnetic properties of these intermetallics. Hence in this study mechanisms for defect formation during annealing of cold deformed FePd intermetallics have been investigated. A combination of experimental tools consisting of conventional TEM, in-situ TEM coupled with SEM and orientation imaging microscopy using electron backscattered patterns have been utilized to elucidate the defect evolution during annealing. The results are discussed with respect to previously accepted models for defect structure evolution in disordered FCC alloys. The implications of these results for annealing phenomena in the L1o class of permanent magnets in general are also explored. Support from the National Science Foundation (DMR) is gratefully acknowledged.

S5.7

Crystal Structure and Thermoelectric Properties of Al-containing Re Silicides. Eiji Terada[1], Min-Wook Oh[1], Myung-Hoon Oh[3], Dang-Moon Wee[2] and Haruyuki Inui[1]; [1]Materials Science and Engeneering, Kyoto University, Kyoto, Japan; [2]Materials Science and Engineering, KAIST, Daejon, South Korea; [3]Materials Science and Engineering, KNUT, Gumi, South Korea.

Binary rhenium disilicide is interesting owing to potentials as a promising candidate material for thermoelectric applications. The stoichiometry of the silicide is determined to be $ReSi_{1.75}$ instead of $ReSi_2$ and the crystal structure belongs to the monoclinic system with an ordered arrangement of Si vacancies in the parent C11b lattice. In the microstructure, twins exists with their boundaries strictly parallel to $[001]_{C11b}$. Binary $ReSi_{1.75}$ exhibits significantly anisotropic thermoelectric properties such that the value of Seebeck coefficient along $[100]_{C11b}$ is positive (230μV/K at 330 K) while it is negative (-300μV/K at 600 K) along $[001]_{C11b}$. This may result from the highly

anisotropic electronic structure of $ReSi_{1.75}$. The dimensionless figure of merit (ZT) for binary $ReSi_{1.75}$ is as high as 0.7 at 1073 K when measured along [001] while the ZT value along [100] is moderate (0.15 at 900 K). We have tried to improve the thermoelectric properties of $ReSi_{1.75}$ by adding Al. Al substitution for Si in Re silicides improves the ZT value along [100]. The temperature dependence of electrical resistivity measured along [100] indicates that the conduction mechanism changes from of semiconductor to of metal upon alloying with Al and the value of electrical resistivity at room temperature for Al-added alloys is significantly reduced by one order of magnitude when compared to the binary counterpart. Thin anomalous layers are locally formed between twins. In these layers the arrangement of Si vacancies is different from that in the binary counterpart. The effects of this microstructural change caused by alloying with Al on the thermoelectric properties will also be presented.

S5.8
Identification of the Chirality of Intermetellic Compounds by Electron Diffraction. Satoshi Fujio[1], Hiroki Sakamoto[1], Kastushi Tanaka[2] and Haruyuki Inui[1]; [1]Department of Materials Science and Engineering, Kyoto University, Kyoto, Japan; [2]Department of Advanced Materials Science, Kagawa University, Takamatsu, Japan.

Enantiomorphism is usually referred to and used to describe objects that are lacking in improper rotations (rotoinversions and rotoreflections). The distinction of chirality in enantiomorphic crystals is usually made by X-ray diffraction. In X-ray diffraction, the breakdown of Friedelfs law occurs through anomalous scattering, resulting in different intensities and phase angles for the Friedel pair of reflections. However, distinction of chirality by X-ray diffraction usually needs a relatively large-sized single crystal of high quality that is free from crystal lattice defects. In addition, special techniques, such as the multiple isomorphous replacement (MIR) method, and a sufficiently strong X-ray beam, such as that from asynchrotoron radiation source, are needed in many cases. If the distinction can be made by electron diffraction in the transmission electorn microscope (TEM), such difficulties can be completely avoided owing to the capability of the TEM of using a nanometer-sized electron probe. However, it is generally believed that electron diffraction is not a general method for the chiral identification of enantiomorphic crystals since the intensity difference is not expected to occur for Bijvoet pairs of reflections through anomalous scattering, which does not occur in electron diffraction. Althogh a few method have so far been proposed to determine the chirality of enantiomorphic crystals such as quartz and MnSi by electron diffraction, in particular by the convergent-beam electron diffraction (CBED) method, none of them can be easily extended to other enantiomorphic crystals. Now, we proposed a new CBED method for the identification of chirality of enantiomorphic crystals, in which asymmetry in the intensity of the reflections of Bijvoet pairs in an experimental symmetrical zone-axis CBED pattern is compared with that of a computer-simulated CBED pattern. The intensity difference for reflections of these Bijvoet pairs results from multiple scattering (dynamical nature of electron diffraction) among relevant Bijvoet pairs of reflections, each pair of which has identical amplitude and different phase angles. Therefore, the crystal thickness where chiral identification is made with the present method is limited by the extinction distance of Bijvoet pairs of reflections relevant to multiple scattering to produce the intensity asymmetry, which is usually of the order of a few tens of nanometers. With the present method, a single CBED pattern is sufficient and chiral identification can be made for all the possible enantiomorphic crystals that are allowed to exist in crystallography.

S5.9
Thermal Stability of Binary Cr-Cr_3Si and Ternary NiAl-Mo Eutectic Alloys. Aravind Gali[1], H. Bei[1,2] and E. P. George[2,1]; [1]Materials Science and Engineering, University Of Tennessee - Knoxville, Knoxville, Tennessee; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

The microstructural stability of Cr-silicides and NiAl-Mo eutectics were investigated at temperatures to 1400°C. The starting microstructure of the Cr-silicides was lamellar whereas that of NiAl-Mo was fibrous. The length scales of the lamellae were on the order of 1-2 mm whereas the fibers were on the order of 400-800 nm in diameter. Thermal stability can be improved by lowering the interfacial energy. This can be achieved by directional solidification or by the segregation of alloying elements to the interfacial boundaries. In this work we investigate the effects of microalloying elements such as Ce, Zr, Hf, Ge, Y, and Ti on thermal stability. * Research sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy, Under Contract DE-AC05-00OR22725 with UT- Battelle, LLC.

S5.10
Low-temperature Phase Transition in NiAlM Alloys. Ling Yang[1,2], Xun-Li Wang[2,3], C. T. Liu[3], Jaime A. Fermandez-Baca[4], James W. Richardson[5] and Donglu Shi[1]; [1]Chemical and Materials Engineering, University of Cincinnati, Cincinnati, Ohio; [2]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Metals & Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [5]Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, Illinois.

Previous studies on ternary NiAlM alloys [1] have found a surprising hardening effect that cannot be solely attributed to the mismatch of atomic size or elastic moduli. Instead, the magnetic properties of solute atoms have to be considered. In search for evidence of possible magnetic ordering, we have carried out a systematic study of NiAlM (M=Ni, Fe, Co) alloys using neutron diffraction. The diffraction data show that when Al atoms are partially replaced by transitional metal atoms ($Ni_{60-x}M_xAl_{40}$), there is a phase transition at very low temperature (Tc 20K), while alloys with transitional metal atoms at Ni sites ($Ni_{50-x}M_xAl_{50}$) maintain a stable B2 structure down to 10 K. Clearly, the addition of transitional metal atoms (Ni+M) at Al sites destabilizes the B2 structure and the transition depends on the fraction of (Ni+M) on Al sites. However, the observed transition does not seem to be related to magnetism, since neither Ni-rich nor Co-doped alloys have any significant magnetic moment. The diffraction pattern of the new phase also does not match any of the known martensite. Instead, we have found that the new peaks can be well indexed with a slightly distorted double-lattice superstructure, although their intensities have not been reproduced. These observations suggest that the new phase is formed by re-ordering of the local atoms within a double-lattice superstructure. It is fascinating that local atomic ordering can occur at such low temperatures. Further experiments are underway to characterize this new phase transition. This research was sponsored by Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under Contract DE-AC05-00OR22725 with UT-Battelle, LLC. References [1] C.T. Liu, C.L. Fu, L.M. Pike, and D.S. Easton, Acta Mater., 50, 3205-3212 (2002)

S5.11
Abstract Withdrawn

S5.12
Ab Initio Calculations of Phase Stability, Defect Energetics, and Theoretical Strength in Ductile RM B2 Compounds. James Robert Morris[1], Yiying Ye[2], M. Krcmar[1], C.-L. Fu[1], K. A. Gschneidner[2] and A. M. Russell[2]; [1]Metals & Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Ames Laboratory, Iowa State University, Ames, Iowa.

We have used first-principles to calculate phase stability, elastic constants, defect energies, and theoretical strength of YAg, YCu and YZn. These rare-earth compounds are members of a wide class of stoichiometric line compounds with the B2 (CsCl) crystal structure. A number of such compounds, including YAg and YCu, have extensive polycrystalline ductility. We demonstrate that these compounds have properties that are distinct from other B2 intermetallics, in particular NiAl. The elastic constants of the ductile compounds are significantly more isotropic. APB energies are high, as expected for highly-ordered materials, but defying the conventional idea that low APB energies are needed for ductility in B2 compounds. Unstable stacking fault energies, associated with the active b=<100> slip mode, are much lower than in NiAl. We have also examined the theoretical strength, and demonstrate marked differences from other systems. This research has been sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under contract DE-AC05-00OR-22725 with UT-Battelle, LLC and contract W-7405-ENG-82 with Iowa State University of Science and Technology.

S5.13
B2 Phases and their Defect Structures: Part II. Ab initio Vibrational and Electronic Free Energy in the Al-Ni-Pt-Ru System. Raymundo Arroyave, Sara Prins and Zi-Kui Liu; Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania.

Over the past decades, CALPHAD modeling has been increasingly used to describe the thermodynamic properties of a great number of material systems. Thanks to these models, the time required for the development of a given material can be significantly reduced, as the knowledge of the thermodynamic stability of the different phases in any given system allows the focusing of the experimental work on only the relevant compositional and thermal regions of the phase diagram. Unfortunately, in many cases, especially in high temperature materials, experimental information needed as input in CALPHAD models is lacking. Fortunately, thanks to recent progress in computational materials science, the gap in experimental knowledge

can be filled with self-consistent ab-initio studies. Considerable progress has been made regarding total energy calculations at 0 K of condensed phases. However, an accurate knowledge of the electronic and vibrational properties of crystalline materials is needed if one is to develop a complete thermodynamic description of any given phase, as they allow the description of the thermodynamics of crystals at finite temperatures. Due to their excellent thermal stability and low mass density, ordered B2 phases are often used in high-temperature applications. In this work, a systematic study of the vibrational and electronic properties of the ordered B2 phases in the Al-Ni-Pt-Ru system is presented. This complements the ongoing efforts in this group to calculate the 0K energetics of this quaternary system. Density Functional Theory within the GGA (and LDA) approximation is used to calculate the vibrational entropies of the B2 phases via the super cell method. The electronic free energy is calculated by integrating the electronic DOS at different volumes. By combining the 0K energetics with the contributions to the free energy of vibrational and electronic degrees of freedom, thermal properties such as enthalpy, specific heats, entropies and so forth are calculated and compared to the available experimental results. Additional results using the much simpler Mean Field Potential theory are also presented for comparison. The results from this work will be employed as input data in the CALPHAD thermodynamic optimization of the modified A2/B2 sublattice model, which allows the description of both the disordered and ordered bcc structures with a single Gibbs energy function.

S5.14
B2 Phases and their Defect Structures: Part I. Ab initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System. Sara Prins, Raymundo Arroyave, Chao Jiang and Zi-Kui Liu; Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania.

Ordered B2 phases are often used in high-temperature structural applications due to their high melting temperatures, good oxidation resistance in harsh environments, low mass density and superior mechanical properties. B2 phases often exist over a composition range as the result of defects in the crystal structure. Defects are either anti-site atoms or vacancies, or in the cases where the deviation from stoichiometry extends to both composition sides, a combination of defects. A thorough knowledge of the fundamental physical and chemical properties of the different defect structures is essential in the development of B2-based alloys. In a systematic first principle study of the Al-Ni-Pt-Ru system, the enthalpies of mixing for the disordered A2 phases have been calculated with Special Quasirandom Structures (SQS) by mimicking the random bcc alloy with the local pair and multisite correlation functions. The enthalpies of formation for stoichiometric B2 phases (NiAl, PtAl, RuAl) have been calculated using both the GGA and LDA approximations, while the enthalpies of formation for B2 phases with large amounts of constitutional defects (both vacancies and anti-site atoms) were also calculated using the SQS approach. The calculated B2 lattice parameters for the different defect structures were compared with experimental results. It will also be shown how these values, together with vibrational and electronic free energies which were calculated using the density functional theory within the GGA and LDA approximations, can be used as input values for the CALPHAD modified sublattice A2/B2 model. The modified sublattice model describes the bcc phases with one Gibbs energy function and simplifies the CALPHAD model significantly.

S5.15
Thermal Analysis of Relaxation Processes of Supersaturated Vacancies in B2-Type Aluminides. Ryusuke Nakamura, Kyosuke Yoshimi, Akira Yamauchi and Shuji Hanada; Institute for Materials Research, Tohoku Univ., Sendai, Japan.

Relaxation behavior of supersaturated vacancies in B2-type aluminides such as NiAl and CoAl was studied by the differential scanning calorimetry (DSC). Different, irreversible DSC peaks were observed only at first heating runs, depending on alloy composition and quenching temperature. In stoichiometric NiAl and CoAl water-quenched from 1773K, single exothermic peak appeared near 950 K. On the other hand, two exothermic peaks appeared in Al-poor Ni-40at%Al and Co-42at%Al alloys quenched from 1773 K. One of the two exothermic peaks in Co-42at%Al disappeared as quenching temperature decreased from 1773 to 1573 K. The exothermic peak was not observed in the samples furnace-cooled and quenched below 1473 K. In the Al-rich side, no peak was also observed for NiAl and CoAl. Furthermore, the DSC measurements were extended to the rapidly solidified B2-type aluminide ribbons where the vacancies with higher concentrations than bulk should be introduced. Relaxation processes of supersaturated vacancies are kinetically analyzed, and then systematically discussed comparing with properties on diffusion and point defects for the B2 aluminides.

S5.16
The Yield Anomaly and Ductility of Single-Slip-Oriented FeAl Single Crystals. Ian Baker[1], Dongmei Wu[2], Paul R. Munroe[3] and Easo P. George[4]; [1]Dartmouth College, Thayer School of Engineering, Hanover, New Hampshire; [2]Materials and Engineering Physics Program, Ames Laboratory - Iowa State University, Ames, Iowa; [3]Electron Microscope Unit, University of New South Wales, Sydney, New South Wales, Australia; [4]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Many features of the yield strength anomaly in B2-structured FeAl alloys have been successfully described or predicted by the vacancy-hardening model. The model does not predict any orientation dependence for the yield anomaly. Thus, here, we describe the results of testing this prediction by measuring the critical resolved shear stress, CRSS, of three differently-oriented, single-slip-oriented Fe-43Al crystals as a function of temperature. In addition, the effects of boron on the CRSS were examined by comparing these data with results from mechanical tests of a single-slip-oriented Fe-43Al-0.12B crystal. It was found that the CRSS of all the alloys decreased rapidly from 77-300 K; showed a plateau from 300-723 K; increased to a peak at 873 K, and then, once more, decreased with further increases in temperature. Boron increased the strength at all temperatures above 150 K, but had no effect below this temperature. While neither the strength below <300 K nor the yield anomaly depended on orientation (in agreement with the vacancy-hardening model), the CRSS in the yield strength plateau region around room temperature did. The effects of temperature on ductility and fracture are also presented.

