SYMPOSIUM N

High-Temperature Ordered Intermetallic Alloys IX

November 27 – 29, 2000

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* Invited paper

8:30 AM *N1.1
RECENT ADVANCES IN DEVELOPMENT AND PROCESSING
OF TITANIUM ALUMINIDE ALLOYS. Helmut Clemens, Fritz
Appel, Institute for Materials Research, GKSS Research Centre,
Geesthacht, GERMANY.

The mechanistic understanding of damage and failure processes in
two-phase titanium aluminide alloys is critically assessed. Based on
these results metallurgical techniques are proposed and evaluated
which apparently are capable to extend the service range of
gamma-base alloys. Implementation of strengthening mechanisms due
to large Nb additions and perovskite precipitates lead to well
balanced properties, which at room temperature are manifested by
strength levels in excess of 1GPa and appreciable tensile ductilities in
the range of 1-2%. The current achievements in forging, rolling and
extrusion of gamma-base alloys on industrial scale are presented.
Finally, prototype components are shown and the results derived from
component tests are discussed.

9:00 AM N1.2
THE DEVELOPMENT OF DUCTILE AND CREEP RESISTANT
TiAl-BASE ALLOYS. S.C. Deevi, W.J. Zhang, Research Center,
Chrysalis Technologies Incorporated, Richmond, VA; C.T. Liu, Metals
& Ceramics Division, Oak Ridge National Laboratory, Oak Ridge,
TN; B.V. Reddy, Research Center, Chrysalis Technologies
Incorporated, Richmond, VA.

The maximum service temperatures of TiAl-base alloys are limited by
their oxidaion and creep resistances. It is necessary to enhance the
room temperature ductility, and high temperature creep and
oxidation resistances of TiAl-base alloys for a broad range of
applications. In addition, we also need to study the physical
properties of TiAl-base alloys for the designers. In this paper, we
present our recent progress in the development of new TiAl-base
alloys. The alloys exhibit high RT ductility ($\sim$4%), high temperature
strength ($\sim$700MPa) and excellent creep resistance and relatively
good oxidation resistance. This alloy is also promising for sheet
fabication. The physical properties of the alloys were meausred and
compared with superalloys, iron aluminides and other TiAl-base
alloys, including thermal conductivity, electrical resistivity, coefficient
of thermal expansion, and specific heat. The potential applications of
this alloy in aerospace and civil inductries were discussed.

9:15 AM N1.3
CREEP BEHAVIOR OF INVESTMENT CAST GAMMA Ti-Al
ALLOYS. K. Sadananda, C.R. Feng, Physical Metallurgy Branch,
Materials Science and Technology Division, Naval Research
Laboratory, Washington, DC.

Creep behavior of Ti-Al-Cr based gamma TiAl alloys with the
addition of Nb, Ta, Mo and Zr is analyzed to evaluate the effect of
composition, microstructure and its stability, grain size are examined
in terms of Larson-Miller plots. The results indicate specimens with
high Al-content or low Ti- content exhibit better creep resistance. In
general alloying with Cr, Nb and Ta improved creep resistance while
the roles of Mo, Zr are unclear. As expected the grain size played a
major part with increasing creep resistance with increasing columnar
grain size. Stability of initial microstructure played a major role in
creep rates and the composition has strong influence on the stability
of the microstructure. The results are analyzed on the basis of current
understanding of the creep behavior of Ti-Al alloys.

9:30 AM N1.4
CREEP BEHAVIOR AND MICROSTRUCTURAL STABILITY OF
LAMELLAR γ-TiAl (Cr, Mo, Si, B) WITH EXTREMELY FINE
LAMELLAR SPACING. W. Schillinger, Materials Science and
Technology, Technical University of Hamburg Harburg, Hamburg,
GERMANY; D. Zhang, G. Dehm, Max-Planck-Institut für
Metallforschung, Stuttgart, GERMANY; A. Bartels, Materials Science
and Technology, Technical University of Hamburg Harburg, Hamburg,
GERMANY; H. Clemens, Institute for Materials Research,
Geesthacht-Research Center, Geesthacht, GERMANY.

γ-TiAl (Cr, Mo, Si, B) specimens with two different fine lamellar
microstructures were produced by vacuum arc melting followed by a
two stage heat treatment. The average lamellar spacing was
determined to be 25 nm and 200 nm respectively. Creep tests at
700°C showed a very strong primary creep for both samples. After
annealing for 24 hours at 1000°C the primary creep for both materials
is significantly decreased. The steady state creep for the specimens
with the wider lamellar spacing appears to be similar to the creep
behavior prior to annealing while the creep rate of the material with
the previously smaller lamellar spacing is significantly higher. Optical
microscopy and TEM-studies show that the microstructure of the
specimens with the wider lamellar specing is nearly unchanged
whereas the previously finer material was completly recrystallized to a
globular microstructure with a low creep resistance. The dissolution of
the fine lamellar microstructure was also observed during creep tests
at 800°C as an acceleration of the creep rate. TEM investigations give
the indication that dynamic recristallisation occured. It is concluded
that extremely fine lamellar microstructures come along with a very
high dislocation density which causes the observed high primary
creep. The microstructure has a composition far away from the
thermodynamical equilibrium which leads to a dissolution of the
structure even at relatively low temperatures close to the intended
operating temperature of γ-TiAl structural parts, thus this limits the
benefit of fine lamellar microstructures on the creep behavior.

10:15 AM N1.5
THE INFLUENCE OF THE TEXTURE ON THE CREEP
BEHAVIOR OF γ-TiAl SHEET MATERIAL. Arno Bartels, Wolfram
Schillinger, Materials Science and Technology Dept., Technical
University Hamburg-Harburg, Hamburg, GERMANY; Anita
Chatterjee, Inst. f. Metallkunde, Universitat Stuttgart, Stuttgart,
GERMANY; Helmut Clemens, GKSS-Research Center, Geesthacht,
GERMANY.

The sheet material of Ti-47.5at%Al-4at%(Cr,Nb,Ta,B) was rolled at
Plansee AG in Reutte/Austria. After primary annealing in order to
flatten the sheets a strong modified cube texture is found by x-ray
diffraction measurements. The c-axes of the tetragonal unit cells in
the grains are aligned with the transverse direction in the sheets. This
texture causes anisotropies of the yield stress which depend on the
temperature. Especially in the range 700°C to 800°C the yield stress
is higher in transverse direction than in rolling direction. According to
this anisotropy of yield the creep resistance is improved in transverse
direction. Heat treatments with different subsequent cooling rates
were performed in order to obtain lamellar microstructures with a
different spacing of lamellae. Creep experiments exhibit an increase of
the creep resistance which is highest after fast cooling. A small
anisotropy is still observed, but now the rolling direction has a slightly
higher creep resistance. The texture measurements show no longer an
alignment of c-axes after the heat treatment in the α-phase field, but
a weak {110}-fiber texture in rolling direction occurs. Modeling on the
base of single crystal yield surfaces performed with the LAPP-Code
can explain, how the anisotropy of creep is caused by the measured
textures in primary annealed as well as in the lamellar microstructure.

10:30 AM N1.6
CREEP IN TiAl ALLOYS: A STUDY BASED ON MODIFIED-
JOGGED SCREW MODEL. G.B. Viswanathan, and M.J. Mills,
Department of Materials Science and Engineering, The Ohio State
University, Columbus, OH.

The objective of this paper would be to revisit the present status of
the high creep of TiAl-alloys with particular reference to models
based on the motion of jogged screw dislocations. Models based on
this have been previously attempted to describe the creep in pure
metals and alloys. Now, in light of emerging new experimental
evidence, this model, with suitable modifications, appear to be
appropriate for the case of creep in TiAl based intermetallic alloys.
High temperature creep experiments have been conducted in the
power law regime for Ti-48Al alloy. Deformation structures seem to
indicate that the creep is controlled by the motion of jogged-screw
dislocations of the type $\mathbf{b}$=1/2<110] in TiAl intermetallic alloy. It will
be shown that a relatively minor, yet physically reasonable,
modification of the original jogged-screw model on produces a stress
dependence which is in better agreement with experiments. Recent
findings on stress dependence on the jog spacing and jog heights and
the corresponding implications of these parameters on the modified
model are discussed, as are some of the critical measurements that
will be necessary to verify this modified model.

10:45 AM N1.7
AN INVESTIGATION OF THE EFFECTS OF TEMPERATURE
ON FATIGUE CRACK GROWTH IN A CAST LAMELLAR XD$^{\text{TM}}$
Ti-47Al-2Mn-2Nb 0.8vol.%TiB$_2$ ALLOY. J. Lou, C. Mercer and W.O.
Soboyejo, The Princeton Materials Institute and The Department of
Mechanical and Aerospace Engineering, Princeton University,
Princeton, NJ.

This paper presents the results of study of the effects of temperature
on fatigue crack growth in a cast lamellar Ti-47Al-2Mn-2Nb
0.8vol.%TiB$_2$ gamma titanium aluminide intermetallic. The effects of
temperature on fatigue crack growth in air are examined at 25, 450
and 700°C. Slower fatigue crack growth rates at 700°C (compared to
those at 450°C) are also explained by crack/microstructure inter-
actions, oxide-induced wedging, and possible elevated-temperature

creep phenomena. Faster fatigue crack growth rates at 450°C are attributed to the absence of oxide-induced closure and the effects of crack-tip deformation. The implications of the results are discussed for potential applications of cast XD^{TM} gamma alloys in the intermediate-temperature regime between 450 and 700°C.

11:00 AM N1.8
TWINNING IN CRACK TIP PLASTICITY OF TWO-PHASE TITANIUM ALUMINIDES. Fritz Appel, Institute of Materials Research, GKSS Research Centre Geesthacht, Geesthacht, GERMANY.

Intermetallic titanium aluminides based on gamma TiAl are prone to cleavage fracture on low index lattice planes. Unfavourably oriented grains may therefore provide easy crack paths so that the cracks can rapidly grow to a length which is critical for failure. Stable crack growth requires the plastic zone to keep with the cleavage crack, which is difficult if the mobility and multiplication rate of the dislocations are low. In this respect mechanical twinning might be an important mechanism, because the growth rate of the twins is often an appreciable fraction of the elastic wave velocity. The present study describes conventional and high-resolution electron microscope observations of crack tip plasticity in two-phase titanium aluminides. Crack tip shielding due to mechanical twinning was recognized as toughening mechanism, which occurs at the atomic scale and apparently is capable to stabilize partly growing cracks. The potential of the mechanism will be discussed in the context of novel design concepts for improving the strength properties of gamma-base titanium aluminide alloys.

11:15 AM N1.9
AN IN-SITU STUDY OF CRACK PROPAGATION IN BINARY LAMELLAR TiAl. Ping Wang and K.S. Kumar, Division of Engineering, Brown University, Providence, RI.

A binary Ti-46% Al was obtained in the cast and isothermally forged condition, and suitably heat treated to produce a fully lamellar microstructure. Further heat treatments were conducted to produce specimens with a large grain size (3-5 mm) from which sub-scale compact tension specimens (19.8 mm x 19.05 mm x 1-1.3 mm) were electrodischarge machined that were single-colony thick but polycolony areally. These were fatigue precracked and tested to failure in a scanning electron microscope equipped with a loading stage. The fracture process on the specimen surface was followed by taking still photographs of the near crack-tip region at various stages of loading, as well as by documenting the entire fracture process by video photography. The K resistance curve was obtained. Observations on the surface of such specimens more accurately represent the bulk and enable a correlation of fracture resistance with microstructural features such as lamellar misorientation (in-plane and through-thickness) and colony boundary inclination to an advancing crack.

11:30 AM N1.10
EFFECTS OF CONSTRAINT-INDUCED NORMAL STRESS ON THE FAILURE OF NOTCHED TITANIUM ALUMINIDES. Jorge Milke, Jack Beuth, Dept of Mechanical Engineering, Carnegie Mellon Univ; Nicholas Biery, Dept of Materials Science and Engineering, Carnegie Mellon Univ; Huang Tang, Dept of Mechanical Engineering, Carnegie Mellon Univ.

Titanium aluminides are candidate materials for replacing nickel superalloys in aircraft engine components. In unnotched uniaxial tension tests, these materials typically experience plastic strains at failure near 1%, which places them in-between traditional definitions for ductile and brittle materials. The purpose of this study is to shed light on the appropriate failure criterion for these materials under multiaxial loading conditions (based on either the maximum equivalent plastic strain or the maximum normal stress). The material tested is a Ti-47.0Al-2.0Cr-1.9Nb alloy with a predominantly lamellar microstructure and approximately 20 - 25 vol. % equiaxed gamma grains. Cylindrical notched specimens are tested which experience elevated normal stresses in their interiors due to circumferential constraint during plastic deformation. Results are presented which quantify reductions in failure loads due to normal stress, compared to those predicted by a maximum equivalent plastic strain criterion. In order to properly interpret the experimental results, an accounting of notch strengthening effects must be included in the model predictions. Model and experimental results suggest that this TiAl alloy has some sensitivity to normal stress and a combined failure criterion is needed under multiaxial loading conditions. A fracture initiation and failure mechanism requiring a combination of normal stress and plastic straining is suggested that is consistent with observed features at fracture initiation sites.