S5.17
Microstructure and Mechanical Properties of Fe-Ni-Mn-Al Alloys. Markus W. Wittmann[1], Ian Baker[1], James Hanna[1] and Paul Munroe[2]; [1]Dartmouth College, Hanover, New Hampshire; [2]University of New South Wales, Sydney, New South Wales, Australia.

A series of Fe-Ni-Mn-Al alloys with elemental concentrations in the range 15 - 35 at. % were cast and found to have a microstructure consisting of alternating, coherent 50nm wide B2 and b.c.c. plates aligned along <100>. Based on the regular interval and connectivity of the two phases, formation of the microstructure is attributed to spinodal decomposition. Mechanical tests on one of these alloys, Fe-20Ni-25Mn-25Al, revealed yield strengths of 1.3 - 1.5 MPa between 300 and 600K and a strength over 200 MPa at temperatures up to 1073K. Heat treatments of one hour at 1073K resulted in coarsening of the microstructure and formation of an f.c.c.phase within the b.c.c. matrix. The results of an investigation into the effects of both heat treatments and compositional variations on the microstructure and mechanical properties of the multi-phased alloys will be presented.

S5.18
Thermomechanical Treatment of a Fe_3Al alloy. Joachim Konrad[1,2], Andre Schneider[1], Stefan Zaefferer[2], Georg Frommeyer[1] and Dierk Raabe[2]; [1]Materials Technology, Max-Planck-Institut fur Eisenforschung GmbH, Dusseldorf, Germany; [2]Microstructure Physics and Metal Forming, Max-Planck-Institut fur Eisenforschung GmbH, Dusseldorf, Germany.

Fe_3Al-based alloys are regarded as promising for high temperature applications in corrosive atmospheres. Generally Fe_3Al shows higher strength compared to disordered Fe-Al alloys and good corrosion resistance in oxidizing and sulphidising atmospheres. The lack of ductility can be overcome by applying a thermomechanical treatment, such as rolling at high temperatures in the A2 (disordered bcc structure) and in the B2 (ordered structure) regimes. Subsequent recrystallization decreases ductility again. A thermomechanical treatment including stepwise hot (T > 900&degC) and warm (800&degC > T > 400&degC) rolling has been established. Aims of the hot rolling step are the refinement and homogenization of the microstructure and the improvement of formability by strain induced ductilization. The former is achieved by hot rolling conditions leading to a combination of dynamic and post dynamic recrystallization resulting in a characteristic crystallographic texture and a controlled grain size. The latter aim is achieved by the movement of single fold dislocations initiating disorder by generating antiphase boundary trails. During subsequent warm rolling this is utilized to improve the ductility. A controlled final heat treatment is applied to produce a fully recovered microstructure and to stabilize the state of improved ductility by reduction of driving forces for recrystallization. The influence of hot and warm rolling temperatures on microtexture evolution and mechanical properties have been investigated. Significant differences in the microtexture according to in-grain orientation gradients and stored energy in correlation with hot rolling temperature have been observed. Warm rolling has been performed in the of B2 and $D0_3$ regimes. The influence of rolling temperatures on ductility and recrystallization kinetics as well as texture and microtexture of the as-rolled state have been examined. On the basis of microtexture investigations by means of EBSD and Taylor type

texture simulation, a mechanism based on the activation of different slip systems is proposed to explain the observed behavior.

S5.19
Optimisation of Precipitation for the Development of Improved Wrought Fe_3Al Based Alloys. Satoru Kobayashi[1], Stefan Zaefferer[1], Andre Schneider[2], Dierk Raabe[1] and George Frommeyer[2]; [1]Microstructure Physics and Metal Forming, Max-Planck Institute for Iron Research, Duesseldorf, Germany; [2]Materials Technology, Max-Planck-Institute for Iron Research, Duesseldorf, Germany.

Fe_3Al based alloys with bcc structures (α : disordered A2 and ordered B2 or D03) have been considered as a structural material for high-temperature application against high-temperature oxidation and sulphidation. Serious problems for the application are the poor high-temperature strength, creep resistance and the limited ductility at low temperatures. Aim of this work is to optimise the fabrication processes to satisfy both, strengthening by precipitates for an improved high-temperature strength and inhibition of recrystallisation that deteriorates room-temperature ductility as well as strength. A $Fe_{-26}Al_{-5}Cr$ single-phase (α) alloy and two different two-phase (α +TiC) alloys with different volume fractions of TiC have been prepared, homogenised in the α single-phase region and hot-rolled at 800°C in the two-phase region of α+TiC to a reduction of 65%, and the kinetics of static recrystallisation has been examined. Based on the results, an optimised thermo-mechanical process has been proposed for the development of a novel wrought Fe_3Al based alloys with strengthening MC carbides. In $Fe_{-26}Al_{-5}Cr_{-0.3}Ti_{-0.2}C$ alloy with a higher amount of TiC, the transus temperature between α and α+TiC exists just below 1400°C and the kinetics of TiC precipitation is very quick. Needle-like TiC particles with more than 1 μm in length formed during air cooling after homogenisation and coarsened during the hot rolling process. The hot deformation with such large TiC particles causes particle stimulated nucleation (PSN) and hence accelerates recrystallisation. While in $Fe_{-26}Al_{-5}Cr_{-0.1}Ti_{-0.07}C$ alloy with a lower amount of TiC, particles with less than 1 μm formed during cooling after homogenisation and exhibited no acceleration of recrystallisation. Based on the results, the following process is proposed in order to accomplish both, strengthening by particles and inhibition of recrystallisation; hot deformation is performed in α single phase or two phase conditions with a small amount of precipitates followed by a heat treatment for further precipitation of very fine particles. The fine particles would also act to pin the boundaries of growing grains, thus leading to extended recovery rather than recrystallisation. In the ($Fe_{-26}Al_{-5}Cr$)-TiC system this process is difficult to be realised due to the high precipitation temperature and quick precipitation kinetics of TiC. Phase diagram determinations by Thermo-calc and experiments revealed that the addition of (V, C) or (Mo, C) instead of (Ti, C) is effective to lower the precipitation temperature.

S5.20
Effect of Excess Vacancy on Antiphase Domain Growth in Fe_3Al. Yuichiro Koizumi, Takashi Hagiwara, Yoritoshi Minamino and Nobuhiro Tsuji; Department of Adaptive Machine Systems, Graduate School of Engineering, Osaka University, Suita, Osaka, Japan.

Growth of $D0_3$-type antiphase domain (APD) in Fe_3Al was investigated by TEM observation and resistivity measurement focusing on the effect of excess vacancies introduced in the quenching process from disordered state. The variation of APD size exhibited considerable deviation from the conventional 'parabolic-growth-law' in the early stage. The variation of the APD size was numerically calculated using diffusion data on the assumption that the migration of the APD boundaries was enhanced by non-equilibrium excess vacancies and the vacancy concentration decreased during the isothermal annealing for APD growth. The calculated variations of APD size could be successfully fitted to the experimental results in the cases that the quenching temperature (T_q) was in the B2 ordered phase region, but not in the cases that the T_q was in the disordered bcc phase region. The APD growth in the latter case was much slower than expected from the calculation. This discrepancy was attributed to the rapid decrease in the vacancy concentration by vacancy clustering since significant amount of dislocation loops were formed only in the specimens quenched from the disordered state and annealed at relatively low temperatures below 700K.

S5.21
Microstructure, Mechanical Properties and Wear resistance of Fe-Al based alloys with various alloying elements. Han-Sol Kim, Won-Yong Kim and Tae-Yeub Ra; Advanced Materials R&D Center, Korea Institute of Industrial Technology, Incheon, South Korea.

We report on microstructure, mechanical properties and wear result of Fe-Al based alloys with various alloying elements. The microstructures were examined using scanning electron microscope (SEM) equipped with energy dispersive X-ray spectroscope and transmission electron microscope. Two types of alloys were prepared using vacuum arc-melting; One is Fe-28Al based alloys with and without alloying elements such as Mo and Zr. The other one is Fe-35Al based alloys produced with same manner. For both types of alloys, Mo addition had found to exhibit an equiaxed microstructure, while dendritic structure was observed to show the effect of Zr addition. These microstructural features were more evinced with increasing content of alloying elements. Concerning the mechanical properties and wear resistance, Fe-35 based alloys were superior to Fe-28Al based alloys especially in the high temperature region. On the basis of the results obtained, details would be discussed.

S5.22
Microstructures in Cold-Rolled Ni_3Al Single Crystals. Kyosuke Kishida, Masahiko Demura and Toshiyuki Hirano; Materials Engineering Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki, Japan.

Considerable amount of studies on the deformation structures in Ni_3Al base intermetallic alloys have been carried out so far, however, main interests were the dislocation structures near the yield point mainly because the anomalous yield behavior is one of the most attractive properties of Ni_3Al. In contrast, the deformation structures in the Ni_3Al-base alloys after large plastic deformation such as cold rolling have rarely been studied by transmission electron microscopy (TEM). Recently we have carried out systematical studies on cold rolling of binary stoichiometric Ni_3Al single crystals with various initial crystal orientations and revealed that the cold rolling behaviors are strongly dependent on the initial crystal orientations, especially on the initial rolling direction (RD). Very thin foils with good quality in shape are available only when the initial RD is close to <001>, whereas macroscopic curving and cracking hinders high cold reduction for samples with the other initial RD. Such an anisotropic rolling behavior must be closely related to the internal deformation microstructure developed during cold rolling. It is therefore necessary to investigate the characteristics of the microstructures in the cold rolled thin foils for understanding the details of the texture formation mechanisms. In the case of the <001> initial RD, the banded structure is formed. Inside each band, a huge amount of widely extended intrinsic stacking faults on {111} planes is developed from relatively early stage of cold rolling. However, no deformation twins are found at any reduction. The presence of such extensive stacking faults is likely to impede uniform slip activation on the other slip planes, and eventually cause heterogeneous and concentrated shear along the other {111} planes. For further cold rolling, the stacking faults and/or the concentrated shear continues to develop on two {111} planes resulting in the formation of the microbands-like structure, which commonly observed in some rolled fcc metals. Shear bands that composed of nano-sized grains develop only at reductions above 90% in the samples with the banded structure. Based on the results of the TEM observations, we will discuss the reason for the anisotropy in the cold rolling of the Ni_3Al single crystals.

S5.23
Line Width Broadening and Peak Shifts Due to Plastic Deformation and Fault Formation in Micron Size Intermetallic Alloys Under Non-Hydrostatic Pressure. John K. Vassiliou[1], J. W. Otto[2], G. Frommeyer[3] and P. Pinto[1]; [1]Physics, Villanova University, Villanova, Pennsylvania; [2]Joint Research Center for the European Commission, Brussells, Belgium; [3]MPI Eisenforschueng, Dusseldorf, Germany.

The d-spacings and the line widths of Bragg peaks in micron size anisotropic polycrystals of Ni_3Al and Cu_3Au intermetallic alloys have been studied under non-hydrostatic conditions by energy-dispersive X-ray diffraction (EDX) in a diamond-anvil cell. Line shifts and line profiles as a function of pressure were used to analyze the microstructural evolution of elastic and plastic strains. Plastic deformation is due to the onset of non-hydrostatic stresses and the introduction of stacking faults and dislocations. A volume incompressibility in the equation of state due to plastic deformation and the saturation of the stacking fault probability is followed by an elastic compression of a fully plastically deformed state. The compression of this state is isotropic and independent of the presence and type of the pressurizing medium. From the systematic shift of different Bragg peaks the stacking fault probability as a function of the confining pressure is derived. The onset of incompressibility of the equation of state corresponds to the onset of increase of the stacking fault probability. Using finite elasticity, it is shown that the stacking fault probability is proportional to an average of the deviatoric stresses.

S5.24
Development and Characterization of W-Based Nanocomposites Prepared by Mechanical Alloying and a Study of the Formation of Intermetallics in These Systems.

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The present study deals with the synthesis of nanocomposites of W-10, 20, 30% Cu, W-10, 20, 30% NiAl and W-10, 20, 30% Ni3Al by high energy ball milling of elemental blends of W, Cu, Ni and Al and looking at the possibility of formation of intermetallics in these systems by high energy ball milling. Mechanical alloying has been carried out in a Fritsch Pulverisette P-5, using WC milling media. The ball milled powders have been characterized using XRD, TEM and SEM. Formation of intermetallics in these systems have been studied by measuring the lattice parametrs from the corresponding x-ray diffraction plots.The crystallite size and strain in the nanocomposites has been calculated from the x-ray peak broadening using Viogt peak profile analysis. The results indicate that nanocomposites with excellent homogeneity can be synthesized by mechanical alloying. The grain coarsening tendency of the nanocomposites after annealing for 2 hours at 400, 600 and 800oC has also been studied. Lattice parameter calculations in all the systems have been carried out both after milling and heat treatments. Interestingly, W shows an increase in the lattice parameter with decrease in the crystallite size suggesting lattice expansion in the nanocrystalline state. The decrease in the crystallite size of W with milling time is more rapid in case of elemental W in comparison to W-Cu nanocomposites, which can be attributed to the cushioning effect caused by ductile Cu. W-NiAl and W-Ni3Al systems show lower crystallite size of W due to the brittle nature of NiAl and Ni3Al. The grain coarsening rate, on heat treatment, of W is the lowest for elemental W in comparison to W-Cu nanocomposites. The sintering behavior of the nanocomposites will also be discussed.

S5.25

Parameters of Dislocation Structure and Work Hardening of Ni_3Ge. Nina A. Koneva[1], Yulia V. Solov'eva[1], Vladimir A. Starenchenko[2] and Eduard V. Kozlov[1]; [1]Dept. of Physics, Tomsk State University of Architecture & Building, Tomsk, Russian Federation; [2]Dept. of Mathematics, Tomsk State University of Architecture & Building, Tomsk, Russian Federation.

Ni_3Ge intermetallic possesses L_{12} structure and remains fully ordered up to the melting temperature. Among other intermetallics with the L_{12} superlattice, Ni_3Ge is one of the least studied materials. Gliding dislocations in this intermetallic are Marsinkowski dislocations. In the present work, the following mechanical characteristics were studied in tension: yield stress $\tau_{0.2}$ and work hardening coefficient $\theta = d\tau/d\epsilon$ for five orientations of single crystals [001], [-1 3 9], [-4 9 17], [-2 3 4] and [-1 1 1]. Measurements were carried out in the 4.2 K - 1000 K temperature interval. The peak temperature $\tau_{0.2}(T)$ and the amplitude of stress at this temperature decrease strongly upon shifting the deformation axis from [001] to [-1 1 1]. The temperature dependencies of $\tau_{0.2}(T)$ and $\theta(T)$ were compared. In addition, the dislocation structure was studied using TEM. The scalar dislocation density ρ was measured in the deformation interval from the yield stress up to failure. The temperature intervals of octahedral and cubic glide are distinguished. The types of active glide systems were identified using slip lines and data about the shape change of the samples. It was confirmed that the main mechanism of self-locking are Kear-Wilsdorf locks. It was established, that the following well-known relationships is valid at temperatures above 77K: $\tau = \tau_F + \alpha Gbsqrt\rho$, where τ_F is the stress of self-locking (solid solution hardening or crystal lattice resistance) of dislocations, α is a parameter of dislocation interaction. Parameter α decreases linearly with temperature for all orientations of single crystals. At the same time, the dependence $\tau_F(T)$ has a shape of a curve with a maximum. It was established that $\tau_{0.2}(T)$ and $\tau_F(T)$ dependencies change in the same manner with changes of the orientation of the deformation axis. Comparison of $\theta(T)$, $\tau_F(T)$ and $\tau_{0.2}(T)$ dependencies was done on the basis of the modern concepts of work hardening. Using the following relationship: $\theta = d\tau/d\epsilon = d\tau/d\rho \cdot d\rho/d\epsilon$, the rate of dislocation accumulation, $d\rho/d\epsilon$, at different temperatures and different orientations of single crystals of the studied alloy was taken into account. The experiments showed that the maximum in dislocation density is reached at the same temperature as the maximum of τ_F and $\tau_{0.2}$. It was established that the mechanisms of dislocation self-locking play an important role in the temperature dependence of work hardening of the Ni3Ge intermetallic.

S5.26

Crystal Structure, Phase Stability and Plastic Deformation Behavior of Ti-rich Ni_3(Ti,Nb) Single Crystals with Various Long-Period Ordered Structures. Koji Hagihara, Tetsunori Tanaka, Takayoshi Nakano and Yukichi Umakoshi; MS&E, Osaka University, Suita, Osaka, Japan.

The Ni_3X-type intermetallic compounds (X= Al, Ti, Sn, Nb, V, etc.) are known to crystallize in various geometrically closely-packed (GCP) crystal structures: $L1_2$ for Ni_3Al, $D0_{24}$ for Ni_3Ti, $D0_{19}$ for Ni_3Sn, $D0_a$ for Ni_3Nb and $D0_{22}$ for Ni_3V, respectively. The crystal structures of those GCP Ni_3X-type phases are characterized by their two features; the stacking sequence of close-packed plane and the ordered arrangements of X atoms on the close-packed plane. The selection of crystal structure are known to be controlled mainly depending on the valence electron density ratio (e/a) and the atomic radius ratio (R_{Ni}/R_X). The compounds described above have relatively simple crystal structures based on 2-fold hcp, 3-fold fcc or 4-fold dhcp structure, while the existence of GCP phases with longer-period stacking sequences has also been reported in some binary and ternary systems. We investigated the phase stability of $Ni_3(Ti_{1-x}Nb_x)$ single crystals with different Nb content (x=0, 0.01, 0.03, 0.05 and 0.10), and found the formation of some metastable GCP structures with longer-period stacking sequences such as 9-fold, 10-fold and 18-fold stacking sequences. The stacking configuration of close-packed planes in those phases was examined by a direct observation using high-resolution TEM, and we determined their crystal structure. The formation of those long-period ordered structures can be explained by the periodic insertion of hexagonal-type stacking faults into the $D0_{24}$-Ni_3Ti phase. Plastic deformation behavior of those long-period ordered phases was examined by compression tests between RT and 1200°C using single crystals. Yield stress anomaly (YSA) was observed in all the crystals by slip on the close-packed plane, which was caused by the Kear-Wilsdorf locking of screw dislocations, similarly to those observed in other binary Ni_3X-type compounds. The extent of YSA is, however, different depending on their crystal structures. The relation between the crystal structure and YSA behavior is discussed especially focusing on the anisotropy of APB energy in those long-period ordered phases.

S5.27

Formation and Migration of Thermal Vacancies in $Ni_{75}Al_{25-x}Fe_x$ Intermetallic Compounds. Ewa Partyka[2,1], Rafal Kozubski[2], Wolfgang Sprengel[1] and Hans-Eckhardt Schaefer[1]; [1]Insitute of Theoretical and Applied Physics, Stuttgart University, Stuttgart, Germany; [2]Insitute of Physics, Jagiellonian University, Krakow, Poland.

Chemical ordering in intermetallic compounds is predominantly controlled by atomic jumps to nearest neighbor vacancies. An important factor controlling the dynamics of the processes is the concentration of thermal vacancies . In the present contribution, the intermetallic $Ni_{75}Al_{25-x}Fe_x$ system ($0 \leq x \leq 25$) with a $L1_2$ structure is studied. The admixture of Fe destabilizes the ordered phase and the "order-disorder" transition temperature decreases. This is accompanied by the decrease of the activation energy E_A for the ordering kinetics. By isochronal residual resistometry at 77 K and the analysis based on the Schulze - Lücke formalism we arrived at a good estimation of the formation (E_F) and migration (E_M) energies for vacancies which contribute to the activation energy E_A for the ordering process. These data suggest that E_F in Ni_3Al is lowered when alloying the compound with Fe. More specific information on the variation of the activation energies for vacancy formation and migration upon alloying Ni_3Al with Fe is expected from positron lifetime and coincident Doppler broadening studies of the positron-electron annihilation radiation.

S5.28

Ab Initio Calculation of Point Defect Energies and Atom Migration Profiles in Varying Surroundings in $L1_2$-Ordered Intermetallic Compounds. Wolfgang Pfeiler[1], Doris Vogtenhuber[2], Jana Houserova[3], Walter Wolf[3,2], Raimund Podloucky[3,2] and Wolfgang Pueschl[1]; [1]Materialphysik, University of Vienna, Vienna, Austria; [2]Center of Computational Materials Science, University of Vienna, Vienna, Austria; [3]Physikalische Chemie, University of Vienna, Vienna, Austria.

$L1_2$-ordered intermetallics, being the main constituent of many superalloys, bear technological relevance and promise as high-temperature structural materials. One is therefore led to study the stability and kinetics of their atom configuration for which the knowledge of defect formation energies and migration profiles is fundamental. Vacancy and antisite defect formation energies were thus calculated for the chemically analogous $L1_2$-ordered intermetallics Ni_3Al, Ni_3Ga, Pt_3Ga, Pt_3In by a supercell ab initio approach. The ground state energy values were incorporated in a grand canonical thermodynamical treatment to obtain their correct interaction due to conservation of stoichiometry as a function of temperature. Elastic and bonding properties were also obtained from ab initio calculations which together with arguments based on atom sizes are used to explain the results. Energy profiles for atom jumps were calculated by statically displacing the jumping atom and relaxing the surrounding neighbours. The influence of variable atomic neighbourhoods on the migration barrier and the stability of the initial and final states were studied by progressively exchanging

nearest and next nearest neighbour atoms, starting from a perfectly ordered structure. Some of the tendencies observed can be made plausible by arguments of atom size, diffusion barriers generally becoming lower as larger atoms are replaced by smaller ones. A modification of the common Börtz-Lebowitz (residence-time) kinetic Monte-Carlo algorithm is proposed so as to account for varying barrier heights and atom surroundings of the jumping atom. The problems of detailed balance and of obtaining the correct thermodynamic equilibrium state are discussed, as is a kinetic ansatz for the co-operative movement of two atoms which seems to play a role in the generation of antisite pairs in a disordering step.

S5.29
Modeling of Creep in Heterogeneous Metal/Intermetallic Composites. William A. Curtin[1], H. Kumar[1], C. L. Briant[1], B. P. Bewlay[2] and L. Cretegny[2]; [1]Division of Engineering, Brown University, Providence, Rhode Island; [2]General Electric Global Research, Niskayuna, New York.

High-temperature creep response is a critical technological requirement for advanced intermetallic systems aimed at replacing superalloys. These advanced systems are typically composites of a refractory metal (e.g. Nb) and a metal-silicide (e.g. Nb5-Si3), with a complex microstructure. Previous work has established the creep behavior of the basic constituents (MRS Symp. Proc. 753, 321 (2003)). However, correlation of the composite creep to the constituent creep behavior needs to be improved. Here, realistic Nb/Nb-Silicide microstructures are mapped onto a 2d computational mesh and creep is modeled explicitly using Finite Elements. The dependence of creep on microstructure and second-phase volume fraction, and the steady-state stress distributions, are assessed. A microstructure-reconstruction technique is then used to generate 3d microstructures using statistical correlation functions extracted from 2d micrographs of the real materials. Creep of the 3d microstructures is then studied, and compared to experiments and the previous 2d models. Stress distributions and hot spots under quasistatic loading are also analyzed. Directions for microstructure optimization to enhance creep and avoid excessive local stress concentrations under quasistatic loading at low temperatures are discussed.

S5.30
Phase Equilibria Predictions in Nb-Silicide Based Composites. Ying Yang[2], Bernard P. Bewlay[1], Melvin Jackson[1] and Austin Chang[2]; [1]General Electric Global Research, Schenectady, New York; [2]Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin.

Nb-silicide based in-situ composites are promising materials for future high-temperature structural applications. Nb-Si alloys are typically alloyed with Hf, Ti, Cr, and Al to provide a balance of mechanical and environmental properties. In order to develop an improved understanding of phase equilibria in Nb-Hf-Ti-Si quaternary system, a methodology coupling the CALPHAD-type computational thermodynamics with experimental measurement of phase equilibria was used in this study. This paper first describes phase equilibria in the Hf-Ti-Si ternary system determined by experiments. Microstructural and microchemical evidence provided a clear definition of the Hf-Ti-Si liquidus surface and indicated that the metal-rich end of the ternary phase diagram possesses one transition reaction. This data was then used to develop a thermodynamic description of the Hf-Ti-Si system. A thermodynamic description of the Nb-Ti-Hf-Si quaternary system was then obtained by extrapolating the thermodynamic descriptions of Hf-Ti-Si, Nb-Hf-Ti, Nb-Ti-Si and Nb-Hf-Si into the quaternary space. The phase equilibria and solidification paths predicted from the currently obtained Nb-Ti-Hf-Si quaternary thermodynamic description are compared with experimental results.

S5.31
Effect of Temperature and Ternary Additives on the Crystallographic Orientation Relationships among Phases Related to the Eutectoid Decomposition of Nb_3Si. Seiji Miura, Kenji Ohkubo and Tetsuo Mohri; Mat. Sci. and Eng., Hokkaido Univ., Sapporo, Japan.

Authors have reported in the previous study that the sluggish decomposition of Nb_3Si phase is effectively accelerated by Zr addition [1]. This effect is obvious at lower temperature range than the nose temperature of the TTT curve. The crystallographic orientation relationships among phases, such as eutectic Nb and product phases of eutectoid decomposition of Nb_3Si (eutectoid Nb and Nb_5Si_3 phases) in the Zr-containing samples heat treated at various temperature ranges were investigated by FESEM/EBSD to understand the decomposition process. Also the effects of additives other than Zr on both decomposition rate and crystallographic orientation relationship were studied. [1] S. Miura, M. Aoki, Y. Saeki, K. Ohkubo, Y. Mishima and T. Mohri, submitted to Met. Mat. Trans. A (2004).

S5.32
Annealing Induced Structural Changes and Microcracking in Mo-Mo_3Si. Xun-Li Wang[1,2], Joachim H. Schneibel[2], Yandong Wang[1], Alexandru D. Stoica[1] and James W. Richardson[3]; [1]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, Illinois.

An outstanding issue in the processing of Mo-Mo_3Si intermetallic composites is that microcracks develop after annealing at high temperatures, which significantly degrade the mechanical properties of the composite materials. The formation of microcracks is difficult to understand from the view point of differential thermal stresses that develop during cooling, which were estimated to be 100 MPa for both phases. It is unlikely such a level of residual stress would cause microcracking at any stage during cooling. In order to determine the nature of microcracking in Mo-Mo_3Si, we have conducted a systematic study of Mo-Mo_3Si composites using a combination of in-situ neutron diffraction, composition analysis, and scanning electron microscopy. In-situ neutron diffraction measurements at 1300°C revealed a significant increase of the lattice parameter in the α-Mo phase as a function of annealing time, whereas the lattice parameter of the Mo_3Si phase shows a corresponding decrease. At the same time, the diffraction peak widths of both phases increased, unexpectedly, with increasing annealing time, giving evidence that plastic deformation occurred at high temperature. X-ray and neutron diffraction measurements made before and after annealing confirmed that the changes in lattice parameters are irreversible, i.e., due to plastic deformation. Because the as-cast materials were obtained off-equilibrium by fast cooling, the α-Mo phase is known to be super-saturated with Si. The in-situ neutron diffraction data therefore suggest that high-temperature plastic deformation during annealing was due to diffusion of Si atoms from α-Mo to Mo_3Si. This finding was corroborated by microscopy studies which demonstrated that the microcracks almost always started at the interface of α-Mo and Mo_3Si grains and grew into the Mo_3Si. Furthermore, crack density measurements via microscopy indicated that as the annealing time increased more cracks were formed. Based on these experimental observations, it is clear that mcirocracking in Mo-Mo_3Si occurred at high temperature. Quite possibly, the diffusion of Si during high-temperature annealing created a highly inhomogeneous stress distribution at the interface where cracks were initiated when the elastic energy exceeded the tensile limit of the Mo_3Si phase. This research was supported by the Division of Materials Science and Engineering, U.S. Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

S5.33
Abstract Withdrawn

S5.34
High Temperature Oxidation Behavior of Al added Mo/Mo_5SiB_2 *in − situ* composites. Akira Yamauchi, Kyosuke Yoshimi and Shuji Hanada; Institute for Materials Research, Tohoku Univ., Sendai, Japan.

Isothermal oxidation behavior of Al added Mo/Mo_5SiB_2 *in − situ* composites was investigated under an Ar-20%O_2 atmosphere over the temperature range of 1073-1673 K. The Al added Mo/Mo_5SiB_2 *in − situ* composites($(Mo\text{-}8.7mol\%Si\text{-}17.4mol\%B)_{100-x}Al_x$; x=0, 1, 3, and 5mol%) were prepared by arc-melting, and homogenized at 2073 K for 24 h in an Ar-flow atmosphere. The ternary Mo/Mo_5SiB_2 *in − situ* composite exhibited a rapid mass loss at the initial oxidation stage and then the passive oxidation after the substrates were sealed with borosilicate glass in the temperature range of 1173-1473 K, whereas it exhibited a rapid mass gain around 1073 K. On the other hand, the Al addition, especially of 1mol%, significantly improved the oxidation resistance of Mo/Mo_5SiB_2 *in − situ* composites at temperatures from 1073-1573 K. These excellent oxidation resistances are considered to be due to the rapid formation of a continuous, dense scale of Al-Si-O complex oxides. The protective oxide scale partially contained crystalline oxides, and the amounts of the crystalline oxides obviously increased with Al concentration.

S5.35
Nucleation of (Mo) Precipitates on Dislocations during Annealing of a Mo-rich Mo_5SiB_2 Phase. Nobuaki Sekido, Ridwan Sakidja and John H. Perepezko; Department of Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin.