11:45 AM N1.11
STRAIN-RATE DEPENDENCE OF THE BRITTLE-TO-DUCTILE TRANSITION TEMPERATURE IN TiAl. M. Khantha, V. Vitek and

D.P. Pope, Department of MS&E, University of Pennsylvania, Philadelphia, PA.

The brittle-to-ductile transition (BDT) and the strain-rate dependence of the brittle-to-ductile transition temperature (BDTT) has been recently investigated in single crystal TiAl (Ti-54.7% Al) [1]. It was found that the activation energy associated with the BDTT is 1.4 eV when the slip is dominated by ordinary dislocations and 4.9 eV when it is dominated by superdislocations. Despite this difference in the activation energies, the BDTT, while varying with the strain-rate remains in the same temperature range, viz., between 516-750C and 635-685C for ordinary and superlattice dislocations, respectively. We propose a new mechanism of the BDT that explains the important features of the transition and predicts the BDTT and its strain-rate dependence in TiAl. The massive dislocation activity which commences near the crack tip at the BDTT is modeled in terms of a strain-rate dependent mechanism of cooperative dislocation generation. In contrast to the large temperature-independent energy barrier associated with the thermal activation of individual dislocation loops, this process is marked by an activation barrier that decreases dramatically with temperature becoming zero at the critical temperature. The strain-rate dependence originates from the glide of pre-existing and thermally nucleated dislocations below the critical temperature. Depending on their relative contributions, the apparent activation energy associated with the BDTT is either equal to or larger than the activation energy for dislocation motion. This model also helps to explain why a high value of the activation energy is not always associated with correspondingly high values of the BDTT. The results are in good agreement with observations. This research was supported by U.S. Air Force Office of Scientific Research grant F49620-98-1-0245.
1. A.S. Booth and S.G. Roberts, Acta Mat. 45, 1045 (1997).

SESSION N2: TITANIUM ALUMINIDES II AND METAL SILICIDES I
Chairs: Haruyuki Inui and Joachim H. Schneibel
Monday Afternoon, November 27, 2000
Room 208 (Hynes)

1:30 PM *N2.1
A NEW ASPECT OF MICROSTRUCTURE CONTROL FOR GAMMA TiAl ALLOYS BASED ON THE PHASE DIAGRAMS. Masao Takeyama, Satoru Kobayashi, Akane Suzuki and Takashi Matsuo, Tokyo Institute of Technology, Dept. of Metallurgy and Ceramics Science, Tokyo JAPAN.

The mechanical properties of gamma alloys are very sensitive to the microstructure, and the microstructure control has been generally done using the decomposition of the high-temperature α-Ti phase along the pathway of $\alpha \to \alpha_2 + \gamma$. However, alloying creates new transformation pathways, such as $\alpha \to \beta + \gamma$ for example, which opens possibility for novel method of microstructure control using β-Ti phase. This paper first reviews our recent studies on the phase diagrams of Ti-Al-M (M: V, Nb, Cr, Mo) ternary systems at elevated temperatures. In any system, the three-phase coexisting region of $\beta + \alpha + \gamma$ present above 1473K changes to that of $\beta + \alpha_2 + \gamma$ as temperature lowers, with its location approaching to the Ti-Al binary edge. The change in phase equilibria is not just because of the second order phase transition of $\alpha \to \alpha_2$ ordering, but caused by a temperature invariant reaction of $\beta + \alpha \to \alpha_2 + \gamma$. The experimental evidence is presented and the cause of this reaction will be discussed in terms of the relative phase stability between α and α_2 phases. Based on these phase diagram studies, the microstructure evolution and formation mechanisms along the pathway of $\alpha \to \beta + \gamma$ are demonstrated. The decomposition of the α phase occurs by either (i) a eutectoid reaction or (ii) a two-step reaction through the precipitation of γ plates, depending on the supersaturation of the solute elements in the α phase, resulting eventually in a β/γ lamellar structure. In latter case, the β phase always forms at the α/γ interface. Some other reactions for microstructure control of gamma based alloys such as $\beta + \alpha \to \alpha_2 + \gamma$ and $\beta \to \alpha_2$ martensitic transformation will be discussed.

2:00 PM N2.2
EXPERIMENTAL AND THEORETICAL INVESTIGATIONS OF THE PHASE TRANSFORMATION IN Al-RICH TiAl INTERMETALLIC COMPOUNDS. Toshiyuki Koyama, Minoru Doi, Dept of MS&E, Nagoya Institute of Technology, Nagoya, JAPAN; Shizuo Naito, Gifu Shotoku Gakuen Univ, Faculty of Economics and Information, Gifu, JAPAN.

Recently, the Ti-Al system has been investigated as a next candidate of the high strength heat resistant materials. However, there are still remained a lot of uncertain points of the morphological stability of microstructure and the dynamics of the microstructure changes in this

alloy system. In the present work, we investigate microstructure changes experimentally to obtain a fundamental knowledge about the phase decomposition of the Al-rich γ-TiAl intermetallic compounds in the two phases region of γ-TiAl(L1$_0$) and Ti$_3$Al$_5$(I4/mbm), then the dynamics of the microstructure developments are analyzed by means of the computer simulation. When the volume fraction of the Ti$_3$Al$_5$ precipitates is low, the plate-shaped precipitate on the (001) plane of the matrix is observed at the early stage of the aging. These precipitates coarsen by the Ostwald ripening (sometimes encountered each other), and then become the complex shape having the {113} habit. On the other hand, the alloy composition (Al content) is increased, i.e., high volume fraction of the precipitates, the tweed-like structure including the very fine Ti$_3$Al$_5$ zone is observed at the beginning of aging. The Ti$_3$Al$_5$ particles encounter each other with progress of aging, finally the microstructure becomes the large layered structure with a zigzag-shaped interface. The direction perpendicular to the zigzag-shaped plane is {113}. We simulated these microstructure changes based on the Phase-field method. The morphology and the time dependence of the simulated microstructure are in good agreement with the experimental observations above mentioned. The computer simulation result indicates that the complex shape of the precipitate phase is mainly controlled by the elastic strain energy.

2:15 PM N2.3
A THREE-DIMENSIONAL PHASE FIELD MODEL FOR COMPUTER SIMULATION OF LAMELLAR STRUCTURE FORMATION IN γTiAl INTERMETALLIC ALLOYS. Youhai Wen, Dept of Materials Science and Engineering, the Ohio State University, Columbus, OH; Long-Qing Chen, Dept of Materials Science and Engineering, The Pennsylvania State University, University Park, PA; Peter M. Hazzledine, Air Force Research Laboratory, Materials and Manufacturing Directorate, AFRL/MLLM, WPAFB, OH; Yunzhi Wang, Dept of Materials Science and Engineering, the Ohio State University, Columbus, OH.

The γTiAl intermetallic alloys are the leading candidates for high-temperature structural materials because of their high specific mechanical strength and good oxidation resistance. Recent interest has been focusing on Ti-rich two-phase alloys that contain a small amount $\alpha_2(Ti_3Al)$ phase, forming a typical self-accommodating lamellar structure. The lamellar structure is what gives the alloys their outstanding combined properties of high-temperature strength and room-temperature ductility, but the processing rotes and heat treatment are still largely empirical and, as a result, a particular lamellar structure cannot be produced in a controlled fashion. In this presentation we describe a three dimensional phase field model developed for computer simulation of the lamellar structure formation in γTiAl alloys. The model takes into account the effect of coherency strain associated with the lattice rearrangement accompanying the phase transformation and the anisotropy in interfacial energy. Without any a priori assumptions on the transformation path and morphological evolution, the simulation studies based on the model have successfully predicted the essential features associated with the lamellar structures observed experimentally. For example, it is shown that the coherency strain accommodation is responsible for the formation of the lamellar structure. The neighboring lamellae of g phase are found to have either a twin or a pseudo-twin relationship, with the former being dominant. It is found that strain-induced interactions result in correlated nucleation which contributes to the formation of the twined lamellae. The lamellar thickness is determined by the interplay among the elastic strain energy, interfacial energy and bulk chemical free energy.

3:00 PM *N2.4
METAL-SILICIDE MICROLAMINATES FOR HIGH-TEMPERA-TURE APPLICATIONS: FABRICATION, STABILITY, AND PROPERTIES. T.P. Weihs, D. Van Heerden, Johns Hopkins University, Department of Materials Science & Engineering, Baltimore, MD; T. Foecke, National Institute of Standards and Technology, Metallurgy Division, Gaithersburg, MD.

Metal-silicide and metal-intermetallic alloys are currently being evaluated for use at high temperatures, beyond those presently attainable with nickel-based superalloys. While these alloys can be fabricated into several different composite geometries using casting, high-temperature extrusion, or physical vapor deposition, this presentation focuses on microlaminated composites that have been vapor deposited and therefore can be considered for use in advanced, thin-walled turbine blades. We will begin by considering the physical vapor deposition and high-temperature processing of metal-silicide and metal-intermetallic microlaminates. Critical issues such as contamination, microstructure, deposition defects, growth stresses, and residual stresses will be addressed. Next, we will review the chemical, phase, and microstructural stability of these layered composites at temperatures ranging from 1100°C to 1600°C. Breakdown mechanisms and their impact on mechanical properties

will be noted using examples from Nb/Nb$_5$Si$_3$, Nb/NbCr$_2$, and Nb/Nb$_3$Al systems. Finally, since the mechanical properties of these microlaminates are strongly dependent on their composite geometry, we will review the impact of layer thickness and volume fraction on the strength, toughness, and creep resistance of several different microlaminate systems.

3:30 PM N2.5
ANOMALOUS STRENGTHENING MECHANISM IN NbSi$_2$-BASED SILICIDE SINGLE CRYSTALS. Yukichi Umakoshi, Takayoshi Nakano and Masafumi Azuma, Osaka Univ., Graduate School of Engineering, Dept. of Materials Science and Engineering, Suita, Osaka, JAPAN.

Anomalous strengthening behavior in NbSi$_2$-based silicides with the C40 structure was examined. NbSi$_2$-based silicide single crystals containing various amounts of Mo were grown by a floating zone method. In compression tests, the temperature and strain rate dependence of yield stress were examined. The silicides deformed by $(0001) <1\bar{2}10>$-slip and the CRSS for the slip did not depend on orientation. Serrated flow in the stress-strain curves was often observed in the temperature range where yield stress showed a positive temperature dependence. The amplitude of sudden stress drop in the stress-strain curve depended strongly on deformation temperature strain rate and alloying elements. The anomalous strengthening is closely related to the formation of dragging atmosphere of substitutional impurity atoms around moving dislocations containing a SISF. To examine effect of the solute atmosphere, the amplitude of stress drop in specimens prestrained at various temperatures was investigated at 400°C. Some specimens were annealed at various temperatures for 1h after 1% prestraining at 600°C to know the effect of formation of dragging atmosphere on the motion of dislocations. Anomalous strengthening mechanism will be discussed focusing on formation of dragging atmosphere, effect of diffusion path, phase stability and interaction between moving dislocations and solute atmosphere.

3:45 PM N2.6
CREEP STUDIES OF THE MONOLITHIC PHASES IN Nb-SILICIDE IN-SITU COMPOSITES. B.P. Bewlay, M.R. Jackson, GE Research and Development Center, Schenectady, NY; C.L. Briant, A.W. Davis, G. Xaio, Division of Engineering, Brown University, Providence, RI.

Nb-silicide composites combine a ductile Nb-based matrix with high strength silicides, and they show great promise for aircraft engine applications. With appropriate combinations of alloying elements it may be possible to achieve the required balance of room temperature toughness and high temperature creep rate. Advanced alloys may contain several different intermetallics including silicides, Laves phases, and the boron rich T-2 phase. To understand the role of each phase on the creep resistance of these composites, we determined their individual creep rates and the dependence of creep rate on composition. To this end we have prepared monolithic alloys with compositions similar to the Nb-based solid solution and the intermetallic phases. We determined their creep rates under a constant compressive load at 1100 and 1200C. We found that the Nb-based matrix creeps readily at 1100C at stresses below 70 MPa. At 1100C the intermetallic phases had creep rates that were too low to be measured in a 24 hour test. At 1200C some of the intermetallics had measurable creep rates. These included the Laves phase with a composition of Nb-15Si-55Cr and the T-2 phase. A 5:3 silicide that contained only Ti,Nb, and Si also had a low but measurable creep rate. These results allow us to quantify the load bearing capability of the individual phases in the Nb-silicide based in-situ composites.