Ever since the discovery of the significant improvement in oxidation resistance of the Mo_5Si_3 phase by small boron additions, the intermetallic compound Mo_5SiB_2 (T2) has received considerable attention for an ultra-high temperature application. In the present study, of particular interest are the two-phase alloys such as a

Mo-10Si-20B alloy where the T2 phase with a non-stoichiometric composition is in equilibrium with Mo solid solution (A2) phase. Previous studies have demonstrated that the plate shaped A2 precipitates are formed in the T2 matrix upon prolonged annealing at 1600°C. The present study was carried out to elucidate heterogeneous nucleation of the A2 phase on dislocations in the T2 matrix. For the examination a Mo-10Si-20B alloy was annealed at 1550°C for 2, 5, 20 and 100 hours, followed by furnace cooling. The dislocations formed in the T2 phase were characterized by TEM using the thickness fringe method, invisibility criterion and stereo observations. The lattice parameters of the T2 phase are determined by powder XRD. TEM observations have revealed that many dislocations have developed during annealing in the T2 phase, though few dislocations and no precipitates are present in the T2 phase of the as-cast alloy. It is found that the dislocation density in the T2 phase qualitatively increases with annealing time. The dislocation network is mainly composed of the edge dislocations with Burgers vectors of <100] and <110]. XRD measurements have demonstrated that the lattice volume of T2 phase increases by about 0.9% after the annealing at 1550°C for 100 hours. Judging from the following two results; (i) dislocations are developed only by heat treatments, and (ii) the lattice volume of T2 phase increases after the annealing, it is concluded that some amount of structural vacancies are introduced during solidification, and the vacancies in excess of the equilibrium concentration are annealed out to form dislocations within the T2 matrix. It is therefore possible that the character and mobility of dislocations are strongly influenced by the composition of the T2 phase. In addition the A2 particles have preferentially precipitated on these dislocations. This suggests that these dislocations are the preferential nucleation sites for the A2 phase. The support of Air Force Office of Scientific Research (F49620-03-1-0033) is gratefully acknowledged.

S5.36

Octahedral twins in L1o-ordered manganese-aluminum intermetallics. Jorg M. K. Wiezorek[1], William A. Soffa[1], Cagatay Yanar[2], Eric A. Stach[3] and Velemir Radmilovic[3]; [1]MSE, University of Pittsburgh, Pittsburgh, Pennsylvania; [2]ALCOA Technical center, ALCOA, Pittsburgh, Pennsylvania; [3]NCEM, LBNL, Berkley, California.

The ferromagnetic L1o-ordered intermetallic phase tau-MnAl appears near equiatomic compositions after appropriate heat treatment. This metastable phase, exhibiting high uniaxial magnetocrystalline anisotropy, is the basis for attractive magnetic properties in these materials. The technologically important properties of these alloys are highly structure-sensitive, depending strongly on the microstructure and defect structure produced by transformation from the high-temperature disordered epsilon-phase (A3, hcp) to the ordered tau-phase (L1o). The tau-phase product exhibits characteristically a plethora of crystal defects resulting from the phase transformation, including a profusion of twin boundaries and twin-related variants. Recently the nature of the transformation mode has been elucidated and as part of this study the mechanism of twin formation and defect generation have been investigated in detail, using CTEM, HREM and in-situ hot-stage TEM. The results of this analysis will be discussed. Support from the National Science Foundation (DMR) is gratefully acknowledged.

S5.37

Phase Equilibria and Lattice Parameters of Fe_2Nb Laves Phase in Fe-Ni-Nb Ternary System at Elevated Temperatures. Nobuyuki Gomi, Sumio Morita, Takashi Matsuo and Masao Takeyama; Dept. of Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, Japan.

Fe_2M TCP compounds are potential strengthener in austenitic heat-resistant steels to be used above 973 K for steam turbine component beyond USC power plant. Among the Laves phases, $Fe_2Nb(\epsilon)$ with hexagonal C14 structure is the most attractive because of high congruent melting temperature (1914K) and relatively large composition homogeneity region. In Fe-Nb binary system, however, the austenite (γ-Fe) region in equilibrium with ϵ phase is limited above 1228K and not stable at lower temperatures, i.e. transformed to ferrite (α-Fe). In this study, thus, phase equilibria in Fe-Ni-Nb ternary system at elevated temperatures have been examined first, in order to identify the γ+ϵ two-phase region. Since we found the extended ϵ single phase region in the ternary system, the lattice parameters of the phases in equilibrium in each other have also been studied. In the binary system, the ϵ single phase region exists in the range of 27.5 to 35.5 at% Nb, and it extends toward the equi-niobium concentration direction up to 44 at% Ni in the ternary system at 1473 K, indicating that more than half of the Fe atoms in Fe_2Nb can be replaced with Ni. As the result, the γ+ϵ two-phase region exists extensively, and the solubility of Nb in γ phase increases from 1.5 to 6.0 at% with increase in Ni content. The lattice parameters of a and c in the C14 Laves phase decrease with increasing Ni content. Supposing that all Ni atoms occupy Fe sublattice site, the change in a axis is in good agreement with calculation based on Vegard's law, whereas that of c axis is much larger than the calculated value. These results clearly suggests that atomic size effect is responsible for a-axis change and the binding energy is dominant factor for the c-axis change. To extend these findings to development of new class of austenitic steels strengthened by Laves phase, an attempt has been made to control the c/a ratio by alloying. The addition of Cr is effective to make the c/a ratio close to the cubic symmetry value (1.633), and very fine ϵ Laves phase particles are homogeneously nucleate within the γ matrix in Fe-Ni-Nb-Cr quaternary alloys aged at 1073 K. The morphology and stability of the Laves phase in two-phase alloys will be discussed in conjunction with the lattice misfit strains.

S5.38

Sputtered coatings based on the Al_2Au phase. Christian Mitterer[1], Helmut Lenhart[1], Paul H. Mayrhofer[1] and Martin Kathrein[2]; [1]Department of Physical Metallurgy and Materials Testing, University of Leoben, Leoben, Austria; [2]CERATIZIT Austria GmbH, Reutte, Austria.

Transition metal nitride-based, wear-resistant hard coatings on cutting tools and other substrates often lack self-lubricating properties at elevated temperatures and distinct colorations allowing product differentiation. In the present work, the possibility of achieving these objectives using coatings based on the purple-red Al_2Au phase within the Al-Au system was investigated. Coatings within this system have been deposited onto cemented carbide and Inconel substrates using unbalanced magnetron sputtering. The coatings were characterized with respect to their topography and morphology, chemical and phase composition, hardness, optical, oxidation and tribological properties. Al_2Au-containing coatings have been deposited with dense, fine-grained structures yielding a hardness of 4 GPa and pink coloration. Vacuum annealing at temperatures of 500°C results in a change to a pronounced purple coloration. The coatings are stable up to about 850°C, where the onset of oxidation occurs. Low friction coefficients when testing against alumina counterparts were achieved in the temperature range between 500 and 700°C. The concept of applying Al_2Au-containing coatings as a colored self-lubricating layer on top of a hard coated cemented carbide tool warrants further investigations.

S5.39

Coatings and Bulk Nanostructured $TiAl_3$-X Intermetallics Produced by Mechanical Milling. Eric Hernandez-Ferreira[1,2], Hector Alfredo Calderon[1], Koichi Tsuchiya[2] and Minoru Umemoto[2]; [1]Ciencia de Materiales, ESFM-IPN, Mexico, DF, Mexico; [2]Production Systems Dept., Toyohashi University of Technology, Toyohashi, Japan.

Bulk materials and coatings made of $TiAl_3$-X nanostructured intermetallics have been produced by mechanical alloying and sintering. X represents 8 at. % of Fe, Cr or Mn. Spark plasma sintering (SPS) has been used at temperatures ranging from 973 to 1173 K in order to preserve a grain size in the nanoscale. Characterization of the nanostructure has been performed including grain size distribution, porosity, hardness, strength in compression and ductility as a function of temperature in the case of bulk materials. High strength and brittleness is found at room temperature but as temperature is increased, these materials become ductile. Remaining porosity apparently prevents ductility at room temperature. A quasi-superplastic behavior is found at temperatures above 973 K. SPS between mechanically alloyed powders and the corresponding supporting material, has been used to produce coatings with a thickness varying from 0.1 to 0.3 mm. Steel, Cu and Al are used as substrate. Characterization of the coating nanostructure includes chemical analysis of the interface between coating and substrate. High hardness across the interface with the support is found. The chemical reaction with the supporting material creates different phases that have been identified.

S5.40

Compressive Creep Behavior in Coarse Grained Polycrystals of Ti3Al and its Dependence on Binary Alloy Compositions. Tohru Takahashi[1], Yuki Sakaino[2] and Shunzi Song[2]; [1]Department of Mechanical Systems Engineering, Tokyo University of Agriculture and Technology, Koganei, Tokyo, Japan; [2]Graduate Student, Tokyo University of Agriculture and Technology, Koganei, Tokyo, Japan.

Compressive creep behavior has been investigated on coarse grained Ti3Al alloys with aluminum contents ranging from 23at.%Al to 42at.%Al, in order to obtain basic experimental information concerning the chemical composition effect on creep of Ti3Al. Pure aluminum and titanium of 99.99% purity were arc-melted into small ingots weighing about 10grams under an argon atmosphere. Small pieces were hot deformed at 1300K by about 50% reduction of height in air and subsequently vacuum annealed at 1400K for 100ks. The resulting microstructures contained equiaxed grains of alpha 2 single phase whose average diameter ranged from 125 to 192 micrometers

except alloys containing 40 and 42 at.% aluminum. The microstructures in 40Al and 42Al materials contained small amounts of gamma phase. Compressive creep tests were performed in vacuum on parallelepiped specimens with dimensions of 2mmx2mmx3mm. The amount of creep deformation was measured by an LVDT sensor attached straight upon the load-conveying rod above the specimen. Based on the recorded contraction in height of the specimen, the applied load was intermittently adjusted in order to keep the true stress constant within about 1% error. The applied compressive stress was mainly 159MPa, and the test temperature ranged from 1100K to 1200K. A very small primary transient and the minimum creep rate region followed by a gradual creep acceleration were observed in the materials containing aluminum up to 25at.%. In contrast to this, the alpha 2 single phase materials containing more aluminum than 25at.% showed greater primary transient where creep deceleration continued up to about 0.1 true strain and its following quasi-steady creep region. Two phase materials containing the gamma phase showed small primary transient probably due to the constraint from the harder gamma phase. When the minimum creep rates are utilized as a representing parameter to illustrate the chemical composition efects upon creep strength, there seems to be 3 or 4 domains in the composition dependence of minimum creep rates upon aluminum contents of the tested alloys. Around 25at.% aluminum the minimum creep rate showed a peak where the creep rate decreased as the aluminum content got further from the stoichiometric composition. The minimum creep rate in the materials containing 27-32at.% aluminum hardly showed a siginificant effect. Increasing creep rate was observed from 32at.% up to 35at.% aluminum. And, finally, the minimum creep rate decreased as the aluminum content exceeded 40at.% where the gamma phase formed.

S5.41 TRANSFERRED TO S7.9

S5.42
Microstructure of Bimetallic Joints of Orthorhombic Titanium Aluminide and Titanium Alloy. Bella A. Greenberg[1] and Valerey V. Rybin[2]; [1]Institute of Metal Physics. Ural.Div.RAS, Ekaterinburg, Sverdlovsk region, Russian Federation; [2]CRISM Prometey, St.-Petersburg, Leningrad region, Russian Federation.

An excellent set of strength properties, which is inherent in orthorhombic titanium aluminides, makes one believe they can be beneficial for construction of bimetallic joints. One more favorable factor is that orthorhombic aluminides (unlike other aluminides) contain a disordered phase, which has a relatively high plasticity. Bimetallic joints of orthorhombic titanium aluminide and a titanium alloy were produced (diffusion and explosion welding). The phase composition and the microstructure of the joints were studied by the methods of X-ray diffraction analysis, X-ray spectrum microanalysis, metallography, scanning and transmission electron microscopy. In the case of explosion welding the phase composition differed little from the initial composition. However, the structure changed drastically. Structural elements, which are typical of strongly deformed materials, were observed. The concurrent presence of a cellular structure and a band structure with a high density of dislocations and new grains pointed to different stages of fragmentation, which were due to an inhomogeneous plastic deformation. Different variants of the interrelation between recrystallization and phase transformations in the heterophase structure under shock-wave loading were considered. In the case of diffusion welding a multilayered structure of bimetallic joint was found. Layer-forming phases were identified. It was found that the titanium alloy mostly regained its initial state, while the aluminide turned into a disordered BCC phase. The corresponding BCC phases appeared on approaching to the contact surface on both sides. Their compositions differed from compositions of the initial alloys because Nb and Al diffused to the titanium alloy and Ti diffused to the orthorhombic aluminide. The mutual adjustment of the BCC lattices, which took place during diffusion welding, was beneficial to a high quality of the bimetallic joint. One more important factor was the absence of a continuous intermetallic layer, which could cause embrittlement, near the contact surface. These two factors were revealed earlier in the study of a bimetallic joint of a titanium alloy of a similar composition and a stainless steel (diffusion welding). Thus, two techniques, which were used for welding together one and the same orthorhombic aluminide and a titanium matrix, provided bimetallic joints having absolutely different structures. After diffusion welding, the structures near the contact surface contained BCC β-phases of the corresponding composition and plate-like inclusions of α2-phases. After explosion welding, structures near the contact surface were free of BCC phases, but contained HCP phases, namely, the titanium α-phase, the aluminide α2-phase and, in addition, the aluminide O-phase.

S5.43
Twin-Transformed Lattice Defects in γ-TiAl. Patrick Veyssiere[1], Haruyuki Inui[2] and Yu-Lung Chiiu[3]; [1]LEM, CNRS-ONERA, Chatillon, France; [2]Fusion Technology - PSI, Ecole Polytechnique Federale de Lausanne, Villigen PSI, Switzerland; [3]Materials Science and Technology, Kyoto University, Kyoto, Japan.

Twins traversing a pre-existing deformation microstructure transform the lattice defects intersected into defects whose nature is either unaffected or changed in terms of Burgers vector, crystallographic direction and/or habit plane. Several examples of such transformations are shown and discussed. The case of a faulted dipole is examined in some detail for it may yield a stacking fault configuration that cannot form spontaneously in the alloy. Transformed faulted dipoles evolve in several ways that inform on the stability of this feature. Conditions of twin propagation and twin growth are examined. A model is provided for spontaneoous growth beyond a critical twin size; the model makes use of forest dsilocations and reactions between partials belomgimg to the twin front.

S5.44
Micro-Fracture Toughness Testing of TiAl Based Alloys with a Fully Lamellar Structure. Kazuki Takashima[1], Discar Rudinal[1], Timothy Halford[1], Yakichi Higo[1] and Masao Takeyama[2]; [1]P&I Laboratory, Tokyo Institute of Technology, Yokohama, Japan; [2]Dept. of Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, Japan.