4:00 PM N2.7
THE EFFECT OF SILICIDE VOLUME FRACTION ON THE CREEP BEHAVIOR OF NIOBIUM-SILICIDE BASED IN-SITU COMPOSITES. B.P. Bewlay, M.R. Jackson, General Electric Co. R&D Center, Schenectady, NY; C.L. Briant, A.W. Davis, Brown University, Division of Engineering, Providence, RI.

This paper will describe the creep behavior in high-temperature niobium-silicide in-situ composites based on quaternary Nb-Hf-Ti-Si alloys. The creep behavior of composites generated from binary Nb-Si alloys and the effect of Hf and Ti additions will be described. The composites were tested in both compression and tension at temperatures up to 1200°C and stress levels in the range of 70 to 280 MPa. The effect of volume fraction of silicide and silicide chemistry on the creep behavior will be described. At high Nb-phase volume fractions the creep behavior is controlled by deformation of the (Nb) and as the volume fraction of silicide is increased the creep behavior is improved. However, at large silicide volume fractions (>0.7) damage in the silicide begins to degrade the creep performance. The creep rate has a minimum at a volume fraction of ∼0.6 silicide. The creep performance of the monolithic and silicide phases will also be

described. The sensitivity of the creep rate / damage accumulation in the composites will also be discussed.

4:15 PM N2.8
METASTABLE PHASE FORMATION IN Nb/Nb_5Si_3 COMPOSITES. David Van Heerden, Timothy P. Weihs, Johns Hopkins University, Dept. Materials Science and Engineering, Baltimore, MD; Timothy J. Foecke, National Institute of Standards and Technology, Metallurgy Division, Gaithersburg, MD.

Microlaminate and in-situ composites are now being developed to serve in future high-temperature turbine blades. These composites consist of a refractory metal that imparts room temperature toughness and an intermetallic phase that instills high temperature creep resistance. One of the most promising of these composite systems is $Nb-Nb_5Si_3$. This system is particularly attractive because the two phases remain in equilibrium up to 1660°C with relatively little Si solubility in the Nb layers at these temperatures (1.3at%). When annealing Nb/Nb_5Si_3 microlaminates at 1400°C, the two phases are stable as expected; the same is true for in-situ composites. However, a third phase appears when Nb/ Nb_5Si_3 microlaminates are annealed at 1500°C or 1600°C. The observed third phase is the non-equilibrium $L1_2$ Nb_3Si m'' phase and not the high temperature equilibrium Nb_3Si phase observed at temperatures exceeding 1660°C. The non-equilibrium Nb_3Si m'' phase forms predominantly within the Nb layers, in the vicinity of the microlaminate interfaces. Given this phase is likely to have a deliterious effect on the high temperature properties of the composites, it is important to understand the conditions that promote its formation. Post anneal XRD, SEM, and TEM investigations suggest that the metastable phase forms during cooling, precipitating from the supersaturated Nb. In-situ XRD studies support this hypothesis. Based on a knowledge of residual thermal stresses and phase densities, Nb_3Si would be stabilized by residual tensile stresses. This raises the following question: is the nucleation and growth of Nb_3Si m'' simply kinetically favored over Nb_5Si_3 or is it thermodynamically favored due to residual stresses and a reduction in elastic strain energy. The importance of this non-equilibrium phase formation will be discussed in light of structural applications of Nb-based, metal-silicide composites.

4:30 PM N2.9
MICROSTRUCTURES AND THERMOELECTRIC POWER OF THE HIGHER MANGANESE SILICIDE ALLOYS. Kimiko Kakubo, Yoshisato Kimura, Yoshinao Mishima, Tokyo Institute of Technology, Dept of Materials Science and Engineering, Yokohama, JAPAN.

Some of transition-metal silicides are candidate materials for thermoelectric generation at high temperatures because of their excellent oxidation resistance. Higher manganese silicide (hereafter denoted as HMS) is known as a p-type thermoelectric material that can be used at high temperature at around 1000 K without any special protection against oxidation. Low cost of compositional elements would be an advantage in commercial use since we are interested in the application of this material as a component of the micro gas turbine engine based co-generators on the distributed electric generation system. The HMS is a line compound having a complicated crystal structure and its chemical composition Mn:Si is reported ranging from 1:1.71 to 1:1.75. Manganese content is a little higher than Mn:Si=1:2, by which reason it is called as HMS. In the present work, we have investigated microstructures and thermoelectric power of the binary HMS base alloys prepared by arc-melting in Ar gas atmosphere. Alloys with 63.0, 63.5, 64.0 and 64.5 at% Si have a small amount of second phase either the primary solid solution (Si) or metallic MnSi phase. A slight revision was made on the HMS single phase region of the Mn-Si binary phase diagram. The MnSi seems to decrease the thermoelectric power while (Si) enhances it. The alloy having the HMS/(Si) eutectic microstructure, 67.9 at% Si, shows the highest thermoelectric power in the Mn-Si binary alloys measured in this work. Moreover, effect of doping the p-type element, Fe and Cr, on thermoelectric power and microstructural feature has been investigated using alloys prepared by ingot metallurgy. Both elements, especially 0.5 at% Cr addition, effectively enhance the thermoelectric power. Microstructures of doped alloys are HMS/(Si) two-phase, almost HMS single phase with a small amount of (Si) phase.

4:45 PM N2.10
DIRECTIONALLY SOLIDIFIED LAMELLAR SILICIDES BASED ON $Cr-Cr_3Si$. E.P. George, L. Heatherly, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

Single crystals of A15-structured Cr_3Si were grown by directional solidification (DS) in a xenon-arc-lamp optical floating zone furnace. Pieces were cut from the Cr_3Si rods and used as seed crystals to directionally solidify $Cr-Cr_3Si$ eutectics. In addition to the eutectic composition, alloys on both the Cr- and Si-rich sides were investigated. The effects of growth rate and rotation speed on solidification microstructures were also investigated. Specimens were

fractured transverse and longitudinal to the DS direction and the resulting fracture surfaces were analyzed by Auger electron spectroscopy to determine whether fracture occurred along the interfaces or by cleavage through one of the phases. We will discuss the correlations among DS parameters, microstructure, and mechanical properties of the $Cr-Cr_3Si$ alloys investigated.
Research sponsored by the Division of Materials Science and Engineering at the Oak Ridge National Laboratory managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

SESSION N3: IRON ALUMINIDE, IRIDIUM AND
OTHER ORDERED INTERMETALLIC ALLOYS
Chairs: Ian Baker and K. Sharvan Kumar
Tuesday Morning, November 28, 2000
Room 208 (Hynes)

8:30 AM N3.1
THE ROLE OF CARBON AND VACANCIES IN DETERMINING THE HARDNESS OF FeAl INTERMETALLIC IN THE QUENCHED AND THE AGED STATES. C. Garcia Oca, D.G. Morris, M.A. Muñoz-Morris, Department of Physical Metallurgy, CSIC, CENIM, Madrid, SPAIN; S.C. Deevi, Chrysalis Technologies, Richmond, CA.

The role of quenched-in vacancies in FeAl intermetallics on producing considerable hardening is well known, as is the softening achieved by annealing as the vacancies are annihilated. The present study examines the quench hardening and anneal softening produced by such quenched-in vacancies and by interstitial carbon solution in a Fe-40Al-C alloy. The interstitial carbon is shown to be a more potent solution hardening agent that the vacancy, while during annealing the co-annihilation of vacancies and carbon atoms in solution leads to dislocation loop debris, equiaxed carbide precipitates or plate-like precipitates, according to the annealing conditions considered. The processes occurring have been followed by detailed TEM studies, and will be discussed in terms of the relative solubilities and diffusion rates of vacancies and carbon. The relevance of such interstitial solute hardening to the behaviour of other FeAl intermetallics, including the effect on the anomalous stress peak, will be briefly considered.

8:45 AM N3.2
STRAIN-INDUCED FERROMAGNETISM IN FeAl SINGLE CRYSTALS. Dongmei Wu and Ian Baker, Thayer School of Engineering, Dartmouth College, Hanover, NH.

It has been known for forty years that B2-structured FeAl can undergo a paramagnetic to ferromagnetic transition upon cold working. The current work examined a number of cold-rolled single crystals of B2-structured FeAl alloys. Magnetic and calorimetric measurements were made on the alloys, using a vibrating specimen magnetometer and a differential scanning calorimeter, respectively. It was found that the strain-induced ferromagnetism is markedly lower for single crystals containing lower iron contents. For a particular composition, the saturation magnetization was found to depend on the orientation along which the single crystal was cold rolled. In-situ annealing experiments were performed in the TEM. These suggest that the APBs residing between gliding dislocations have little influence on the strain-induced ferromagnetism. Instead, evidence will be presented that the ferromagnetic behavior arises from APB tubes. This research is funded by the National Science Foundation grant DMI-9973977.

9:00 AM N3.3
SYNTHESIS AND CHARACTERIZATION OF MECHANICALLY ALLOYED AND HIP-CONSOLIDATED Fe-25Al-10Ti INTER-METALLIC ALLOY. Su-Ming Zhu, Makoto Tamura, Kazushi Sakamoto, Kunihiko Iwasaki, Japan Ultra-high Temperature Materials Research Institute, Ube, Yamaguchi, JAPAN.

Ti addition has been reported to be very effective in improving the tribological properties of Fe_3Al. The present study is concerned with the processing, microstructural characterization, mechanical and tribological properties of ultrafine-grained bulk Fe-25Al-10Ti intermetallic alloy. The Fe-25Al-10Ti alloy was synthesized from elemental powders by mechanical alloying and hot isostatic pressing (HIP). An ultra-high pressure (1 GPa) hot isostatic pressing (HIP) facility was used in an effort to consolidate the mechanically alloyed powders into fully dense compacts while retaining the nanocrystalline microstructure. Fully dense Fe-25Al-10Ti compacts with a grain size of about 200 nm were produced after HIP treatment at 800°. Mechanical properties of the alloy were evaluated by compression test from room temperature to 800°. At room temperature, the alloy exhibits significantly higher flow stress and considerable rupture strain. The yield strength decreases monotonically with increasing test temperature with no positive temperature dependence observed. The grain growth after high temperature deformation is not severe,

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indicating that the alloy has a relatively high thermal stability. Finally, tribological properties of the alloy were evaluated by using a pin-on-disk type wear tester and compared with those of a cast iron.

9:15 AM N3.4
INTERACTION OF BORON WITH CRYSTAL DEFECTS IN B2-ORDERED FeAl ALLOYS. Anna Fraczkiewicz, Anne-Sophie Gay, Emmanuel Cadel[a], Didier Blavette[a], ENSMSE, Centre SMS, URA CNRS, St. Etienne, FRANCE. [a]Universite de Rouen, UMR 6634 CNRS, Faculte des Sciences de Rouen, Mont St-Aignan, FRANCE.

Doping with small boron additions is a well-known way to suppress the intrinsic room-temperature intergranular brittleness of intermetallic alloys. The commonly admitted mechanism of this effect, i.e. an intergranular segregation of boron, seems not to be the only important feature. In this work, an extended study of boron interactions with crystal defects (point defects, dislocations, APB, grain boundaries) will be shown in FeAl (B2), B-doped alloys containing 40 at.% Al. The intergranular segregation of boron is characterized; both an equilibrium and a non-equilibrium (due to a solute atom / thermal vacancy interaction) segregation mechanisms are identified. Thanks to a study by 3D atom probe field ion microscopy, a strong tendency of boron to segregate to other kinds of crystal defects, like dislocations, stacking faults or APB, could be obtained. Especially, the first experimental evidence of boron segregation to an edge $< 100 >$ dislocation will be shown. An evidence of local depletion in Al in the vicinity of segregated dislocation was also obtained. Boron segregation to crystal defects strongly modifies the elementary mechanisms of plastic deformation of FeAl crystals. An example of this effect will be shown by an experimental observation of yield point in room temperature tensile tests. Moreover, an important effect of boron on the high temperature yield stress (yield stress anomaly, presented in details in [1]) will be shown and discussed. [1] Yield Stress Anomaly in FeAl and FeAlNi B2-ordered alloys Olivier Calonne, David Colas, Anna Fraczkiewicz and Francois Louchet, this conference.

9:30 AM N3.5
THE YIELD ANOMALY IN COBALT-TRANSITION METAL B2 COMPOUNDS. M. Wittmann, I. Baker, Thayer School of Engineering, Dartmouth College, Hanover, NH.

Compression tests performed on CoTi and CoHf over a range of temperatures and strain rates from 5×10^{-6} s^{-1} to 1 s^{-1} show a positive temperature dependence of the yield stress, which shifts to higher temperatures with increasing strain rate. In the region of the peak yield stress, serrated yielding, a negative rate sensitivity of the yield stress, and an increased work hardening rate were observed. These observations are consistent with strong solute-dislocation interactions. The occurrence of static strain aging, and results from quenching experiments, strain rate change tests, and TEM observations made below, at, and slightly above the peak temperature will be presented. The results suggest that the yield anomaly in CoTi and CoHf can be accounted for by a classical dynamic strain aging mechanism. This work was funded by the National Science Foundation, Division of Materials Research through grant DMR-9812211

10:15 AM *N3.6
HIGH TEMPERATURE STRENGTH OF Ir-BASED REFRACTORY SUPERALLOYS. Y. Yamabe-Mitarai, National Research Institute for Metals, Tsukuba, Ibaraki, JAPAN.

We suggested refractory superalloys based on Ir or Rh with an fcc and L1$_2$ two-phase coherent structure that are potentially useful at ultra-high temperatures at which Ni-based superalloys cannot be used. In the Ir-based binary alloys, precipitate morphology depends on the lattice misfit between the fcc matrix and the L1$_2$ precipitate. When the lattice misfit is about 2%, plate-like L1$_2$ precipitates forms in the fcc matrix. Cuboidal L1$_2$ precipitates form in the alloy with small lattice misfit about 0.3%. The dependence of precipitate morphology on compressive strength and compressive creep of Ir-based binary alloys up to 1800°C will be reported in this study. Two kinds of alloys with different precipitate morphology were selected among refractory superalloys; that is, the Ir-Zr alloy with plate-like L1$_2$ precipitates and the Ir-Nb alloy with cuboidal L1$_2$ precipitates. Precipitation hardening was main strengthening mechanism of Ir-based refractory superalloys. The precipitation-hardening effect was larger in the Ir-Zr alloy than in the Ir-Nb alloy. Shearing and bypass of precipitates were observed in the Ir-Zr alloy and Ir-Nb alloy, respectively. This difference of the deformation mode attributes to strength behavior. On the other hand, the creep strain of the Ir-Zr alloy was larger than that of the Ir-Nb alloy. This is because the coarse lamellar structure was formed at grain boundary and grew into grains by discontinuous coarsening during creep. Design of the alloy with both high strength and high creep resistance will be discussed in terms of precipitate morphology and lattice misfit.

10:45 AM N3.7
HIGH-TEMPERATURE MATERIALS QUATERNARY Ir-Nb-Ni-Al ALLOYS. X.H. Yu, Y. Yamabe-Mitarai, Y. Ro, S. Nakazawa, H. Harada, National Research Institute for Metals, High-Temperature Materials 21 Project, Tsukuba, Ibaraki, JAPAN.

Refractory superalloys was proposed by using platinum group metals as a matrix. Ir was considered because its some excellent advantages, e.g., high melting temperature (2440°C) and good oxidation resistance. Quaternary Ir-Nb-Ni-Al alloys were prepared by combining two kinds of binary alloys Ir-Nb and Ni-Al in different proportions, which located from Ni-side to Ir-side in the diagram of quaternary Ir-Nb-Ni-Al alloys. The two binary alloys, Ir-Nb and Ni-Al, consisted of fcc and L1$_2$ two phases and can form fcc/ L1$_2$ coherent structure. We expected that the two-phase region, fcc L1$_2$, could connect to each other from Ni-side to Ir-side and the fcc/L1$_2$ coherent structure can be formed in the quaternary Ir-Nb-Ni-Al system. The object is to take the advantages of Ir-base alloys (high-temperature strength) and Ni-base alloys (good ductility and relatively lower density and cost). The microstructure evolution, high-temperature strength behavior and lattice misfits of the 17 kinds of quaternary alloys were investigated systematically. The results were unexpected. There was a three-phase volume (fcc Ir$_3$Nb Ni$_3$Al) existing in the quaternary Ir-Nb-Ni-Al system. Two kinds of L1$_2$ phase (Ir$_3$Nb and Ni$_3$Al) was observed. And two kinds of fcc/ L1$_2$ coherent structures were also observed in some alloys. These alloys improved the ductility drastically. The alloys, located in the Ir-rich side, exhibited excellent balance of high-temperature strength (above 1000MPa) and ductility (about 20%). The phase stability was also very good. Up to 2000°C, the fcc/ L1$_2$ two-phase structure still existed. They are promising for using at ultra-high-temperature.

11:00 AM N3.8
DENSITY OF THERMAL VACANCIES IN L1$_2$ Al$_3$Sc-M, M=Mg, Zr, Y OR Ti. C. Woodward[a], Air Force Research Laboratory, Wright Pattterson AFB; Mark Asta, Dept. of Materials Science and Engineering, Northwestern Univ, Evanston, IL; [a]Materials and Processing Div, UES Inc, Dayton, OH.

Modifications to alloy chemistry are often used to tailor the intrinsic flow behavior of structural materials. Models of creep in intermetallic alloys must account for the influence of chemistry on the available intrinsic creep mechanisms. As in simple metals the presence of vacancies strongly influences bulk diffusion processes in these materials. Limiting the density of constitutional and thermal vacancies by alloying may produce materials with enhanced creep properties. The energy of intrinsic and substitutional point defects in $L1_2 Al_3 Sc$ are calculated within a first principles, local density functional theory framework. Relaxed structures and energies for vacancies, antisites and solid solutions are calculated using a planewave pseudopotential method. Calculated defect energies are used within a grand-canonical ensemble formalism (the Dilute Solution Model) to estimate the point defect densities as a function of temperature and composition. The density of vacancies is found to be sensitive to the underlying stoichiometry. The dependence of the vacancy concentration for solid solutions of Mg, Zr, Y and Ti is predicted.

11:15 AM N3.9
THE ORIGIN OF LOW TEMPERATURE TWINNING IN HFV$_2$-BASED LAVES PHASES. Won-Yong Kim, David P. Pope and David E. Luzzi, Department of Materials Science, University of Pennsylvania, Philadelphia, PA.

The occurrence of twinning in Laves phase alloys is sensitive to alloy composition and deformation conditions such as strain rate and temperature. HfV$_2$ Ta Laves phase based alloys with various compositions are produced by arc-melting and float-zone-melting. X-ray diffraction is used to analyze the crystal structures and lattice parameters for each sample investigated. Compression tests are conducted at temperatures down to near liquid helium temperatures using a specially designed testing apparatus. A complex mechanical behavior is found with a ductility maximum below room temperature. At this temperature, Laves matrix alloys achieve a ductility in compression in excess of 12%. The softening effect is also found in room temperature-tested specimens that are previously annealed or tested at the lower temperature. The original hardness and low ductility is recovered upon annealing at higher temperatures. In all cases, TEM analysis shows that the deformation is carried by twinning in the Laves phase. The evidence points to the presence of an incipient phase transformation as the origin of the low temperature ductility in these Laves phases. The results in the ternary system will be compared with that of the binary HfV$_2$ system and with other ternary Laves phases.

11:30 AM N3.10
COMPRESSION BEHAVIOR IN L1$_2$ MODIFIED TITANIUM TRIALUMINIDES ALLOYED WITH CHROMIUM AND IRON.

Tohru Takahashi and Tadashi Hasegawa, Department of Mechanical Systems Engineering, Tokyo Univeristy of Agriculture and Technology, Koganei, Tokyo, JAPAN.

$L1_2$ modified titanium trialuminides have been reported to form when a fraction (8 - 10 at.%) of aluminum was substituted by the third elements such as chromium and iron. In the present study, chromium and iron modified quaternary intermetallics have been prepared in addition to chromium- and iron-modified ternary titanium trialuminides. Microstructures and compression behavior have been investigated on recrystallized polycrystalline materials whose average grain diameter was adjusted to about 40 micrometers. X ray diffraction measurement revealed no evident indication of phase separation into two phases singly modified by chromium or by iron. This might suggest that the $L1_2$ modified trialuminide phase forms a continuous and mutually substitutional solution phase in the Al-Ti-Cr-Fe system. Lattice parameters of the $L1_2$ modified phases showed a linear relationship with chemical composition, and slightly decreased with increasing iron content. Mechanical behavior was investigated under compression tests at temperatures ranging from the ambient temperature to 1300K. The yield strength showed moderate decrement with increasing temperature, and they were about 150-200MPa at 1100-1300K. In the medium temperature range from 600 to 800K a small fluctuation of flow stress was observed immediately after yielding, and it ceased after compression to some strain. The materials showed full deformability at temperatures higher than 800-1000K. The yield strength and deformability were both insensitive to the chemical composition.

11:45 AM N3.11
DEVELOPMENT OF TOUGH AND STRONG CUBIC TITANIUM TRIALUMINIDES. Robert A. Varin, University of Waterloo, Dept of Mechanical Engineering, Waterloo, Ontario, CANADA; Les Zbroniec, National Institute of Materials and Chemical Research, Higashi, Tsukuba, JAPAN; Zhi Gang Wang, Inst of Aeronautical Materials, Beijing, PR CHINA.

The $L1_2$-ordered titanium trialuminides are derived from $D0_{22}$-ordered Al_3Ti by alloying with fourth-period transition elements such as Cr, Mn, Fe, Co, Ni, Cu and Zn. They have attracted much attention as high temperature structural materials because of their low density, high melting point, oxidation resistance better than that for TiAl-based alloys, and expected improvement of room temperature tensile ductility and fracture toughness due to their cubic lattice structure. Unfortunately, despite numerous efforts in the last ten years their fracture toughness has not been improved. Most surprisingly, such brittle materials also exhibit quite a low strength (hardness). The first breakthrough that has been achieved in our laboratory demonstrates that, as opposed to many other intermetallics and specifically those with the $L1_2$ crystal structure, the $L1_2$ titanium trialuminides are immune to the moisture-induced environmental embrittlement. This important finding allowed us to focus further research efforts on other factors. Very recently, the second breakthrough has been achieved that demonstrates that by manipulating the concentration of (Ti+Mn) combined with boron doping, the room temperature fracture toughness of Mn-stabilized titanium trialuminide can be improved by a whopping 100% from $\sim$4 $MPam^{1/2}$ to $\sim$8 $MPam^{1/2}$ with a simultaneous, almost three fold, increase in yield strength to $\sim$550MPa, and by 150 - 250% at 1000°C to $\sim$10 - 12 $MPam^{1/2}$ with a simultaneous suppression of intergranular fracture (IGF) to $\sim$50%. It is expected that by optimizing chemical composition and microstructure additional improvements in fracture toughness and yield strength are possible. In this work, these breakthroughs will be described and discussed.

SESSION N4: METAL SILICIDES II
Chairs: Easo P. George and Matthew J. Kramer
Tuesday Afternoon, November 28, 2000
Room 208 (Hynes)

1:30 PM *N4.1
STRUCTURAL AND THERMOELASTIC PROPERTIES OF Mo-Si COMPOUNDS: THEORY AND EXPERIMENT. C.L. Fu, J.H. Schneibel, C.J. Rawn, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN.

Critical issues for Mo-Si compounds ($MoSi_2$, Mo_5Si_3, and Mo_3Si) as ultra-high-temperature materials include the understanding of their defect structures and the reduction of high anisotropy in the coefficient of thermal expansion (CTE) of many 5-3 silicides. We address these issues by first-principles calculations, and X-ray and neutron powder diffraction. Both the heat-of-formation and site-exchange energy are found to increase progressively as the Si content increases. The dominant point defect types in Mo_3Si and Mo_5Si_3 are antisite defects on both sublattices. The antisite defect

formation energies are high as would be expected from the existence of covalent bonds in these compounds. We then address the physical origin for the high CTE anisotropy of 5-3 silicides (contrasting with that of nearly isotropic disilicides). The CTE along the c-direction is more than twice that in the a-direction for Mo_5Si_3. The CTE anisotropy is due to an elastically more rigid basal plane and a higher anharmonicity along the c-axis. This higher anharmonicity along the c-axis is attributed to the existence of [001] transition-metal chain structures in the $D8_m$ structure. As these chain structures are modified (by alloying additions) or eliminated (by structural modification from $D8_m$ to $D8_l$), we find a significant decrease in the CTE anisotropy. Work sponsored by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, and by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Transportation Technologies, as part of the High Temperature Materials Laboratory User Program, ORNL. ORNL is operated by UT-Battelle, LLC, for the U.S. DOE under contract DE-AC05-00OR22725.

2:00 PM N4.2
ELASTIC AND PLASTIC MECHANICAL PROPERTIES OF Mo_3Si DETERMINED BY NANOINDENTATION. J. Gregory Swadener, Isai Rosales, Joachim H. Schneibel, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN.

The anisotropic elastic constants of single crystal Mo_3Si (A15) were determined from nanoindentation experiments on multiple surface orientations. During indentation, the material exhibited "pop-in" behavior, which is characterized by a rapid jump in displacement, at a load of approximately 1 mN for several orientations. Yielding was found to occur at loads lower than 0.5 mN, which is consistent with Rice's unstable stacking energy criterion for the nucleation of dislocations [2]. The residual impressions produced by the "pop-in" behavior were measured using atomic force microscopy. For different surface orientations, large differences in impression depth and pile-up on the surrounding surface were found. These differences and the plastic behavior can be explained by considering the resolved shear stresses for the limited number of available slip systems in this material. [1] Research at the Oak Ridge National Laboratory SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC. [2] J.R. Rice, J. Mech. Phys. Solids, 40, 239 (1992).