TiAl based alloys with a fully lamellar structure exhibit superior fracture properties compared to those with other microstructures. This is mainly due to the activation of extrinsic toughening mechanisms including crack deflection and shear ligament bridging. These extrinsic toughening mechanisms are controlled by the mechanical properties of lamellae, in particular the lamellar interface fracture strength. It is, therefore, extremely important to evaluate the fracture properties of lamellar colonies to improve the fracture toughness of such TiAl based alloys. In this investigation, a micro-sized testing technique is applied to investigate the fracture properties of lamellar colonies in a TiAl based alloy. A fully lamellar, Ti-46Al-5Nb-1W, alloy and a Ti-48Al two-phase single crystal (PST) were used in this work. Micro-sized cantilever specimens with a size $\approx$ 10 x 15 x 50 μ^3 were prepared from one lamellar colony by focused ion beam machining. Notches with a width of 0.5 μm and a depth of 5 μm were also introduced into the micro-sized specimens by focused ion beam machining. Fracture tests were successfully completed using a mechanical testing machine for micro-sized specimens (MFT-2000) at room temperature. The fracture toughness values were obtained in the range 0.2 - 6 MPam$^{1/2}$. Fracture surface observations indicate that these variations are attributable to differences in local lamellar orientations ahead of the notch. These fracture toughness values are also lower than those having been previously reported in conventional samples. This may be due the absence of significant extrinsic toughening mechanisms in these micro-sized specimens. Fracture mechanisms of these alloys are also considered on the micrometer scale. The results obtained in this investigation give important and fundamental information on the development of TiAl based alloys with high fracture toughness.

S5.45
High-Temperature Environmental Embrittlement of Isothermally Forged TiAl-Based Intermetallic Alloys with Various Kinds of Microstructures. Takayuki Takasugi, Yasuhiro Hotta, Satoshi Shibuya, Yasuyuki Kaneno and Hirofumi Inoue; Department of Metallurgy and Materials Science, Osaka Prefecture University, Sakai, Osaka, Japan.

Isothermally forged TiAl-based intermetallic alloys with various microstructures (gamma grain, duplex, dual phase and fully lamellar microstructures) were prepared. These TiAl-based intermetallic alloys were tensile tested in vacuum and various atmospheres (such as air containing water vapor, O_2 gas, N_2 gas and H_2 gas) as functions of temperature and strain rate. Some intermetallic alloys and microstructures showed reduced tensile strength (or elongation) in air and H_2 gas at low temperature, and also in air, H_2 gas and O_2 gas at high temperature. Also, the observed fractography depended on not only the testing temperature and microstructure but also the testing atmospheres. The observed microstructural effect on the high-temperature environmental embrittlement was discussed, in association with hydrogen and oxygen properties and kinetics in the constituent phases and at some interfaces.

S5.46
Abnormal Deformation Behavior in Polysynthetically-twinned TiAl Crystals with A and N Orientations: An AFM Study. Yali Chen and David P. Pope; Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.

Polysynthetically-twinned TiAl crystals were deformed by compression with loading axis parallel and perpendicular to the lamellar interfaces. The deformation structures on the free surfaces were scanned using a dimension AFM with scan directions parallel

and perpendicular to the lamellar interfaces. Abnormal deformation behaviors were observed to occur in both orientations. When the compression axis is parallel to the lamellar interfaces, the gamma and alpha lamellae deform primarily by shear in planes inclined with the lamellar interface, while the shear vectors lie in the interface. However, in-plane shear, shear in slip planes parallel to the lamellar interfaces, also occurs along the lamellar interfaces. When the loading axis is perpendicular to the lamellar interface, in-plane shear was found to be dominant at the beginning stage of plastic deformation and contributes more to the macroscopic strain. These behaviors are controversial to the Schmid Law since the applied resolved shear stress for these deformation systems is zero. The abnormal phenomenon was explained by the large coherency stresses along the lamellar interfaces.

S5.47

Experimental Studies and Thermodynamic Modelling on the Phase Transformations in γ-TiAl Based Alloys.

Harald F. Chladil[1], Harald Leitner[1], Arno Bartels[2], Rainer Gerling[3], Wilfried Marketz[4] and Helmut Clemens[1]; [1]Department of Physical Metallurgy and Materials Testing, University of Leoben, Leoben, Austria; [2]Materials Science and Technology, TU Hamburg-Harburg, Hamburg, Germany; [3]Institute for Materials Research, GKSS-Research Centre, Geesthacht, Germany; [4]Research & Development, Boehler-Schmiedetechnik GmbH&CoKG, Kapfenberg, Austria.

Current γ-TiAl based alloys are complex multi-phase materials. Effective alloy development, hot working, and subsequent heat treatments require the knowledge of the constituent phases and their transformation kinetics. For casting the solidification path has to be known, whereas for thermomechanical processing the α and β transus temperatures, which sensitively depend on alloy composition, are of particular importance. The knowledge of the influence of alloying elements on the amount and the thermodynamical stability of the phases present is the basis for heat treatments, which are applied for optimization of mechanical properties. For example, β/B2 phase stabilizing elements can be harmful for creep resistance. The present study combines light-optical and scanning electron microscopy, X-ray diffraction and differential scanning calorimetry for the characterization of phase transformations in low alloyed γ-TiAl alloys (so-called 2nd generation alloys showing total alloying concentrations < 5 at%) and high Nb containing γ-TiAl based alloys. In particular, these high Nb bearing alloys with the baseline composition Ti-(42-45)Al-(5-10)Nb+X (at%) have attracted a lot of attention because they combine high creep strength, good ductility at room temperature and excellent oxidation resistance. The term X stands for small amounts of metallic and non-metallic alloying elements. Here, carbon is of particular interest because of its applicability to precipitation hardening. In addition to the experimental investigations, thermodynamic modelling based on the CALPHAD method was used for phase prediction. The results derived from experiments conducted on a variety of γ-TiAl based alloys are compared to thermodynamic calculations. Finally, the influence of carbon on the transition temperatures will be presented. Carbon is currently not available in the commercial TiAl database.

S5.48

Massive Transformation in High Niobium Containing TiAl-Alloys.

Arno Bartels[1], Slawomir Bystrzanowski[1], Harald Chladil[2], Helmut Clemens[2], Rainer Gerling[3], Harald Leitner[2] and Frank-Peter Schimansky[3]; [1]Materials Science and Technology, TUHH, Hamburg, Germany; [2]Physical Metallurgy and Materials Testing, Montanuniversitaet, Leoben, Austria; [3]Materials Research, GKSS Research Centre, Geesthacht, Germany.

Two high Nb containing γ-TiAl-based alloys with chemical composition of Ti-45Al-7.5Nb (at.%) and Ti-46Al-9Nb (at.%) were massively transformed to single phase γ-TiAl by rapid cooling from the α-phase field, i.e. from temperatures above 1300°C. Using a quenching dilatometer the influence of cooling rate and starting temperature on a successful massive transformation was studied. In addition, the required undercooling to start massive transformation could be determined by means of dilatometer measurements. With a high cooling rate from a high starting temperature, for example, an incomplete massive transformation is obtained, characterized by small transformed areas situated at the grain-boundary triple points of the parent α-grains. The orientation map of these embedded massively transformed γ-islands and of the surrounding α-grains was determined by electron back-scattered diffraction. The γ-phase was analysed as cubic phase and the α-phase as hexagonal α. The analyses of these measurements resulted in the orientation relation between the close-packed planes and directions of the parent α-grains and those of the massively transformed γ-areas. In order to investigate the thermal stability of the microstructure, massively transformed material was annealed for one hour at temperatures, increased in steps of 100°C, between 400-1200°C. After the various annealing treatments the microstructural changes caused by recovery, recrystallization and precipitation of $\alpha/\alpha 2$-phase were analyzed by hardness tests and X-ray diffraction measurements. The onset of these processes is reflected in a drop of hardness which starts at about 800°C. X-ray diffraction patterns of massively transformed microstructure do not show separated γ-200 and γ-002 reflections as expected from a tetragonal γ-TiAl lattice. At 800°C separation of the γ-200 and γ-002 reflections starts and increases with increasing annealing temperature. This phenomenon, the increase of the c/a-ratio, is attributed to relaxation of internal stresses and formation of $\alpha 2$-Ti3Al. The appearance of $\alpha 2$-phase is associated with an increase of the Al-content in the γ-TiAl phase.

S5.49

Abstract Withdrawn

S5.50

Different Creep Behaviors of Two Fine-Grained XD TiAl Alloys Prepared by Similar Heat Treatments.

Hanliang Zhu[1], D. Y. Seo[2] and K. Maruyama[1]; [1]Graduate School of Environmental Studies, Tohoku University, Sendai, Japan; [2]Institute for Aerospace Research, National Research Council of Canada, Ottawa, Ontario, Canada.

TiAl-based alloys are potential candidate structural materials for high temperature applications in turbine and automotive engines due to their low density and good elevated temperature properties. However, the poor ductility at ambient temperature has limited their applications. To overcome this obstacle, some developments of TiAl alloys have been focused on refining the lamellar microstructure. Investment cast XD TiAl alloys have uniform cast microstructures with relatively fine grain size by adding boron. Furthermore, the lamellar structure can be further refined by appropriate heat treatment. In this study, microstructural characteristics and creep behaviors of two XD TiAl alloys with nominal composition of Ti-45Al-2Nb-2Mn+0.8vol%TiB2 (at%) (45XD) and Ti-47Al-2Nb-2Mn+0.8vol% TiB2 (at%) (47XD) were investigated. A near lamellar microstructure and two fine-grained fully lamellar (FGFL) microstructures in both alloys were prepared by selected heat treatments. Microstructural examination and tensile creep tests showed that the near lamellar microstructure of 45XD alloy possessed inferior creep resistance due to its coarse lamellar spacing and larger amount of equiaxed gamma grains at colony boundaries. The fine lamellar spacing as well as the fine lamellar colony size gave a major contribution to lower the minimum creep rates in the fully lamellar 45XD TiAl alloy. In contrary to 45XD TiAl alloys, the near lamellar microstructure of 47XD exhibited the best creep resistance though it has coarsest lamellar spacing and largest amount of gamma grains at colony boundaries. Furthermore, the fully lamellar microstructure with finer lamellar spacing showed inferior creep resistance compared to that with coarser lamellar spacing in 47XD TiAl alloy. Based on the examination of the deformed microstructures, it is suggested that the interlocked grain boundaries and relatively coarse colony sizes in 47XD TiAl alloy were responsible for its different creep behaviors compared with 45XD TiAl alloy. Therefore, good microstructural stability is significantly important to improve the creep resistance in the FGFL TiAl alloys.

S5.51

Phase Transformation in Orthorhombic Ti2AlNb Alloys Under Severe Deformation.

Nataliya V Kazantseva[1], Bella A Greenberg[2] and Vitaliy P Pilugin[2]; [1]Ural Division RAS, Institute of Metal Physics, Ekaterinburg, Russian Federation; [2]Institute of Metal Physics, Ekaterinburg, Russian Federation.

The structure and phase transformations of polycrystalline orthorhombic Ti-22 %Al-26,6 %Nb, Ti-25 %Al-22 %Nb (initial phase content O-phase, ordered for Ti, Al, and Nb), and Ti-25,62 % Al-13,89% Nb-0,34% Zr-0,32% Mo (initial phase content B2-phase) alloys after severe plastic deformation by shear under pressure and pulse shock loading with steel plate were studied. It was found that severe plastic deformation of orthorhombic alloys caused phase transformations of the displacement type and those associated with a change in the degree of long-range order, namely B2-omega (B82), B2 -B19 and B2- beta (BCC) (in the case of alloy with initial B2-phase structure) and O- B19- A20 (initial O-phase structure, Ti2AlNb). Unlike to ordinary metals, severe plastic deformation of the titanium aluminum intermetallics leads to decreasing of the strength of the material. Upon severe deformation by the shear under pressure of the orthorhombic alloys, as the degree of deformation increases, the phase transformation order-disorder occurs. Phases formed under severe deformation: B19, A20, B82 - are metastable. They are absent in the equilibrium phase diagrams of the compounds studied. The beta (BCC) phase is also metastable, it is absent in the equilibrium phase diagrams at room temperature. Upon shear under pressure deformation of the alloy with initial O-phase, as the degree of deformation increases, the content of the B19 phase disordered for niobium decreases, whereas the content of the completely disordered

A20 phase content increases. At a grain size of 20 nm, the initial orthorhombic O-phase is completely transformed into the A20 phase. Fine particles of the B19 phase were also found in the orthorhombic alloys with initial O-phase after shock wave loading. The ways of improving the room temperature plasticity of the titanium aluminides are discussed.

S5.52
Mechanical Behavior of a Pt-Cr Jewelry Alloy Hardened by Nano-Sized Ordered Particles. Kamili Jackson, Mielani Nzula and Candace Lang; Centre for Materials Engineering in Mechanical Engineering, University of Cape Town, Cape Town, South Africa.

Annual platinum jewelry sales exceed a billion dollars but South Africa, the largest supplier of platinum, exports minimal finished jewellery. UCT aims to change this by increasing the scientific knowledge of platinum-rich alloys. Mechanical testing as related to microstructure and processing can provide properties useful to both researchers and jewelers. Platinum jewelry alloys are based on binary systems that have not been well characterized. The phase diagrams are often incomplete and mechanical data is missing. The focus of this research is to provide mechanical data of a Pt-Cr alloy by small-scale tensile testing. The materials engineering of platinum jewelry is interesting because only 5wt% can be used for alloying in order to maintain hallmarking. However, pure platinum is very soft and must be alloyed in order be used effectively as jewelry. In several binary systems an increase in hardness has been found after cold working and annealing at low temperatures. The hardening in these alloys has shown to be a result of nano-sized ordered particles. In particular, the existence of the ordered particles has previously been confirmed for a Pt-Cr alloy by TEM. Extensive work has been done on the Pt-Cr alloy to understand the crystal structure and mechanisms of the ordered phase. Hardness tests were performed to measure mechanical properties after various heat treatments. Until recently, most platinum researchers have used hardness tests as the only measure of mechanical properties. A new small-scale tensile testing machine has made the measurement of other mechanical properties economically possible. An 8mm long specimen is used, which significantly reduces the cost of the specimens. Mechanical properties other than hardness are important to jewelers since they determine how easily the alloys will be formed, how well they can be polished and resist scratches, and how well the final piece will hold stones. It also gives basic data that scientists can understand and relate to the hands-on experience of jewelers. In addition, researchers can use mechanical data as selection criteria when choosing alloys for future work. The information gathered on the microstructure of the Pt-Cr binary alloy combined with the results of the mechanical studies will give a more complete picture of behavior to both jewelers and researchers. Preliminary tests on an annealed and cold rolled Pt-Cu alloy show a clear relationship between strength and hardness. In addition, data like strain to fracture and strain hardening was also obtained. It will be helpful to see if the hardening in the Pt-Cr alloy will affect other properties like ductility and strain hardening. It is expected that the increase in strength will have little effect on the low ductility of the cold rolled specimens but elastic strain energy will be improved. Considering that a finished item is cold worked but a higher hardness is useful this will be an excellent result.