2:15 PM N4.3
REFINEMENT OF CRYSTALLOGRAPHIC PARAMETERS IN REFRACTORY METAL DISILICIDES. Katsushi Tanaka, Keigo Nawata, Haruyuki Inui, Masaharu Yamaguchi, Masahiro Koiwa, Dept of Materials Science and Engineering, Kyoto University, Kyoto, JAPAN.

The crystal structures of seven binary refractory metal disilicides, RSi_2, with the $C11_b$ ($MoSi_2$ and WSi_2), C40 (VSi_2, $CrSi_2$, $NbSi_2$ and $TaSi_2$) and C54 ($TiSi_2$) structures have been refined through analysis of single-crystal X-ray diffraction data. Crystallographic parameters refined are space groups, lattice constants and atomic coordinates. In most previous studies, silicon atoms have been assumed to locate at the ideal positions so that the refractory metal atoms are perfectly six-fold coordinated in RSi_2 layers prevailing in all the three structures. The present analysis shows that the silicon atoms are displaced from the ideal positions. The magnitude of such displacement is found to be closely related to the interatomic distance in these pseudo-hexagonally arranged RSi_2 layers. In addition, the space group of three of the four C40 disilicides, VSi_2, $CrSi_2$ and $TaSi_2$, is determined to be $P6_422$, which is of chirality with respect to that ($P6_222$) assigned in the previous studies. The displacement of silicon atoms from the ideal positions indicates that all the six R-Si bonds in RSi_2 layers are not equivalent.

2:30 PM N4.4
INFLUENCE OF BORON IN IMPROVING THE OXIDATION RESISTANCE OF Mo_5Si_3. P.F. Tortorelli, B.A. Pint, K.L. More, Oak Ridge National Laboratory, Oak Ridge, TN; M. Akinc, Iowa State University, Ames, IA.

It has been previously reported that the addition of boron to Mo_5Si_3 results in substantial improvement in high-temperature oxidation resistance (cf. work of Meyer et al., 1999). Using similar alloys based on the Mo_3Si-T1-T2 and $MoSi_2$-T1-MoB phase regions as well as Mo_5Si_3 without B, this boron effect was demonstrated under thermal cycling conditions (1200°C, oxygen, 1-h cycles). Furthermore, scanning electron microscopy, electron microprobe analysis, and transmission electron microscopy of focused-ion-beam-prepared specimens have been used to evaluate microstructural changes that occurred due to the high-temperature exposures. In particular, the microstructural characterization focused on determination of the amount and disposition of borosilicate glass and, for the compositions

displaying oxidation resistance, a detailed analysis of the protective oxide layer that formed. In this way, the roles of boron and associated glass formation in improving the oxidation resistance of Mo_5Si_3 can be better understood.

3:15 PM *N4.5
PHASE STABILITY IN PROCESSING AND MICROSTRUCTURE CONTROL IN HIGH TEMPERATURE Mo-Si-B ALLOYS. J.H. Perepezko, R. Sakidja and S. Kim, Univ. of Wisconsin-Madison, Dept. MS&E, Madison, WI.

For applications at ultrahigh temperatures the multiphase microstructural options that can be developed in the Mo-Si-B system have demonstrated an effective and attractive balance of essential characteristics. The coexistence of the high melting point ($>2100^\circ$C) ternary intermetallic Mo_5SiB_2 (T2) phase with Mo provides a useful option for in-situ toughening. A further enhancement is available from a precipitation reaction of Mo within the T2 phase that develops due to the temperature dependence of the solubility behavior of the T2 phase. However, direct access to Mo T2 microstructures is not possible in ingot castings due to solidification segregation reactions that yield nonequilibrium boride and silicide phases with sluggish dissolution. Alternate routes involving rapid solidification of powders are effective in suppressing the segregation induced phases. The processing and microstructure options can also be augmented by selected refractory metal substitutional alloying, such as the incorporation of Nb or Cr, that alters the solubility of the T2 phase and the relative phase stability to yield solidification of two phase refractory solid solution T2 structures directly. The observed alloying trends highlight the role of atomic size in influencing the relative stability of the T2 phase. A key component of the overall microstructural control and long term microstructural stability is determined by the kinetics of diffusional processes. The analysis of selected diffusion couples involving binary boride and silicide phases has been used to assess the relative diffusivities in the T2 phase and coexisting phases over the range of solubility and to provide a basis for the examination of the kinetics of reactions involved in coatings and oxidation. The support of the AFOSR (F49620-00-1-0077) is gratefully acknowledged.

3:45 PM N4.6
PLASTIC DEFORMATION OF SINGLE CRYSTALS WITH THE $C11_b$ STRUCTURE: EFFECT OF THE c/a RATIO. Kazuhiro Ito, Hironori Yoshioka, Masaharu Yamaguchi, Kyoto Univ, Dept of MS&E, Kyoto, JAPAN.

$MoSi_2$ has a great potential for very high temperature applications. Plastic deformation of $MoSi_2$ single crystals with the $C11_b$ structure is extremely anisotropic; the [001]-oriented crystals can be plastically deformed only at 900°C, while plastic flow is possible at ambient temperature for single crystals with orientations other than [001]. It is caused by non-Schmid behavior of slip on $\{013\}<331>$ with the higher CRSS values for orientations close to [001]. The $C11_b$ structure is derived by stacking up three bcc unit cells (c/a=3) and then compressing them along the c-axis yields $MoSi_2$ (c/a=2.45). In order to provide a better understanding of key factors on such non-Schmid behavior, we chose $PdZr_2$ with the c/a ratio higher than 3 (c/a=3.3) and characterized the plastic deformation. Compression tests were conducted at various temperatures along [001], [010] and [110] axes. Slip on $\{013\}<100>$ has the shortest Burgers vector and the largest plane distance in $PdZr_2$ and was observed to be activated with the lowest CRSS for [110] orientation. While slip on $\{013\}<331>$ can be activated even at -196°C for [001] orientation. Although the Schmid factors of $\{013\}<331>$ slip for [001] and [010] orientations are the same, the yield stress of the [010]-oriented crystals is about twice higher than that of the [001]-oriented crystals. Thus non-Schmid behavior of slip on $\{013\}<331>$ is also observed in $PdZr_2$, but the manner is opposite to that in $MoSi_2$. Plastic anisotropy in the $C11_b$ structure will be discussed in terms of the c/a ratio.

4:00 PM N4.7
MECHANICAL BEHAVIOR OF MOLYBDENUM DISILICIDE-BASED ALLOYS. A. Misra, J.J. Petrovic, T.E. Mitchell, Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM; A.A. Sharif, University of Michigan, Department of Engineering Science, Flint, MI.

Intermetallic compounds such as $MoSi_2$ are potential materials for structural applications at temperatures above the melting points of typical superalloys. However, monolithic intermetallic compounds typically have very low strengths at temperatures greater than 1200°C and low ductility (even in compression) at near-ambient temperatures. We have investigated the mechanical behavior of the following single-phase alloys with the $MoSi_2$ body-center tetragonal structure: $MoSi_2$ alloyed with 1 to 2.5 at.% Re, $MoSi_2$ alloyed with 2 at.% Al, $MoSi_2$ alloyed with 1 at.% Nb, and $MoSi_2$ alloyed with 1 at.% Re and 2 at.% Al. Several anomalies in the mechanical behavior of alloyed materials were observed. For example, (i) addition of only

$\sim$2 at.% Re results in an order of magnitude increase in compressive strength at 1600°C, (ii) additions of Nb and Al cause solution softening at near-ambient temperatures, and (iii) quaternary $MoSi_2$-Re-Al alloys show strengthening at elevated temperatures and reduction in flow stress with enhanced plasticity at near-ambient temperatures in compression. Experiments on single crystals as well as polycrystals and transmission electron microscopy studies of the dislocation substructures are used to gain insight on the deformation behavior. The mechanisms of anomalous solution hardening and softening will be discussed. This research was funded by Department of Energy, Office of Basic Energy Sciences.

4:15 PM N4.8
SIMULATION OF A TENSILE TEST IN TRANSITION METAL DISILICIDES. M. Friak, M. Sob, Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, CZECH REPUBLIC; V. Vitek, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA.

Detailed self-consistent ab initio study of electronic structure of transition metal disilicides is performed using the Full Potential Linear Augmented Plane Wave method (FLAPW). Tensile test with loading along the [001] axis is simulated for disilicides with both $C11_b$ structure ($MoSi_2$, WSi_2, $ReSi_2$) and C40 structure (VSi_2, $TaSi_2$, $NbSi_2$). The necessity to include the relaxation of internal structure parameters is emphasised. Different tendencies of behavior of Si-Si bonds in disilicides studied are analysed.

4:30 PM N4.9
EFFECTS OF TERNARY ADDITIONS ON THE DEFORMATION BEHAVIOR OF SINGLE CRYSTALS OF $MoSi_2$. Haruyuki Inui, Koji Ishikawa and Masaharu Yamaguchi, Department of MS&E, Kyoto University, Sakyo-ku, Kyoto, JAPAN.

Effects of ternary additions on the compression deformation behavior of single crystals of $MoSi_2$ have been investigated in the temperature range from room temperature to 1500°C. The alloying elements studied include V, Cr, Nb and Al that form a C40 disilicide with Si and W and Re that form a $C11_b$ disilicide with Si. The addition of Al is found to decrease the yield strength of $MoSi_2$ at all temperatures while the additions of V, Cr and Nb are found to decrease the yield strength at low temperatures (below 800°C) and to increase the yield strength at high temperatures (above 1300°C). When slip on $\{110\}<111>$ is operative, the extent of the decrease in low-temperature yield strength seems to be best correlated with the decrease in stacking fault energy on $\{110\}$. In contrast, the additions of W and Re ($C11_b$ formers) are found to increase the yield strength at all temperatures. Although the extent of the increase in yield strength is small for a small amount of W addition, the yield strength significantly increases upon large amounts of W additions. The extent of the increase in yield strength is significantly larger for Re additions than for W additions. Of the ternary elements investigated, Al and Nb seem to be the most effective in improving the low-temperature deformability of $MoSi_2$ while Re and Nb seem to be the most effective in improving the high-temperature strength, when judged from the observed yield strength.

4:45 PM N4.10
DISLOCATION INTERACTIONS WITH VACANCIES AND VACANCY CLUSTERS IN TRANSITION-METAL DISILICIDES. Man H. Yoo, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN.

Energetic aspects of the formation of jog-pairs and kink-pairs on a straight dislocation are analyzed using the anisotropic elasticity theory for the equivalent slip systems of $(1\bar{1}0)[111]$, $(0001)[11\bar{2}0]$, and $(001)[110]$ in MSi_2 of $C11_b$ (M = Mo or W), C40 (M = V, Nb, Ta, or Cr), and C54 (M = Ti) structures, repectively. In cases of $MoSi_2$ and WSi_2, other slip systems reported in the literature are also included, and temperature effects are taken into account for $MoSi_2$. The results show that glide loops of the active slip systems are stable in all cases, having positive line tensions. The interaction energies in kink-pairs and jog-pairs are found to be generally very anisotropic with respect to the screw axis and the non-screw character, respectively. These results indicate that the elastic anisotropy plays an important role in the formation of pinning points by cross-slip and/or dislocation-vacancy interactions. Similarities and differences in the available deformation characteristics and microstructures of MSi_2 crystals will be discussed in view of the present results. Possible role of vacancy-type Frank loops in strengthening of $MoSi_2$ and WSi_2 will be also discussed.

SESSION N5: POSTER SESSION
HIGH-TEMPERATURE ORDERED
INTERMETALLIC ALLOYS
Chairs: Shuji Hanada, Kevin J. Hemker,
Ronald D. Noebe and Gerhard Sauthoff
Tuesday Evening, November 28, 2000
8:00 PM
Exhibition Hall D (Hynes)

N5.1
THE EFFECTS OF ENVIRONMENT ON THE ROOM
TEMPERATURE DEFORMATION OF SINGLE-SLIP-ORIENTED
FeAl SINGLE-CRYSTALS. I. Baker, D. Wu, Thayer School of
Engineering, Dartmouth College, Hanover, NH; Y. Yang, Hypertherm,
Inc., Hanover, NH; E.P. George, Metals and Ceramics Division, Oak
Ridge National Laboratory, Oak Ridge, TN.

The effects of environment (air, oxygen and vacuum) and of hydrogen
charging on the fracture strain and fracture strength have been
studied in single-slip-oriented FeAl single crystals tensile-tested at 2.5
$\times 10^{-3}$ s^{-1}. Fracture strains greater than 40% have been obtained in
specimens tested in oxygen whereas elongations of $\sim$10% and $\sim$20%
were obtained in air and vacuum, respectively. Hydrogen-charged
specimens showed little ductility. Fractography showed that testing in
different environments produced marked differences in the fracture
surfaces. Intermittent loading of tensile specimens in air and in
alternating air/oxygen environments has also been performed at 5 $\times$
10^{-5} s^{-1}. Intermittent loading in air, with unloading periods of a few
hours, produced greater fracture strains than continuous loading.
Alternately loading in air/oxygen showed changes in the flow stress
between the two environments. The results will be discussed in terms
of the effects of moisture-produced hydrogen on FeAl. Research
supported at Dartmouth College by NSF grant DMR-9973977 and
DOE contract DE-FG02-87ER45311, and by the Oak Ridge
Associated Universities SHaRE program contract
DE-AC05-76OR00033; and by the Division of Materials Science and
Engineering at the Oak Ridge National Laboratory, managed by
UT-Battelle, LLC, for the U.S. Department of Energy under contract
DE-AC05-00OR22725.

N5.2
THE INFLUENCE OF SOME MICROSTRUCTURAL AND TEST
PARAMETERS ON THE TENSILE STRESS AND DUCTILITY OF
A MA FeAl INTERMETALLIC. J. Chao, M.A. Munoz-Morris, J.L.
Gonzalez-Carrasco and D.G. Morris, Department of Physical
Metallurgy, CENIM, CSIC, Madrid, SPAIN.

The present study examines the influence of some microstructural
parameters (grain size, dispersoid size, and vacancy content) and
some tensile test parameters (strain rate, protective oxide coatings,
air and water vapour excluding films, and surface geometrical quality)
on the tensile behaviour (yield stress, work hardening rate, tensile
stress, tensile ductility) of a mechanically-alloyed, fine grained
Fe-40Al intermetallic. Major changes of tensile strength and ductility
are obtained by changing grain size (ductility increased from 1% to
10% for grain sizes of 100mm and 1mm) and by avoiding premature
stress/strain concentrators (ductility increased from 5% to 10% for
imperfectly machined to prepolished sample surfaces). Ductility
variations are interpreted using a slow-crack-propagation-to-instability
model, where the respective roles of environment, deformation
processes, and fracture mechanisms can be distinguished.

N5.3
YIELD STRESS ANOMALY IN FeAl AND FeAlNi B2-ORDERED
ALLOYS. Olivier Calonne, David Colas, Anna Fraczkiewicz and
Francois Louchet[a], ENSMSE, Centre SMS, URA CNRS 1884, St.
Etienne, FRANCE. [a]LTPCM, INPG, UMR CNRS 5614, St. Martin
d'Héres, FRANCE.

The stress anomaly of as-cast B2-ordered FeAl and FeNiAl alloys,
B-free and B-doped, is investigated through mechanical testing
between RT and 900°C. Both boron doping and Ni addition are
efficient for improving the high temperature mechanical resistance of
studied materials. Boron addition significantly increases the stress
peak temperature TP (200°C) and the corresponding stress maximum
(200 MPa). In Ni-alloyed (5 wt.%) materials, an additional hardening
(100 $\sim$200 MPa) is observed, especially at low temperatures, resulting
in a high and almost constant YS value on a wide plateau from about
400 up to 700°C. No shift of TP due to nickel addition is observed.
Origins of YSA anomaly were studied by TEM. Both post-mortem and
in situ TEM observations in FeAl show that the slip direction changes
from $< 111 >$ below TP to $< 100 >$ above. $< 110 >$ dislocations are
also observed around TP in the B-doped material. These results are
consistent with a model based on Saka's and Yoshimi's decomposition
scheme of $< 111 >$ superdislocations into $< 110 >$ and $< 001 >$,
resulting in superdislocation locking. The locking rate increases with
temperature, and is balanced by multiplication, which yields both

YSA and a zero strain rate sensitivity. The reinforcing effect of boron
may be explained by solute segregation to dislocation lines, especially
to the $< 110 >$ edges, which hinders multiplication and therefore
shifts towards higher temperatures the alternative deformation
mechanism. Further work is necessary to explain the strong additional
hardening of B-doped FeAl due to Ni; in particular, Mills's hypothesis
of APB energy decrease due to Ni will be tested.

N5.4
CALCULATION OF THERMAL EXPANSION COEFFICIENTS OF
IRON-ALUMINIDES. T. Seletskaia, L. Muratov, B.R. Cooper, West
Virginia University, Morgantown, WV.

The iron-aluminides Fe$_3$Al and FeAl have been among the most
widely studied intermetallics because of their low cost, low density,
good corrosion resistance and exceptional strength retention at high
temperature. The thermal expansion behavior has many consequences
both in phase development during processing and in application of
these materials. For this reason we calculated the thermal expansion
coefficients (CTE) of both intermetallic compounds over a wide range
of temperature and assessed the dependence of the CTE's on the most
commonly used additives such as molybdenum, chromium and
niobium. In our calculations we used two independent techniques: the
Local Harmonic Approximation and the Monte Carlo method. The
first technique allowed us to test the validity of our potentials within
a short period of time, and the second technique improved the
accuracy of calculations and increased the range of temperature. The
required total energy of the sample for both techniques was computed
by using a semi-empirical tight-binding method originally developed
by NRL and modified by us. The parameters of the tight-binding
Hamiltonian were fitted to reproduce the band structure and the
total-energy obtained from our ab-initio full-potential linear
combination of muffin-tin orbitals (FPLMTO) calculations. The
question of the phase stability was carefully examined, and we will
discuss the influence of the specific additives on the phase formation.

N5.5
LOW TEMPERATURE POSITRON LIFETIME AND DOPPLER
BROADENING MEASUREMENTS IN B2-TYPE FeAl ALLOYS.
Tomohide Haraguchi, Osaka Prefecture Univ, Dept of Materials
Science, Osaka, JAPAN; Fuminobu Hori, Ryuichiro Oshima, Osaka
Prefecture Univ, Research Institute for Advanced Science and
Technology, Osaka, JAPAN; Mineo Kogachi, Osaka Prefecture Univ,
Dept of Materials Science, Osaka, JAPAN.

Positron lifetime and Doppler broadening measurements have been
carried out systematically for B2-type intermetallic compounds FeAl
with composition range from 41.2 to 50.7 at%Al so as to clarify the
feature of lattice defects of the alloys. By using specimens quenched
from various temperatures, the measurements were performed at a low
temperature, 100K, in order to inhibit the atomic vibration effects as
well as possible. Two lifetime components are unable to obtain with
the conventional two-lifetime component analysis except for a few
data, indicating a saturation trapping of positron at the vacancy sites.
Few composition and temperature dependences of mean positron
lifetimes are found. The values are in a range of about 180-200 psec
and well similar to the published data. These values do not correspond
to vacancy clusters, but to mono or di-vacancies. From Doppler
broadening measurement, tendency for the S-parameter to increase
with increase in Al content is noticed for each quenching temperature.
It was confirmed from our previous density measurements that large
amount of vacancies are easily retained in this FeAl system, and the
concentration amounts to about 1% in the alloys with higher Al
content even after a long time annealing at 573K. Therefore, it is
suggested that such an increase of S-parameter are attributed to
change in the defect configuration or the fraction of atoms around the
vacancies, not to increase in vacancy concentration. Furthermore, the
Al concentration dependence of S-parameter seems to be grouped into
three; rapid increases in the first stage (41.2-45.0 at%Al), flat or slight
decrease in the second stage (45.0-47.5 at%Al) and then a rapid
increase in the third (47.5-50.7 at%Al). This may reflect the change in
defect situation with composition as describes above.

N5.6
VOID FORMATION, MORPHOLOGY AND STABILITY IN NiAl.
M. Zakaria and P.R. Munroe, Electron Microscope Unit, University of
New South Wales, Sydney, AUSTRALIA.

Void formation, morphology and stability in stoichiometric NiAl was
studied through controlled heat treatments over a range of annealing
temperatures from 400°C to 900°C. Specimens were first annealed at
1300°C to retain a supersaturation of vacancies at room temperature.
Structural analysis was performed using transmission electron
microscopy. Voids were observed to form at temperatures as low as
400°C, but were noted to dissolve during annealing at 900°C. Two
distinct void morphologies were noted: cubic and rhombic
dodecahedral. No clear correlation between void type and the heat

treatment conditions used was established. In some instances both morphologies were observed at the same annealing temperature. At higher annealing temperatures ($>800°C$) extensive dislocation climb was noted, and this became the dominant mechanism for the removal of excess vacancies. The relative incidence of void formation and dislocation climb at each annealing temperature has been related to the mobility of vacancies. The variations in the shape of voids can be described in terms of their relative surface energy of each void type and its mode of nucleation.

N5.7
ADVANCEMENT OF THE DIRECTIONAL SOLIDIFICATION PROCESS OF A Ni-Al-ALLOY. F. Scheppe, I. Wagner and P.R. Sham, Giesserei-Institut, RWTH Aachen, Aachen, GERMANY.

In order to improve the efficiency of modern gas turbines for energy transformation with simultaneously decreasing ecological damage, higher material demands are inevitable. These demands are today met by the application of single-crystal Ni-base-superalloys. Intermetallic compounds, such as NiAl, offer new opportunities for developing low density, high-strength structural alloys which might be used at higher temperatures when compared to conventional titanium- and nickel-base alloys.
Simple geometry were assembled in production size clusters. A special SiO_2-poor ceramic shell mold system, compatible with the alloys regarding temperature, thermal expansion and chemical resistance, was used to determine pouring and process parameters (pouring temperature, mold temperature, lowering speed) for the directional solidification process of a NiAl-Cr alloy.
The attempts show that only a narrow range of tolerance exists, in which the variation of the process parameters led to a directional solidified casting. However it was possible to produce crack free directional solidified NiAl-components.

N5.8
MICROSTRUCTURES INVESTIGATION OF IN-SITU TiB_2 PARTICLES REINFORCED NiAl ALLOY COMPOSITE. G.H. Cao, Z.G. Liu, G.J. Shen[a], J.M. Liu, National Laboratory of Solid State Microstructures, Nanjing University, Nanjing, PR CHINA. [a]Analysis and Testing Centre, Southeast University, Nanjing, PR CHINA.

The TiB_2 reinforced NiAl alloy composite was fabricated by exothermic dispersion (XD) technique and condensed by hot isostatic pressing (HIP). The interface between TiB_2 and NiAl was studied by transmission electron microscopy (TEM). The experimental results show that there is no reaction product formation at the TiB_2/NiAl interface and the relationships between TiB_2 and NiAl have no specific orientations. In addition, a fcc phase with lattice constant a=1.038nm was observed in NiAl matrix. The X-ray diffraction directing to composite shows that it mainly consists of TiB_2 and NiAl, and no abnormal peaks were found out, which shows that the small volume fraction of this fcc phase. TEM energy dispersive X-ray spectroscopy (Philips, CM200 FEG, spot size: 5nm) analysis to this fcc phase indicated that it contains element Ni, Al and B with atomic ratio 6:3:1.

N5.9
THE EFFECT OF Cu-MACROALLOYING ON RAPIDLY SOLIDIFIED NiAl INTERMETALLIC COMPOUND. Sergio Garcia, Carlos Gonzalez, Julio Juarez, Universidad Nacional Autonoma de Mexico, Instituto de Investigaciones en Materiales, D.F., MEXICO.

Intermetallic compounds have long been recognized as potentially useful structural materials for high temperature applications, however their utilization have been limited by poor toughness and damage tolerance at room temperature, and inadequate strength and creep resistance at elevated temperature. On the other hand, solidification processing of intermetallic compounds upon equilibrium phase diagram appears to be quite limited. With conventional melt processing of intermetallic compounds one or more peritectic reactions and wide liquidus-solidus separation are encountered and lead to large-scale composition segregation which is difficult to eliminate during post-solidification treatments. At the same time the characteristics which make intermetallic compounds unattractive for conventional processing qualify then as suitable candidates for rapid solidification processing. This work present results, on the effect of Cu-macroalliying additions to the NiAl intermetallic compound in its rapidly solidified condition, in terms of the variation of lattice parameter and microhardness Vickerss measurements as a function of Ni/Cu concentration ratios. STEM microanalyses and microstructure variations are also included.

N5.10
MULTI-MODAL ORDER-ORDER KINETICS IN Ni_3Al AS STUDIED BY MONTE CARLO COMPUTER SIMULATION. P. Oramus, R. Kozubski, Institute of Physics, Jagellonian University, Krakíow, POLAND; V. Pierron-Bohnes, M.C. Cadeville, Institut de Physique et Chimie des Matériaux de Strasbourg, Strasbourg, FRANCE; W. Pfeiler, Institut für Materialphysik, University of Vienna, Vienna, AUSTRIA.