S5.53
Formation of Plate-Like Tetragonal Tau Phase in MnAl-C Alloys. Alla S. Sologubenko[1], Helge Heinrich[2], Peter Muellner[1] and Gernot Kostorz[1]; [1]Angewandte Physik, ETH Zurich, Zurich, Switzerland; [2]AMPAC, University of Central Florida, Orlando, Florida.

The metastable tau phase of MnAl is of interest for its magnetic properties. The tau phase forms from the supercooled high-temperature epsilon phase. The epsilon-to-tau transformation has been studied by transmission electron microscopy with the goal of clarifying details of the microscopic mechanisms of nucleation and growth of the plate-like tau phase in MnAl-C alloys. Small amounts of C (within the solubility limit) were added to delay the decomposition of both tau and epsilon to the equilibrium phases beta and gamma. The plate-like tau phase (L10 structure) of MnAl forms from the epsilon phase (A3 structure) in a step-like process. The displacive mode of the plate-like tau formation results in definite crystallographic relationships between the matrix epsilon and the product tau. The crystallographic correspondence is transmitted by the intermediate epsilon-prime phase (B19 structure). The structural domains of epsilon-prime nucleate and grow coherently within the epsilon matrix. As epsilon-prime domains evolve, elastic strains increase at the epsilon-prime interfaces until shear by the formation of stacking faults reduces these strains. A shuffling of the stacking faults by motion of partial dislocation within a single epsilon-prime domain diminishes the elastic strains further. As a result, polytypes appear. The transformation field is limited to a single epsilon-prime domain. Finally, the epsilon-prime domain boundaries are overcome by the collective motion of transformation dislocations which form twinned tau plates. The epsilon-prime domain boundaries are nucleation sites for successive transformation steps and limit the spatial extension of the transformation for the intermediate steps.

SESSION S6: Other Intermetallics and Titanium Aluminides I
Chairs: F. Appel and J. M. K. Wiezorek
Wednesday Morning, December 1, 2004
Room 208 (Hynes)

8:30 AM *S6.1
Alloy Design Concept using TCP and GCP Intermetallics for Austenitic Heat Resistant Materials. Masao Takeyama, Dept. of Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, Japan.

Why there are no austenitic heat-resistant steels strengthened by intermetallic compounds? For energy efficiency and environmental protection, there is a strong demand for developing new austenitic steels applicable to steam turbine components beyond state-of-the-art USC power plants. This talk will provide some ideas for the alloy design how we use intermetallics as a strengthener for the development of a new class of austenitic steels to be used above 973 K. TCP and GCP compounds are of great potential to achieve this goal. Most of transition metals M form both Fe_2M Laves (TCP) and Ni_3M (GCP) compounds, so that the phase equilibria among these compounds together with γ-(Fe, Ni) austenite phase at elevated temperatures in Fe-Ni-M ternary systems are extremely important for design of multi-component alloys. In particular, for the TCP compounds as a strengthener, the partition coefficient of Ni between γ and Fe_2M phases is a key factor, and it has to be large enough to stabilize γ against both Fe_2M and α-Fe, since M is in general α stabilizer. However, very limited studies on the phase equilibria have been reported. We reveal that the single-phase region of Fe_2Nb with hexagonal C14 structure extensively penetrates into the ternary field toward equi-niobium concentration direction, and more than 40at% Ni can dissolve into it at 1473 K. This result makes it possible to disperse the Laves phase finely in the γ matrix by controlling the c/a ratio of C14 through alloying in Fe-Ni-Nb-Cr alloys. For GCP, a Kurnakov type compound of Ni_3V with $D0_{22}$ structure is the most attractive because of relatively high disordering temperature (1318 K) as well as the lattice parameters with respect to the disordering fcc phase: $a_{D022} \langle a_\gamma \langle c_{D022}/2$. The volume fraction as well as coherent morphology of the $D0_{22}$ phase in the two-phase alloy can widely be changed through the fcc$\rightarrow D0_{22}$ phase transformation and misfit control. The knowledge can apply to the multi-component system by replacement of Ni with Fe and V with Nb, making it possible to design a new class of austenitic alloys. The detail of the alloy design concept together with experimental results will be presented.

9:00 AM S6.2
RuAl-Ru Eutectics. Todd Reynolds and David Johnson; MSE, Purdue University, W. Lafayette, Indiana.

The fracture toughness of two phase alloys of RuAl-Ru(Mo,Cr) processed by arc-melting then directionally solidifying using a cold crucible Czochralski technique or a modified Bridgman process were investigated. Due to different amounts of aluminum loss, volume fraction of phases varied. The fracture toughness values for these B2-hcp alloys ranged from 23 to 38 MPa$sqrt$m. Increasing the volume fraction of RuAl was found to decrease the fracture toughness. The oxidation resistance was poor at 1100°C for the RuAl-Mo alloys but was considerably better for the RuAl-Mo-Cr alloys. Mechanical property data from compression and four point bend tests as well as oxidation tests will be reported for alloys of these systems.

9:15 AM S6.3
Formation and Morphology of Kurnakov Type $D0_{22}$ Compound in Disordered fcc γ-(Ni, Fe) Matrix Alloys. Akane Suzuki[1] and Masao Takeyama[2]; [1]Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan; [2]Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, Japan.

Ni_3M type GCP compounds are attractive as strengtheners in heat-resistant austenitic steels as well as Ni base superalloys. In this study, formation and morphology of $D0_{22}$ compound Ni_3V in γ-fcc alloys were investigated as a model case in order to understand fundamentals for microstructure control of new class of austenitic steels. Because of a Kurnakov type compound, Ni_3V becomes disordered γ-fcc phase above disordering temperature (1318 K at stoichiometric composition). The formation process of the $D0_{22}$ phase in γ matrix varies, depending on the composition and heat treatment temperature; precipitation of $D0_{22}$ takes place at temperature above

T_0 (allotropic phase boundary between γ and $D0_{22}$ in the two-phase region), while allotropic transformation to $D0_{22}$ accompanied by multi-variant structure occurs when cooling below T_0. The morphology of coherent precipitates of the $D0_{22}$ compound is sensitive to misfit strains against matrix and can be controlled by alloying addition. The habit planes between the two phases become irrational, parallel to both directions of the invariant line and an a-axis of $D0_{22}$, since the lattice misfit becomes negative along a-axis (δ_a) and positive along c-axis (δ_c) of the $D0_{22}$. The calculation based on the lattice invariant theory as well as experimental results clearly demonstrate that the misfit strain ratio δ_c/δ_a is a dominant factor to determine the habit plane. In addition, the shape of $D0_{22}$ phase, either prism or plate, depends strongly on the magnitude of $|\delta_a|$. These findings will extend to Ni-Fe-Nb-V quaternary system, by partial replacement of Ni with Fe and that of V with Nb, and possibility to develop austenitic steels strengthened by the compound will be discussed.

9:30 AM *S6.4
A New Paradigm: Ductile Intermetallic Compounds.
Karl A. Gschneidner[1,2], Alan M. Russell[1,2], Alexandra O. Pecharsky[1], Zhehua Zhang[1], James R. Morris[1,3], Tom A. Lograsso[1], C.H. Chester Lo[1] and Yiying Ye[1,4]; [1]Ames Laboratory, Iowa State University, Ames, Iowa; [2]Materials Science and Engineering, Iowa State University, Ames, Iowa; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Center of Analysis and Testing, Wuhan University, Wuhan 430072, Hubei, China.

Recently, we discovered a family of rare earth intermetallic compounds (RM, where R = rare earth and M = non-rare earth metal), which exhibit unprecedented large ductilities at room temperature, up to 25% elongation at failure. These compounds have the B2 CsCl-type structure and they are fully ordered, stoichiometric line compounds. To date, we have made quantitative measurements on five of these materials: DyCu, ErCu, YCu, (Tb0.88Dy0.12)Zn, and YAg. Of the five compounds only the (Tb0.88Dy0.12)Zn phase exhibits brittle failure with no ductility. Preliminary examination studies indicate that at least eight other RM B2 phases also exhibit ductile behavior: HoCu, YRh, CeAg, NdAg, ErAg, YIn, ErIr, and ErAu. YAg is the most ductile compound examined to date, with an elongation of 27% at failure with a maximum tensile strength of 150 MPA (comparable to a standard commercial grade aluminum alloy) and a KIC fracture toughness of 19 MPa·m0.5. DyCu and YCu also exhibit significant ductilities and fracture toughnesses. The results of single crystal tensile and compression tests on YCu, YAg, and (Tb0.88Dy0.12)Zn will be discussed. First principles calculations of several of these compounds have been made. As expected for a highly ordered intermetallic compound, the antiphase boundary energies are high, but in contrast the unstable stacking fault energies are remarkably low. The calculated values for the RM B2 phases will be compared with those of the brittle NiAl B2 phase. Since there are about 100 B2 RM phases, in addition to those noted above, there are lots of opportunities to explore various mechanical behaviors and correlate them with their electronic structures. This discovery of ductile intermetallic compounds has opened a new area of fundamental research on the mechanical behavior of solids, and should lead to many new commercial uses. This research has been sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under contract W-7405-ENG-82 with Iowa State University of Science and Technology and under contract DE-AC05-00OR-22725 with UT-Battelle.

10:15 AM S6.5
Rationalization of the plastic flow behavior of Polysynthetically-twinned (PST) TiAl crystals based on slip mode observation using AFM and Schmid's law. Yali Chen and David P. Pope; Materials Science and Engineering, University of Pennsylvania, Philadelphia, Pennsylvania.

PST TiAl samples of different orientations were prepared and deformed by compression at room temperature. The deformation structures on the free surfaces were scanned using an AFM. It was found that when the angle between the lamellar interfaces and the loading axis is between 20 degree and 80 degree, PST samples deform primarily by shear in slip planes parallel to the lamellar interfaces. When the angle is below 20 degree, both the gamma phase and the alpha 2 phase deform by shear in slip planes inclined with the lamellar interfaces, but the shear vectors lie in the interface. When the angle is close to 90 degree, complex deformation behavior occurs. Shear in planes parallel to the lamellar interfaces contributes more to the overall strain in the directions perpendicular to the loading axis and the out-of-plane shear contributes to the strain in the compression direction. The characteristic U-shape curve of the yield stress versus the angle between the loading axis and the lamellar interfaces can be explained quite well using different C.R.S.S. for the three different deformation modes.

10:30 AM S6.6
The Correlation of Slip between Adjacent Lamellae in TiAl.
Patrick Veyssiere[1], M. Sundararaman[2], G. Molenat[3], J. B. Singh[2] and A. Couret[3]; [1]LEM, CNRS-ONERA, Chatillon, France; [2]Materials Science Division, Bhabha Atomic Research Centre, Mumbai, India; [3]CEMES, CNRS, Toulouse, France.

In polycrystalline lamellar Ti-47Al-1Cr-0.2Si compression tested at RT and 600 C, deformation is achieved by ordinary dislocations and twins. Alloys cooled down from 1400 C at about 15 C per minute exhibit one prevalent variant O accompanied by its twin-related variant OT yet under a lesser proportion (average lamellar thickness 110 nm). In such a microstructure, the propagation of strain is explained by the notion of pilot and driven orientations. In a number of situations of adjacent pairs of variants O/OT, deformation takes place in one variant of these pairs, either O or OT, by activation of the slip system that is the most favoured under the applied stress. This slip plane is unique irrespective of the thickness of the lamellae; the nature of the favoured slip system is also independent of lamellar environment including adjacent alpha2 lamellae. In case of multiple slip families as is the case of the present investigation, the operating slip plane is not necessarily the slip system with lowest critical resolved shear stress. When ordinary dislocations are activated by the applied stress in variant O, then slip occurs by ordinary dislocations in variant OT too with the peculiarity that this is not necessarily the slip system with lowest resolved shear stress within that family. The variant that responds according to the Schmid law is regarded as the pilot variant, its companion twin-related variant is dubbed driven. The property holds true whether the operating Burgers vector is parallel or inclined to the interface. The same behaviour is encountered for twinning defining a pilot and a driven orientation in the same way. An additional property is that twinning and not ordinary slip, is activated in the driven variant even though the resolved shear stress for ordinary slip is larger than its critical resolved shear stress. Finally, a property common to ordinary slip and twinning is that the operating systems are in mirror orientations in the pilot and driven variants and that includes the slip directions. In particular the orientation of the <110] slip direction to the interface (parallel or inclined) is conserved.

10:45 AM S6.7
Study of the Deformation Behavior of Lamellar γ-TiAl by Numeric Modeling. Thomas Schaden[1], F. D. Fischer[1], H. Clemens[2] and F. Appel[3]; [1]Institute for Mechanics, University of Leoben, Leoben, Austria; [2]Department for Physical Metallurgy and Materials Testing, University of Leoben, Leoben, Austria; [3]GKSS Geesthacht, Geesthacht, Germany.

Processing of titanium aluminides often starts with the break down of the coarse-grained lamellar microstructure of the ingot. The lamellar microstructure consists of alternating layers of γ-TiAl and α_2-Ti_3Al. After large compressive deformation at temperatures above 1000°C samples were analyzed by means of scanning electron microccopy. The lamellar colonies show, depending on their orientation, more or less marked buckling-type deformation modes according to an instability mode of big wave length. Both structural defects of the lamellae as well as their somewhat irregular arrangement trigger such a deformation behavior. In addition, a shear band-type deformation mode occurs according to an instability mode exhibiting a short wave length. These two deformation modes interact in a rather subtle way, which leads to a very inhomogeneous deformation pattern. In order to simulate the microstructural development during hot working we have established a finite element unit cell model, which is a representative volume element (RVE). The model describes the deformation behavior of the material on a micro-, meso- and macroscopic level. The microscopic level represents the local deformation behavior inside single lamellar colonies taking into account the anisotropic deformation behavior of the γ-TiAl lamellae. At the mesoscopic level six grains are considered to describe the material behavior over a length scale of 100μm. Here, the topological anisotropic material behavior is described by means of Hill-plasticity, which combines the anisotropy due to the existence of the lamellae with the anisotropy of the γ-TiAl lamellae. The numerical model is able to reflect the very inhomogeneously deformed microstructure and demonstrates the concentration of strain in families of shear bands with different amounts of localized shear. The experimentally found deformation pattern can be well predicted by our numerical findings. Due to the high value of imparted deformation energy, recrystallization effects occur, which lead to softening of the material. The energy concentration in the shear bands was calculated in order to predict the onset of recrystallization and to estimate the size of the newly formed grains. From our studies it can be concluded that two softening mechanisms occur: one due to the bifurcation-type deformation pattern and the other due to softening through recrystallization. In addition, we were able to verify the interaction of all these mechanisms and to quantify their specific contributions. Finally, an analysis of the local hydrostatic stress state was conducted to calculate the mechanical driving force in addition to the still

existing chemical driving force with respect to an α_2-Ti_3Al to γ-TiAl transformation. This phase transformation leads to a spheroidization of the lamellar colonies. This mechanism can be considered as a further softening mechanism.