Order-order relaxations in γ-Ni_3Al previously extensively studied by means of resistometry, are simulated within a model of vacancy mechanism of atomic migration in a superstructure implemented with Monte Carlo technique and the Glauber algorithm. The experimentally observed contribution of two simultaneous relaxation processes showing different rates, as well as the theoretically predicted effect of vacancy ordering have been definitely reproduced and analysed in details in terms of the dynamics of particular kinds of atomic jumps. The processes following an increase and decrease of temperature resulted only partially symmetric in time. The proposed model scenario for the creation and elimination of antisite atoms in the relaxing $L1_2$-type superstructure shows that the experimentally observed features of the "order-order" processes in Ni_3Al follow from an interplay between two dominating and coupled modes of long- and short-range ordering: the creation/elimination of nn pairs of antisites (SRO) and the change of the "overall" number of antisites (LRO). High profile of the first process results in a high contribution of the fast component in LRO kinetics. The studies stimulated a development of a workshop for computer simulation of atomic migration in superstructures both in a steady-state and structural relaxation conditions.

N5.11
FIRST PRINCIPLES CALCULATION OF CORRELATED ATOM MIGRATION IN $L1_2$-Ni_3Al. H. Schweiger, R. Podloucky, Center for Computational Materials Science and Department for Physical Chemistry, University of Vienna, Vienna, AUSTRIA; W. Püschl and W. Pfeiler, Institut für Materialphysik, University of Vienna, Vienna, AUSTRIA.

Recent Monte-Carlo simulations of order relaxations in $L1_2$-ordered Ni_3Al reproduced the simultaneous action of two processes as experimentally observed by residual resistometry. It was shown that the fast process is related to the fast annihilation/creation of nearest neighbour antisite pairs. These findings are now strongly corroborated by a new supercell approach of *abinitio* quantum mechanical calculations describing the simultaneous displacement of Ni- and Al-atoms on their way to their respective antisite positions. Studies of single jumps suggest that such a correlated migration of Ni and Al is necessary in order to prevent Al-antisites from jumping back into their regular position. Relaxation of neighbouring atoms was taken into account. Thus a minimum migration barrier of about 3 eV was derived which together with the calculated formation energy of a Ni vacancy of 1.5 eV amounts to 4.5 eV in remarkable agreement with the unusually high activation enthalpy of 4.6 eV as observed experimentally.

N5.12
Ni_3Al THIN FOIL BY COLD ROLLING. Toshiyuki Hirano, Masahiko Demura, Kyosuke Kishida, National Research Institute for Metals, Tsukuba, Ibaraki, JAPAN; Yozo Suga, Nippon Cross Rolling Co., Mobara, Chiba, JAPAN.

Ni_3Al has attractive high-temperature properties as structural materials. The major problem of this compound, grain boundary brittleness, has been overcome by boron addition and directional solidification. Particularly, the directional solidification we found is very effective. Recently we successfully fabricated thin foil below 100 μm in thickness by cold rolling. With these thin foils, it is possible to construct honeycomb structure, which posses a potential as high-temperature lightweight materials. Here we present the fabrication of thin foil by cold rolling using directionally solidified binary stoichiometric Ni_3Al. Thin foils of 70 μm in thickness were successfully fabricated with 95% reduction at room temperature without intermediate annealing, having a strong {110}texture. The surface is smooth and shinny with a metallic luster. Though intensively work-hardened, the as-rolled foils posses some ductility: it is possible to bend them almost double. Considering the high temperature applications, the loss of ductility due to recrystallization is of great concern since the recrystallized equiaxed grain boundaries are normally brittle. Fortunately, the foils posses more than 3% room-temperature tensile ductility after heat treatment at higher temperatures above 1073 K. Thus, it is considered that the foils have a potential for high-temperature honeycomb structure.

N5.13
CREEP BEHAVIOR OF Ni_3Al: COMPARISON OF MONOTONOUS AND TRANSIENT TESTS. B. Lo Piccolo, J.L. Martin, T. Kruml, Ecole Polytechnique Fédérale, Département de Physique, Lausanne, SWITZERLAND; J. Bonneville, Université de Poitiers, Futuroscope, FRANCE.

In an attempt to improve the understanding of the deformation

mechanisms of Ni_3Al, transient creep experiments are performed along the stress-strain curves of binary polycrystals ($Ni_{76}Al_{24}$, $Ni_{75}Al_{25}$). Logarithmic creep is observed at temperatures of 300K and 550K, at different strains along the stress-strain curve, for creep durations of about 300s. These yield values of the activation area of the dislocation mobility which agree well with those measured using load relaxation experiments. They provide in addition unique and quantitative information about the substructural changes as a function of strain, including the mobile dislocation exhaustion-rate. High dislocation exhaustion-rates are found as compared to ordinary metallic materials. These can be explained in terms of the Kear-Wilsdorf lock mechanism, well established in Ni_3Al. These results are in fair agreement with previous publications about monotonous creep tests. Indeed, the latter indicate a short primary stage during which dislocations gliding along the primary octahedral plane are exhausted. At the highest temperatures explored and stresses of about 330 MPa, instabilities are sometimes observed along the transient creep curve. They are thought to correspond to the appearance of inverse creep which has been reported as taking over during monotonous creep tests at intermediate temperatures. Etch-pit experiments on single crystals of similar compositions are underway to measure the corresponding dislocation velocities and to identify their slip planes as a function of the imposed conditions.

N5.14
SLIP TRACE CHARACTERISATION OF Ni_3Al BY ATOMIC FORCE MICROSCOPY. C. Coupeau, J. Bonneville, Universite de Poitiers, Faculte des Sciences, Futuroscope Cedex, FRANCE; T. Kruml, Swiss Federal Institute of Technology, Lausanne, SWITZERLAND.

The intermetallic compound Ni_3Al exhibits over a certain temperature range a positive temperature dependence of its flow strength. A large majority of the proposed models consider that a thermally activated cross-slip process plays a key role in this anomalous behaviour. However, these models disagree in the description of the cross-slip mechanism and, in particular, in the height of the cross-slipped segment. It is well known that a crystalline material sheared by dislocations displays slip traces at its surfaces. These slip traces are intimately associated with the processes controlling plastic flow and may contribute to a better understanding of the material plasticity. In this study, we examined by using an atomic force microscope (AFM) the slip traces produced on Ni_3Al single crystalline specimens after 1% plastic strain. Three temperatures have been investigated in the anomalous domain: 293K, 500K and 700K, which respectively corresponds to the onset, intermediate and nearly 100K below the peak temperature. The overall features of the slip traces are analysed. Particular attention is paid to observe the temperature evolutions of cross-slip events, the slip trace deviations from the primary octahedral slip plane and to quantify the slip trace lengths. It is observed that the number of cross-slip traces does not significantly evolve with deformation conditions and, in a correlated manner, that the slip traces essentially belong to the primary octahedral slip system. However, the lengths of the slip traces become shorter and shorter with increasing temperatures, indicating a decreasing mean free path. These results will be discussed and compared with the predictions of the models.

N5.15
MICROSTRUCTURAL EVOLUTION AND MECHANICAL PROPERTIES OF Al_3Ti-BASED MULTI-PHASE ALLOYS. Seiji Miura, Juri Fujinaka, Rikiya Nino and Tetsuo Mohri.

A preliminary study on the phase relations in Al-Mo-Ti-X quaternary systems in the vicinity of tri-aluminide phases is carried out. In the Al-Mo-Ti ternary system, a bcc-phase field extends from the Ti-Mo edge to high Al region at high temperatures and it equilibrates with a $D0_{22}$-Al_3Ti phase containing a large amount of Mo. It is found that, by additions of X=Mn or Cr, an $L1_2$-(Al, X)$_3$Ti phase appears in the two-phase region composed of $D0_{22}$-Al_3Ti and bcc phases of the Al-Mo-Ti ternary system. The bcc phase is also found to be stabilized by these quarternary additions. The mechanical properties of these alloys will be presented. This research is partially supported by NEDO (New Energy and Industrial Technology Development Organization).

N5.16
HYDROGEN PULVERIZATION IN INTERMETALLICS-BASED ALLOYS. Satoshi Semboshi, Naoya Masahashi and Shuji Hanada, Institute for Materials Research, Tohoku University, Sendai, JAPAN.

Pulverization behavior and microstructure evolution with hydrogenation in hydrogen absorbing intermetallic-based alloys, such as $TiMn_2$ with TiMn, Ta_2Ni with Ta solid solution (Ta_{ss}) and Nb_3Al with Nb solid solution (Nb_{ss}), are investigated to clarify the mechanism of the hydrogen pulverization. Ti -60 at.% Mn consisting of $TiMn_2$ Laves phase and TiMn is remarkably pulverized to fine powder under 30 μm in the first hydrogenation. Crack propagation

parallel to the sample surface is observed throughout both phases after hydrogenation. The lattice constant and the amount of hydrogen retained in $TiMn_2$ increase with the number of hydrogenation, while do not change in TiMn phase. Nano-sized regions with Moire patterns are produced in $TiMn_2$ and Debye rings corresponding to titanium hydride δ-TiH appear in the diffraction pattern. Ta -10 at.% Ni consisting of Ta_{ss} and Ta_2Ni Laves phase is pulverized to coarse powder more than 100 μm in the first hydrogenation. Crack propagation occurs preferentially in the brittle Ta_2Ni phase rather than in the ductile Ta_{ss} phase. In Nb_{ss} / Nb_3Al two phase alloy, when the volume fraction of brittle Nb_3Al increases, the particle size with hydrogenation becomes small, deducing the hydrogen pulverization could be correlated with its toughness. Tantalum hydride with nano-grains is observed in Ta_{ss}, similar to $TiMn_2$. Based on these observations it is concluded that the hydrogen pulverization is attributable to (1) the absorption of a large amount of hydrogen in a hydrogen affinity phase, (2) the strain introduced by lattice expansion and the hydride formation, and (3) the crack propagation in a brittle phase.

N5.17
HIGH TEMPERATURE TENSILE AND COMPRESSION BEHAVIOR OF AN HYDROGENATED Ti_3Al-BASE ALLOY. Yong Zhang, Dept of Physics and Astronomy, Univ of Delaware, Newark, DE; Shaoqing Zhang, Inst of Aeronautical Materials, Beijing, CHINA.

In this article, the effect of hydrogenation on hot deformation has been investigated in a wrought Ti_3Al-base alloy, Ti-25Al-10Nb-3V-1Mo (at%), using high temperature tensile and compression tests at 900°C. Hydrogenation treatment was carried out using high temperature gas charging method. Hydrogen concentration in the alloy was charged up to 0.4 wt%. The microstructure characterization was examined by transmission electron microscopy (TEM), X-ray diffraction (XRD) and optical microscopy (OM). At different deformation rates, hydrogenation can not only decrease the tensile strength or increase tensile plasticity, but also lower the peak hot compression stress. Hydrogen increases the strain rate sensitive coefficience during hot compression test. With increasing the hydrogen concentrations added to the alloy, the volume fraction of α_2 phase in the alloy subjected to tensile or compression deformation, whereas that of β phase increases. TEM results show that hydrogen promotes the globularization or dynamic recrystallization of α_2 phase and dynamic recovery of β phase. After hot deformation, the hydrogen concentration in the alloy can be easily resumed to a safe level by a vacuum annealing treatment. The higher the hydrogen concentrations in the alloy before hot deformation, the finer the microstructures after dehydrogenation treatment. Phase transformation mechanism during hydrogenation-hot deformation-dehydrogenation is also discussed.

N5.18
HIGH TEMPERATURE COMPRESSION PROPERTIES AND DEFORMATION MICROSTRUCTURE OF CAST Fe-25Al-10Ti INTERMETALLIC ALLOY. Su-Ming Zhu, Makoto Tamura, Kazushi Sakamoto, Kunihiko Iwasaki, Japan Ultra-high Temperature Materials Research Institute, Ube, Yamaguchi, JAPAN.

The compression behavior of Fe-25Al-10Ti alloy has been studied as a function of temperature and strain rate. The alloy was prepared by arc melting in an argon atmosphere. The flow behavior was analyzed by the constitutive equation, and the deformation microstructure was examined by optical and transmission electron microscopy (TEM). The alloy exhibited strong tendency of strain hardening at low temperatures. Strength anomaly was observed in this alloy around 600°. The mechanical behavior was interpreted in terms of dislocation structures. Based on the stress-strain response, strain rate sensitivity and deformation microstructure, possible hot working range for the Fe-25Al-10Ti alloy was proposed.

N5.19
MECHANICAL PROPERTIES OF Fe_3Al INTERMETALLIC MATRIX COMPOSITES. Park Bong Gyu, Ko Se-hyun, Park Yong-ho, Tohoku National Industrial Research Institute, Sendai, JAPAN.

Fe_3Al matrix composites were fabricated using mechanical alloying and pulse discharge sintering processes. Selected reinforcement was TiB_2. Volume fractionw of TiB_2 was systematically changed from 0 to 25. Microstructure was observed using optical microscope and TEM. Tensile test was carried out. Room and high temperature mechanical properties were measured and analyzed with the relation to the microstructure. Fracture mode was also discussed.