11:00 AM S6.8
Effect of B Addition on Thermal Stability of Lamellar Structure in Ti-47Al-2Cr-2Nb Alloys. Yukinori Yamamoto, Philip J. Maziasz and C. T. Liu; Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Thermal stability of fully lamellar microstructure in hot-extruded T-47Al-2Cr-2Nb (at.%) alloys with and without 0.15 B has been evaluated for both powder-metallurgy and ingot-metallurgy materials. The lamellar microstructure in the alloy with B becomes unstable after a short period of aging at 800 °C because gamma grains form adjacent to borides (TiB2 or TiB) within the lamellae. The formation of these grains is attributed to less alpha 2 plates around the borides because they scavenge Ti, resulting in coarsening of the gamma lamellar plates during the early stages of aging. In the case of the alloy without B, however, the lamellar microstructure exhibits high thermal stability after long time exposure (> 5000 h) at 800 °C, indicating that the existence of borides is the cause of thermal instability of the microstructure. In the presentation, the formation mechanism for gamma grains will be discussed. This research was sponsored by the Division of Materials Science and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

11:15 AM S6.9
Fatigue Testing of Microsized Samples of $\gamma-$TiAl Based Material. Timothy P. Halford, Kazuki Takashima and Yakichi Higo; Precision and Intelligence Laboratory, Tokyo Institute of Technology, Yokohama, Japan.

High strength $\gamma-$TiAl based alloys, such as Ti$-$46Al$-$5Nb$-$1W (Alloy7), which were originally developed for gas turbine and automotive applications are now being considered for application in Microelectromechanical Systems (MEMS). This requires the evaluation of these materials upon the microscale. As international standards do not currently exist for the evaluation of the mechanical properties of samples with dimensions equivalent to those required by MEMS devices, the development of new methods was required. The method developed here is intended for the fatigue testing of samples measuring $\approx$ 10mm (B) x 20mm (W) x 40mm (L). This is completed using a machine recently developed at Tokyo Institute of Technology to load samples of lamellar $\gamma-$TiAl based material to failure in compressive bending. This method is intended to work alongside methods previously developed for the fracture toughness testing of similar microsized cantilever bend specimens. In this work sample cantilevers of Alloy 7 are Focussed Ion Beam (FIB) machined from foil $\approx$ 20mm thick and their stress $-$ life (S$-$N) fatigue behaviour evaluated. The dependence of fatigue life upon lamellar orientation for given peak stress / stress ranges is considered. The effect of the reduced scale of these samples upon the mean and scatter of these sample lifetimes is also considered through comparison with previous data obtained from the S$-$N testing of macrosized samples of the same material.

11:30 AM S6.10
Texture development during hot working in gamma titanium aluminide alloys of different phase constitution.
Michael Oehring, Fritz Appel, Heinz-Guenter Brokmeier and Uwe Lorenz; Institute for Materials Research, GKSS Research Centre, Geesthacht, Germany.

The evolution of preferred orientations during processing appears to be of significant importance for the use of gamma titanium aluminide alloys, since the desired lamellar microstructures exhibit a strong anisotropy of mechanical properties. In this work tex ture development has been investigated after hot extrusion and sheet rolling, which are considered to be technologically relevant wrought processes. As texture evolution certainly is dependent on several factors, involving deformation properties, recrystallization kinetics and particularly the phase constitution at hot-working temperature, different processing conditions and alloy compositions were investigated. By comparing the results it is indicated that the determined textures can be understood by the deformation modes of the dominating phase at hot-working temperature and the subsequent phase transformations. However, the current understanding of texture evolution is far from being complete as no model can be presented which quantitatively accounts for the contribution of the different processes mentioned.

11:45 AM S6.11
On the Effect of Interstitial Elements on Microstructure and Properties of Ternary and Quaternary TiAl Based Alloys.
Jean-Pierre Chevalier[1,2], Melanie Lamirand[1] and Jean-Louis Bonnentien[1]; [1]CECM - CNRS, Vitry, France; [2]Materiaux Industriels, CNAM, Paris, France.

Interstitial elements, such as carbon, nitrogen and especially oxygen are known to have a significant solubility in alpha2 TiAl, but only slight in the gamma phase. Hence, these elements have a strong influence on the microstructures. Furthermore, many titanium grades have a relatively high initial oxygen content, and due to the high reactivity of these alloys, pickup during processing may also lead to TiAl alloys with typically at least, and often more, 1000 ppm wt oxygen. Using strict clean processing (alloy preparation, melting, remelting, high temperature heat treatment) together with either ultra high purity titanium or commercial purity titanium as starting materials, the effects of interstitial elements on microstructure and mechanical properties (hardness, yield stress and ductility) have been studied systematically. Microstructures have been quantitatively analysed and particular care has been taken to assess relative ductilities of the alloys. Following from previous work on binary alloys, here Ti-Al-Cr ternary and Ti-Al-Cr-Nb quaternary aloys have been studied. The effects of interstitial content has been ascertained both for fully lamellar microstructures obtained by controlled cooling from the alpha phase and for duplex microstructures obtained by heat treatment in the alpha-gamma phase field. The results are clear and similar trends are observed in all cases : oxygen stabilises the lamellar microstructure and affects the kinetics of the alpha-gamma phase transformation, leading to a higher than equilibrium volume fraction of the alpha2 phase for the case of continuous cooling. On the other hand, the volume fractions of alpha2 and gamma are close to equilibrium values for the duplex microstructures. Both the lamellar spacing and the alpha2 volume fraction correlate with increased hardness and yield strength, but with a decreased ductility. The results for oxygen will be briefly compared to those obtained for carbon and nitrogen. Possible mechanisms linking the interstitial element content with the phase transformation kinetics will be discussed. These suggest that the interstitial elements may well play an important role in determining microstructuresl and that their content should be more strictly controlled in general. Fluctuations in interstitial content, together with differences in cooling rate may well give rise to variations in microstructure, which could at least partially explain the scatter in properties encountered for these alloys. Finally the microstructure-yield stress relation will be briefly examined, and the more tenuous link between microstructure and ductility will be broached.

SESSION S7: Titanium Aluminides II
Chairs: D. G. Morris and Patrick Veyssiere
Wednesday Afternoon, December 1, 2004
Room 208 (Hynes)

1:30 PM S7.1
An Electron Microscope Study of Mechanical Twinning and Fracture in TiAl Alloys. Fritz Appel, Institute for Materials Research, GKSS Research Centre, geesthacht, Germany.

Deformation twinning is an important mode of plastic deformation in g(TiAl) based titanium aluminide alloys. The mechanism apparently compensates for the lack of independent slip systems that can operate simultaneously at given stress and, thus, plays an important role in alloy design strategies for mitigating the problems associated with the poor damage tolerance of the material. In spite of the significant progress that has been achieved in this field our understanding is still in many ways imperfect. To some extend this is due to the atomic scale of the processes and the difficulties associated with the complexity of defect structures and constraint stresses that are developed in heavily twinned material. This imbalance of information is addressed in the present paper by a transmission electron microscope (TEM) study of twin structures, utilising high resolution imaging techniques. Consideration will be given in separate sections to the following topics. The major areas of the study are: (i) twin nucleation and propagation, (ii) effects of solutes and precipitates on the kinematics and dynamics of twin propagation, (iii) association of mechanical twinning and fracture.

1:45 PM S7.2
TEM Characterisation of Fatigued TiAl-based Alloys.
Hui Jiang[1], Dawei Hu[2] and Ian Jones[3]; [1]Department of Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom; [2]Department of Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom; [3]Department of Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom.

The fatigue properties of TiAl-based alloys have been studied extensively over the past two decades. However, detailed microstructural examination by TEM of polycrystalline TiAl-based

alloys after fatigue testing is very limited. In this paper we report on the TEM characterisation of fatigued Ti44Al8Nb1B with fully lamellar microstructure (with not more than 2% GB gamma grains) and near lamellar microstructure (with about 12% GB gamma grains). These underwent testing at room temperature at 600 and 500MPa respectively with a stress ratio R= 0.1 and a frequency of 82Hz. The failed testpieces were examined using TEM in order to characterise their micro-deformation behaviour via dislocations density and slip systems in the different gamma constituent components of the lamellar microstructure. Dislocation densities and slip systems have been correlated with the orientations of the gamma components with respect to the stress axis. The results are explored with a view to understanding the initial cracking of the lamellar microstructures and the possible effect of grain boundary gamma grains on the cracking behaviour.

2:00 PM S7.3
Impact Properties of Hot-Worked Gamma Alloys with BCC β-Ti Phase. Kentaro Shindo[1], Toshimitsu Tetsui[2], Toshiro Kobayashi[3], Shigeki Morita[3], Satoru Kobayashi[4] and Masao Takeyama[5]; [1]Nagasaki Research & Development Center, Mitsubishi Heavy Industries, LTD., Nagasaki, Nagasaki, Japan; [2]Nagasaki Research & Development Center, Mitsubishi Heavy Industries, LTD (Present Department : Tohoku University), Nagasaki, Nagasaki, Japan; [3]Department of Production Systems Engineering, Toyohashi University of Technology, Toyohashi, Aichi, Japan; [4]Department of Metallurgy and Ceramics Science, Tokyo Institute of Technology (Present Department : MPI), Meguro-ku, Tokyo, Japan; [5]Department of Metallurgy and Ceramics Science, Tokyo Institute of Technology, Tokyo, Megro-ku, Japan.

Impact damage behavior of a hot-forged TiAl alloy with a composition of 42∼44Al-5∼10X:X=V,Mn(at%), consisting of lamellar, g and b grain of which the hot workability was improved by introducing b phase, has been Investigated using an instrumented Charpy impact test, tensile test at high strain rate and foreign object attack test. In instrumented Charpy impact test the absorbed energies for crack initiation and propagation were measured, and the effect of microstructure on the absorbed energies has been analyzed, by paying attention to the grain size, interlamellar spacing and lamellar area fraction The results were also compared with those from the alloys with fully-lamellar structure (FL), nearly-gamma structure (NG) and equiaxed grain structure (EG). The absorbed energy for crack initiation is much larger than that for the crack propagation. The impact properties of the hot-forged TiAl alloy are superior to those of the alloys with various microstructures. The energy for crack initiation is almost comparable to that of the alloy with EG structure and greater than those of the others, whereas the energy for crack propagation is the greatest among others although the value is almost equal to that for the alloy with FL structures. The energy for crack initiation of the forged alloy depends strongly on the microstructure factors. The value increases with reduction of both grain size and interlamellar spacing although the grain size effect is more obvious than that of the lamellar spacing. However, the value does not necessarily increase with increase in the lamellar area fraction, and the suitable lamellar area fraction is found to be about 70%. These microstructure factors including the fraction of bcc b-Ti phase can easily be controlled by processing route for hot-forged materials, indicating that substantial improvement of toughness should be possible. In tensile test at high strain rate, the dependence of strain rate of hot-extruded TiAl alloy is obtained and compered with that of Nikel based superalloy, Inconel713C. In the renge of strain rate from 4.0*10-3 to 1.7*104(s-1), tensile strength of hot-extruded TiAl alloy increases with increase in the strain rate, but that of Inconel713C decreases. Then, Using impact resistance of TiAl alloy at the low strain rate impact test like Charpy impact test, it is possible to assessed impact resistance at the high strain rate like foreign object attack in the turbine on the safty side. In foreign object attack test with taper plate specimen modified turbine blade and brass ball as foreign object, the relation between impact damege and thickness of specimen at attack point is investgatied. A limite of impact energy, at which there isnf t a crack on buck of attack point, is obtained with each thickness about hot-forged TiAl alloy,42Al-5Mn. Therefore, the method of improvement of tughness and assessment of impact resistance of TiAl alloy is showen in this study.

2:15 PM S7.4
Effect of Long-Period Superstructures on Plastic Properties in Al-Rich TiAl Single Crystals. Nakano Takayoshi[1], Koutaro Hayashi[1], Yukichi Umakoshi[1], Yu-Lung Chiu[2] and Patrick Veyssiere[2]; [1]Department of Materials Science and Engineering, Graduate School of Engineering, Osaka University, Suita, Osaka, Japan; [2]Laboratoire d Etude des Microstructures, CNRS-ONERA, Chatillon cedex, France.

In Al-rich TiAl crystals, some long-period superstructures appear depending on the annealing temperature and Al composition. Among them, the Al_5Ti_3 and $h-Al_2Ti$ superstructures contain pure Al (002) layers as in the $L1_0$ matrix structure, alternating with Ti (002) layers exhibiting an ordered arrangement of excess Al atoms. In single crystals with compositions ranging from Ti-54.7at.%Al to Ti-62.5at.%Al annealed at 1473K, the Al_5Ti_3 long-period superstructure embedded in the L10 matrix develops with increasing Al concentration to finally transform fully into $h-Al_2Ti$ at Ti-62.5at.%Al. The long-period superstructures affect the plastic behavior and deformation microstructure. The CRSS for the 1/2<110] ordinary slip, for example, increases abruptly with development of the Al_5Ti_3 ordering. Dislocations with 1/2<110] Burgers vector group into fourfold configurations to avoid forming APBs in the superstructure. The CRSS for slip in the <110] direction further increases with the formation of the $h-Al_2Ti$ particles in the $L1_0$ matrix phase at Ti-62.5at.%Al. By contrast, the Al_5Ti_3 single-phase single crystal that results from further annealing of Ti-62.5at.%Al at 1023K for 48h, exhibits a CRSS significantly lower than that of the two-phase alloy with same alloy content. <101] superlattice dislocations are primarily activated under both [210] and [1 1 8.6] load axes, independent of the Al concentration, but the dislocation microstructure strongly depended on load orientation and Al composition. The frequency of the decomposed and dissociation reactions of <101] superlattice dislocations is closely related to the degree of development of the Al_5Ti_3 phase and the type of leading partials.

2:30 PM S7.5
TEM analysis of long-period superstructures in TiAl single crystal with composition-gradient. Satoshi Hata[1], Kohjiro Shiraishi[1], Masaru Itakura[1], Yoshitsugu Tomokiyo[1], Noriyuki Kuwano[2], Takayoshi Nakano[3] and Yukichi Umakoshi[3]; [1]Department of Applied Science for Electronics and Materials, Kyushu University, Fukuoka, Japan; [2]Art, Science and Technology Center for Cooperative Research, Kyushu University, Fukuoka, Japan; [3]Department of Materials Science and Engineering and Handai Frontier Research Center, Osaka University, Osaka, Japan.

The microstructure formation in TiAl alloys with Al-rich compositions is complicated and not well understood. This is due to the fact that various long-period superstructures are formed depending on Al concentrations and annealing conditions. In order to study phase relationships and formation mechanisms of the long-period superstructures in wide ranges of Al concentration, the present authors attempted to make a TiAl single crystal with a composition-gradient. After dipping a Ti-54.7 at% Al single crystal into molten Al at 1507 K for 5 min, a reacted area with a composition-gradient from 54.7 to 75 at% Al was formed at the surface of the single crystal. Transmission electron microscopy (TEM) observations revealed that the following long-period superstructures were formed sequentially in the composition-gradient area: short-range order (SRO), h-Al_2Ti, one-dimensional antiphase domain structure (1d-APS) and Al_3Ti ($D0_{22}$). The SRO structure transforms into Al_5Ti_3 superstructure after subsequent annealing at 973 K. All the superstructures except Al_3Ti have clear orientation relationships with the $L1_0$ matrix. The fact is explained in terms of ground state structures in a binary alloy system that are defined using effective pairwise atomic interactions. It was also revealed that microstructures of the h-Al_2Ti and 1d-APS domains depend on the composition-gradient as well as the Al concentrations. Such a dependence of the microstructures suggests that anisotropic diffusion processes and a subsequent formation of strain fields in the $L1_0$ matrix influence the domain growth of the long-period superstructures.

2:45 PM S7.6
Atomisitic Structure of the TiAl/ Ti_3Al Interface Observed During Massive Transformation. William Reynolds and Diana Farkas; Materials Science and Engineering, Virginia Tech, Blacksburg, Virginia.

Empirical interatomic potentials were used to simulate the atomic structure of an ordered TiAl/ Ti_3Al interface formed during massive transformation. The exact orientaion relashinship observed in experiments was generated and the minimum energy configuration was obtained using molecular statics simulations. The observed configuration presents edge to edge matching of atomic sites along one direction and it is shown that this matching is indeed maintained in the relaxed computer simulated structure. The effects of various deviations of this one dimensional matching orientation of the interface energy and structure are discussed.

3:15 PM S7.7
Influence of Micro-alloying on Oxidation Behavior of TiAl. Michiko Yoshihara[1] and Shigeji Taniguchi[2]; [1]Mechanical Engineering and Materials Science, Yokohama National University, Yokohama, Japan; [2]Materials Science and Processing, Osaka University, Suita, Japan.

TiAl-based alloys have attractive properties as light weight

heat-resisting material. Numerous engineering alloys have been developed for structural applications in automotive and aerospace components. The alloys thus developed contain at least several alloying elements that may optimize thermally stable microstructures and/or improved high temperature mechanical properties. However, the influence of alloying element on oxidation behavior has not been well clarified yet. In the present study, the influence of a wide range of elements on oxidation behavior of TiAl was investigated by micro-alloying using ion implantation. The ion implantation was carried out with doses of 10^{19} to 10^{21} ions/m^2 at acceleration voltages of 40 to 340kV. The oxidation resistance was assessed by cyclic oxidation test with temperature varying between room temperature and 1200K, in a flow of purified oxygen under atmospheric pressure. The influence can be classified into a few groups according to their effect. (1) Implantation of beta-phase stabilizing elements, Nb, Mo, Ta and W, improves the oxidation resistance significantly. Formation of a protective Al_2O_3 layer through beta phase formed in modified zone, which was confirmed by TEM observation, and reduced growth rate of TiO_2 by doping effect are responsible for the effect. Fe also forms beta-phase, however the improvement is limited because of the absence of doping effect. (2) Halogen elements, F and Cl, are similarly effective to improve the oxidation resistance by forming convoluted Al_2O_3 scales, under which adherent Al_2O_3 scales remained. Preferential reaction of Ti with the halogen elements seems responsible for the results. (3) Al and Si show limited improvement, while P shows good result. The doping effect seems to be predominant for the improvement by P. (4) Implantation of Se and Ag enhances the oxidation owing to Al depletion in the modified layer. (5) B, C, N, Mg, Ar, V, Cr and Zr are ineffective for the improvement.

3:30 PM S7.8
Creep of TiAl Alloys at 750°C Under Moderate Stress.
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The present paper presents a study of creep of two Ti-48Al-2Cr-2Nb alloys processed by cast and powder metallurgy routes at 750°C under 150 MPa and 80 MPa, two conditions close to the operating conditions in turbine engines and leading to identical creep rates ($10^{-8}s^{-1}$). Creep tests were conducted to measure the creep properties and to determine the internal stress and the activation parameters. The deformation microstructures of samples crept up to 0.5 and 2% were subsequently investigated in a transmission electron microscope (TEM) to determine the deformation mechanisms responsible for primary and secondary creep. Creep curves exhibit the usual three stages. The primary stage is more extended for the near lamellar microstructure of the as-cast alloy as compared to the powder metallurgy alloy with a duplex microstructure. The secondary stage is very short. In these two alloys, stress jumps provide identical values of the activation parameters. Furthermore, these values are constant all along the curve, namely in the primary and secondary stages. Internal back stress measured by strain change dip tests is higher in the as-cast alloy than in the powder metallurgy alloy. TEM observations show that ordinary dislocations are predominantly active and can be separated in two groups. Dislocations in the first group are elongated along their screw orientation, anchored at many points and moving by glide. Type 2 ordinary dislocations are moving by a mixed climb mechanism for which the elementary process is nucleation and propagation of jog pairs. The deformation microstructure is formed in majority by type 2 dislocations, especially after primary stage. From these experimental results, creep is found to be controlled by this mixed climb mechanism on the basis of the good consistency evidenced with the values of the activation parameters. Dislocation glide is activated in some localised areas to relax high local stresses. In addition, the better resistance of the as-cast alloy is due to shorter mean free path for the moving dislocations. Finally, the amplitude of the primary stage appears to be correlated to the amount of internal stress. This stage is thus interpreted as a stage during which the strength of the microstructure is homogenised by the hardening of soft area through the building of an internal stress.

3:45 PM S7.9
Microstructure-Property Relationships of two Ti_2AlNb-based Intermetallic Alloys: Ti-17Al-33Nb and Ti-22Al-28Nb(at%).
Dingqiang Li, Christopher J. Cowen and Carl J. Boehlert; School of Engineering, Alfred University, Alfred, New York.

For Ti_2AlNb intermetallic alloys, which depending on composition and processing treatment may contain any combination of the ordered orthorhombic (O), ordered hexagonal (α_2), or ordered or disordered body centered cubic (BCC) phases, microstructure is of critical importance to the mechanical properties. It has been established that the O phase tends to provide creep resistance while the BCC phase tends to provide processability and ductility. Yet these phases have shown compatibility through slip transmission across their interface boundaries and their orientation relationship which evolves from their phase transformations. This is one reason why two-phase O+BCC microstructures can exhibit a more attractive combination of room temperature (RT) and elevated temperature properties (such as tensile, creep, and fatigue strength and tensile ductility), which are important for structural applications within the biomedical, sports and recreational, and aerospace industries, than other intermetallic and non-intermetallic Ti alloys. However, shortcomings exist in the understanding of microstructure-property relationships of O+BCC Ti_2AlNb alloys. In order to address some of these shortcomings, Ti-17Al-33Nb and Ti-22Al-28Nb(at.%) alloys were processed into sheets, using pancake forging and hot-pack rolling, and evaluated in tension (RT and 650°C), creep (650-710°C), and fatigue (RT) and the properties and deformation behavior were related to microstructure. Some of the microstructural features evaluated were grain boundary character distribution, grain size, phase volume fraction, and morphology. The Al content was important to strength and elongation-to-failure (ϵ_f), where the higher Al content in Ti-22Al-28Nb lead to greater tensile and creep strengths, lower ϵ_f values, and brittle fracture response. However, the RT strengths of the Ti-17Al-33Nb, which always exhibited ductile failure (ϵ_f>8%) due to larger BCC phase volume fractions than for Ti-22Al-28Nb, were adequate for structural applications and always greater than 800MPa. The creep stress exponents, activation energies, and deformation characteristics suggested that at low stresses grain boundary sliding may be active while at higher stresses dislocation creep is probable. Increased lath O-phase volume fractions, which resulted from increased solution treatment temperature (i.e. larger prior-BCC grain sizes) followed by aging, resulted in significantly better creep resistance. The fatigue S/N behavior indicated that both of these alloys exhibit fatigue lives comparable or superior to that of Ti-6Al-4V(wt.%). Overall, the results of this study confirm that lath O+BCC microstructures outperform equiaxed O+BCC microstructures with respect to elevated temperature properties. Combining the creep observations with the tensile response, the Ti-17Al-33Nb lath O+BCC microstructure exhibited the more attractive combination of properties for structural application.

4:00 PM S7.10
Increase in Gamma/Alpha2 Lamellar Boundary Density and its Effect on Creep Resistance of TiAl Alloys.
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Stability of their lamellar microstructure is crucial for creep resistance of TiAl alloys at high temperatures, but degradation of the lamellar microstructure is unavoidable. Coarsening of lamellar spacing and spheroidization of lamellae are the major degradation events, and both of them occur by means of lamellar boundary migration. The lamellar microstructures of TiAl alloys contain four types of boundaries. Among the four types, gamma/alpha2 boundary has the highest stability, and sustains the original lamellar microstructure for longer duration. In the present study it will be discussed how to raise density of the gamma/alpha2 boundaries for improving the microstructural stability. The volume fraction of alpha2 phase increases during heating up to a temperature in alpha+gamma dual phase field, and the excess alpha2 phase transforms back to gamma phase during cooling. New gamma/alpha2 boundaries may be added by the heat treatment. The driving force for the gamma to alpha transformation should be large enough for precipitating a new aplha2 laths, but too large driving force may introduce apha2 laths being not parallel to the original gamma/alpha2 boundaries. A Ti-48mol%Al alloy was heated to 1550K at several heating rate. The density of gamma/alpha2 lamellar boundaries increased with increasing the heating rate, and creep resistance was confirmed to increase by the addition of the new gamma/alpha2 boundaries. On the other hand, too first heating rate resulted in unstable lamellar microstructure due to its less aligned lamellar microstructure.

4:15 PM S7.11
Effect of Long-Term Aging and Creep Exposure on the Microstructure of TiAl-Based Alloy for Industrial Applications.
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The effect of long-term ageing and creep exposure on the microstructural stability of a cast ABB-2 alloy with nominal chemical composition Ti-46Al-2W-0.5Si (at.%) was studied. Before ageing and creep testing the investigated investment cast components in the form of plates, bars and gas turbine blades were subjected to heat treatments. The ageing experiments were performed at temperatures ranging from 973 to 1073 K for various times from 10 to 14000 h in air. Constant load tensile creep tests up to 25677 h were performed at applied stresses ranging from 150 to 400 MPa and at temperatures 973-1123 K. The microstructure of the specimens was characterized by optical microscopy, scanning electron microscopy and transmission

electron microscopy before and after ageing and creep deformation. Before ageing and creep testing the microstructure of the samples was nearly lamellar or duplex. The nearly lamellar microstructure consisted of $\alpha 2$(Ti3Al) and γ(TiAl) lamellae, coarse B2 (ordered Ti-based solid solution) particles and small volume fraction of the γ-phase formed along the grain boundaries. The duplex microstructure consisted of lamellar, feathery and γ-rich regions. Microstructural analysis revealed that the lamellar regions are composed of $\alpha 2$ and γ lamellae, coarse B2 particles and fine needle-like B2 precipitates. The feathery regions contain γ-matrix with $\alpha 2$, B2 and Ti5Si3 particles. Coarse Ti5Si3 particles are identified within the γ-rich regions. During ageing of the samples with duplex initial microstructure, the $\alpha 2$-phase in the lamellar and feathery regions transforms to the γ-phase and fine needle-like B2 precipitates. The microstructural instabilities lead to a softening of the alloy. The measured time exponents and activation energies for softening are discussed from the point of diffusion-controlled transformations and coarsening of the coexisting phases. A possible effect of such microstructural changes on softening kinetics is analyzed. The softening produced at designed operating temperature of 973 K is very slow and cannot affect significantly mechanical properties of the investment cast components during their long-term service. Special attention is paid to the phase analysis and deformation structure of the crept specimens. Significant differences of one order of magnitude in minimum creep rate and time to fracture of the specimens with different initial microstructure (nearly lamellar or duplex) are explained on the basis of deformation structure and microstructural changes affecting the creep deformation processes of the material. The microstructural changes and softening have only negligible effect on the creep strength in the temperature range of interest for industrial applications. Fine precipitates formed due to microstructural instabilities along the $\alpha 2/\gamma$ lamellar interfaces and within the γ-rich regions are effective obstacles to dislocation motion during creep, which enhance the creep strength.

4:30 PM S7.12
Creep Behavior and Microstructural Stability of Ti-46Al-9Nb Material with Different Microstructures.
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In this paper the creep behavior and the microstructural stability of high Nb containing Ti-46Al-9Nb (in at%) sheet material were investigated in the temperature range of 700°C to 800°C. The study involves three different types of microstructure, namely fully lamellar with narrow lamellar spacing, duplex and massively transformed (massive transformation was obtained by fast cooling from the α phase field). Short-term creep experiments at 700°C and 225 MPa confirmed that the fine lamellar microstructure with narrow lamellar spacing exhibits a much higher creep resistance when compared to massively transformed and duplex. During long-term creep tests up to 1500 hours stress exponents (in the range of 4.4 to 5.8) and activation energies (of about 4 eV) have been estimated by means of load and temperature changes, respectively. Both, stress exponents and activation energies suggest that under the applied conditions diffusion assisted climb of dislocations is the dominant deformation mechanism. Furthermore, the beneficial influence of a heat-treatment which stabilizes the fully lamellar microstructure on creep has been proven: At 800°C and 150 to 225 MPa significantly reduced primary and secondary creep rates and prolonged time-to-failure were observed compared with samples without such an additional heat treatment. The thermal stability of the different microstructures under various creep conditions has been analyzed by means of back scatter electron microscopy and X-ray diffraction. Our investigations revealed considerable stress and temperature induced microstructural changes which are reflected in the dissolution of the α 2 phase accompanied by precipitation of new Al- as well as Ti/Nb - rich phases situated on the grain boundaries. It was shown that especially the duplex microstructure is prone to such microstructural instabilities.

4:45 PM S7.13
Internal Friction of a High Nb Gamma TiAl Alloy With Different Microstructures.
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An intermetallic Ti-46Al-9Nb (at%) alloy with different microstructures (fine-grained equiaxed, coarse grained fully lamellar, and duplex) was studied by internal friction measurements at 300K to 1280K using different frequency ranges: (I) 0.01 Hz to 10 Hz and (II) around 2 kHz. The loss spectra in range I show (i) a loss peak of Debye type at T ? 1000K which is only present in fully lamellar and duplex samples; (ii) a high-temperature damping background above ? 1100 K. The activation enthalpies determined from the frequency shift are H = 2.9 eV for the loss peak and H = 4.2 - 4.3 eV for the high-temperature damping background. The activation enthalpies for the viscoelastic high-temperature damping background agree well with values obtained from creep experiments and are in the range of those determined for self-diffusion of Al in TiAl. These results indicate that both properties (high-temperature damping background and creep) are controlled by volume diffusion assisted climb of dislocations. The loss peak is assigned to diffusion-controlled local glide of dislocation segments which, as indicated by transmission electron microscopy observations, are pinned at lamella interfaces. From measurements of the eigenfrequencies in frequency range II the variation of Youngs modulus was determined in the temperature range of 300 K to 1200 K. The modulus decreases only by about 15% proving that gamma TiAl-based alloys retain their elastic stiffness up to high temperatures. The Youngs modulus of Ti-46Al-9Nb is significantly higher when compared to Ti-based alloys. An influence of microstructure on elastic modulus was not found.