N5.20
EFFECT OF $E2_1$-Fe_3AlC PRECIPITATION ON MECHANICAL PROPERTIES OF γ-AUSTENITE STABILIZED BY ADDITION OF Mn AND Co. Seiji Miura, Hiroaki Ishii and Tetsuo Mohri.

An $E2_1$-Fe_3AlC phase has been investigated as a potential high temperature material with a fcc-based structure. However, no sound single-phase Fe_3AlC alloys can be fabricated by a conventional melting and casting method because of a peritectic reaction associated with the formation of a graphite phase. Although, in the Fe-Al-C ternary system, the $E2_1$-Fe_3AlC phase equilibrates with the graphite phase and a B2-FeAl phase or a $D0_3$-Fe_3Al phase it was reported that the Fe_3AlC phase equilibrates with a γ-austenite when a large amount of Mn is added. In the present study it is also found that the addition of both Mn and Co are also effective to stabilize both the $E2_1$-Fe_3AlC phase and the γ-austenite phase, resulting in the Fe_3AlC-γ two-phase field. The volume fraction of the $E2_1$-Fe_3AlC phase precipitated in the γ-austenite phase is as much as 30% and the lattice mismatch is evaluated to be $\approx$3%, rather higher than those of $\gamma/\gamma\prime$ in Ni-base superalloys. The large lattice mismatch causes a plate-like precipitation of the $E2_1$-Fe_3AlC phase in the fcc-austenite phase. Their mechanical properties will also be presented. This research is supported by Kawasaki Steel 21st Century Foundation.

N5.21
MICROSTRUCTURES AND MECHANICAL PROPERTIES OF THE γ / κ TWO-PHASE Fe-Mn-Al-C(-Cr) ALLOYS.
Kazuyuki Handa, Yoshisato Kimura and Yoshinao Mishima, Tokyo Institute of Technology, MS&E, Yokohama, JAPAN.

The $E2_1$ type intermetallic compound $(Fe,Mn)_3AlC_X$, κ phase, would be an excellent strengthener for the fcc γ-Fe base heat resisting alloys for high-temperature application over 1000 K, since the $E2_1$ ordered crystal structure is quite similar to that of the $L1_2$, well-known strengthener of Ni-base superalloys. The only difference in crystal structures is that $E2_1$ has an interstitial carbon atom on the body-center site of the $L1_2$. We can expect to design a new type of Fe base alloys through the microstructure control on the γ/κ two-phase. One advantage of this alloy design is low cost comparing with commercial Fe-base superalloys including considerable amount of high-cost Ni. In the present work, Fe-Mn-Al-C alloys with relatively high carbon contents (higher than 2wt%) were selected in order to stabilize κ phase even above 1000 K and to increase the volume fraction of it. The relationship between mechanical properties and microstructure were investigated for the γ/κ two-phase alloys. A typical microstructure of the γ/κ two-phase alloys is that the $E2_1$ phase precipitates as cubes or plates in the γ-Fe matrix. Microstructural feature depends on chemical compositions and heat treatment conditions. Compressive yield strength of the present alloys is comparable to that of Fe-base superalloys. Tensile test has revealed that coarse κ phase on the grain boundary tends to be an initiation site of micro-crack and works unfavorable for the ductility. To improve relatively poor oxidation resistance, the Cr addition from 2 to 11 at% was conducted on the Fe-Mn-Al-C alloys. Effect of the Cr addition on the stability of the γ/κ two-phase microstructure was evaluated by microstructural observation, and mechanical properties of the Fe-Mn-Al-C-Cr alloys were investigated at temperatures ranging from 300 to 1000 K in tension.

N5.22
ON THE DETECTION OF ORDERING IN HIGHLY STABILISED BETA TiVCrAl ALLOYS. Y.G. Li and M.H. Loretto, IRC in Materials for High Performance Applications, University of Birmingham, Birmingham, UNITED KINGDOM.

The extent of ordering in the Ti-(20-37)V-15Cr-(0-7)Al (all compositions are in wt% unless indicated) alloys has been examined using transmission electron microscopy (TEM), electron diffraction, neutron diffraction, conventional and synchrotron X-ray diffraction. Energy dispersive X-ray analysis has been used to determine site occupancy. It has been found that addition of 5% Al to the TiVCr ternary system led to detectable ordering of the bcc beta matrix (A2) into the B2 structure with all techniques other than conventional X-rays. Between 4-5% Al only electron and neutron diffraction and the presence of dislocation pairs in deformed samples revealed the presence of long range order. At 3% Al the presence of dislocation pairs provided the only evidence for order. No evidence for order was found in alloys containing less than 2% Al. The results are discussed in terms of the site occupancy and the effectiveness of different techniques in detecting order in TiVCrAl alloys.

N5.23
DEFORMATION TWINS IN Ni_3Nb SINGLE CRYSTALS WITH $D0_a$ STRUCTURE. Kouji Hagihara, Takayoshi Nakano and Yukichi Umakoshi, Osaka Univ, Graduate School of Engineering, Dept of MS&E, Suita, Osaka, JAPAN.

Ni_3Nb compound with $D0_a$ structure is of great interest as a strengthening component for Ni-based superalloys. Temperature dependence of yield stress and operative slip systems was investigated using Ni_3Nb single crystals. Single crystals were grown by a floating zone method under Ar gas flow. Compression and tensile tests were performed in a vacuum at temperatures from -196°C to 1200°. Three twinning systems of $\{211\}<\overline{1}0\ 7\ 13>$, $\{011\}<0\overline{1}1>$ and $\{012\}<0\overline{2}1>$ were operative in addition to four slip systems of $(010)[100]$, $(010)[001]$, $(001)[100]$, and $\{201\}<10\overline{2}>$. Such deformation behavior depended strongly on crystal orientation and deformation temperature. The CRSS for these twinning systems monotonously decreased with increasing temperature, while some of the slip systems exhibited anomalous strengthening. Since the CRSS for the twinning systems, particularly, $\{011\}<0\overline{1}1>$ was relatively low, twinning deformation easily occurred singly or accompanied with other systems. Twinning preferentially appeared, for instance, at the loading axes of [270]* and [302]* and often crossed to each other. Operation of additional slips or twinnings was observed at the intersection between twins to accommodate the residual internal strain. Types of intersected twins and accommodated deformation modes at the intersection were classified based on the crystallographic relationship.

N5.24
PROCESSING AND PROPERTIES OF GAMMA LAVES PHASE IN-SITU COMPOSITE COATINGS DEPOSITED VIA MAGNETRON SPUTTERING. Feng Huang, Wesley S. Rollings, Jason K. Morgan, John A. Barnard, Mark L. Weaver, Univ of Alabama, Dept of Metallurgical and Materials Engineering, Tuscaloosa, AL; William S. Epling, Univ of Alabama, Dept of Chemical Engineering, Tuscaloosa, AL.

Recent research efforts have established that Laves phase reinforced gamma titanium aluminides (i.e., γ Laves) offer significant potential as oxidation-resistant coatings in high-temperature structural applications at temperatures up to 1000°C, as wear-resistant coatings for cutting tools or for protecting magnetic storage media. In these applications, these materials will need to exhibit enhanced resistance to oxidation, corrosion, and wear. In the present study, the microstructures, physical properties and tribomechanical properties of γ Laves phase coatings have been investigated. The coatings have been deposited via magnetron sputtering on glass, single crystal silicon, and titanium aluminide substrates. The results are discussed relative to commercially available coating alloys.

N5.25
Transferred to Y11.4

N5.26
ANOMALOUS STRAIN RATE DEPENDENCE OF TENSILE ELONGATION IN MOISTURE-EMBRITTLED $L1_2$ ALLOYS. T. Takasugi, Y. Kaneno and H. Inoue, Department of Metallurgy and Materials Science, Graduate School of Engineering, Osaka Prefecture Univerity, Sakai, Osaka, JAPAN.

The effect of strain rate on tensile ductility of moisture-induced embrittlement of $L1_2$-type ordered intermetallic alloys such as Co_3Ti and $Ni_3(Si,Ti)$ was investigated at ambient temperatures (298K-353K) by tensile test and SEM fractography. The anomalous increase of tensile elongation and ultimate tensile stress was observed in a very low strain rate region and also at high temperatures, accompanied with an increase of area fraction in ductile transgranular fracture pattern. The anomalous strain rate dependence of tensile ductility was shown to become more evident with decreasing grain size and also with deviating from alloy stoichiometry. As a process counteracting to the hydrogen decomposition process from moisture in air, oxidation process on the alloy surface was suggested.

N5.27
TENSILE PROPERTIES OF B2-TYPE CoTi INTERMETALLIC COMPOUND. Y. Kaneno and T. Takasugi, Department of Metallurgy and Materials Science, Graduate School of Engineering, Osaka Prefecture University, Sakai, Osaka, JAPAN.

B2-type CoTi intermetallic compound which was hot-rolled and recrystallized was tensile-tested as a function of temperature. The yield (and ultimate tensile strength) showed a peak at an intermediate temperature ($\sim$800K). The brittle-ductile transition (BDT) for tensile elongation took place at about 800K, above which large tensile elongation was observed. Corresponding to this transition, SEM fractography showed a change from cleavage-like pattern in mixture with intergranular fracture pattern to large cross-sectional reduction, i.e. necking of the tensile specimen. Also, it was found that the observed mechanical properties were independent of heat-treatment procedures, indicating that retained vacancies did not actually affect the mechanical properties of CoTi intermetallic compound.

N5.28
CRYSTAL GROWTH OF RuAl BASE ALLOYS. Sebastien Rosset, Rachel E. Bailey, and David R. Johnson, Materials Engineering, Purdue University, West Lafayette, IN.

Good room temperature toughness is often reported for the high temperature B2 compound RuAl. This unusual toughness is argued to originate from the multiplicity of slip along the $< 110 >$ and $< 100 >$ directions. However, no single crystal work have been reported in the literature. In the present work, different crystal growth techniques were examined with the aim to produce single crystals for future deformation studies. Small single crystals and in-situ composites based on the RuAl-refractory metal eutectic systems were produced using cold crucible Czochralski techniques. Characterization of the crystals and eutectics for alloys containing Mo and W are presented.

N5.29
PARTITIONING AND INTERFACIAL ADSORPTION OF TERNARY ELEMENTS IN TWO-PHASE Al-Al$_3$Sc ALLOYS.

Mark Asta, Dept. of Materials Science and Engineering, Northwestern Univ., Evanston, IL; C. Woodward[a], Air Force Research Laboratory, Wright Patterson AFB; V. Ozoliņš, Sandia National Laboratories, Livermore, CA; [a]Materials and Processing Div, UES Inc, Dayton, OH.

The $L1_2$, Al$_3$Sc intermetallic plays a critical strengthening role as a coherent, coarsening-resistant precipitate phase in a developing class of structural Al-based alloys. Currently, the effects of ternary alloying additions on the mechanical properties are under investigation experimentally and theoretically in order to increase the service temperature of these alloys. We study the partitioning and interfacial adsorption of ternary elements in two-phase Al-Al$_3$Sc alloys from first-principles calculations, within a local-density-functional-theory framework. The structure and energetics of dilute substitutional impurities are calculated using ab-initio methods, and used within a dilute-solution framework to calculate finite-temperature sublattice compositions, equilibrium phase partitioning, and interfacial segregation profiles. Appreciable segregation of ternary elements to coherent Al-Al$_3$Sc interfaces is predicted.

N5.30
THERMOELASTIC PROPERTIES OF SUPER HIGH TEMPERATURE Ru-Ta SHAPE MEMORY ALLOY. Y. Furuya, Hirosaki Univ, Dept of Intelligent Machines and System Engineering, Hirosaki, JAPAN; H. Zhirong, Shaanxi Institute of Technology, Dept of Material Science and Engineering, Shaanxi, CHINA. (at present, Visiting Scientist of Hirosaki Univ.)

It was studied by R. Fonda[1] and Y. Furuya[2] that the equiatomic Ru-Ta alloy can show the thermoelastic phase transformation at super high temperature region above 1000°C. The inverse transformation temperature(Af) associated with shape memory effect seems to be remarkably higher by two times than those of the formerly reported high temperature NiMnAl alloy system whose maximum Af is about 600-700°C, therefore it will be applicable to ultra-high temperature turbine blades for developing higher efficiency jet engine and super heat-resistance component alloy such as the tip material of the wings of aerospace vehicle due to the better ductility, toughness and mechanical strength than the ceramics at super high temperature region over 1000°C. These features seem to be very attractive, however, detail thermoelastic properties of Ru-Ta system alloy have not been clarified. Then, in the present paper, we investigate the change of each transformation temperature that depends on alloy composition by changing the Ru content from 46-54at%. By DSC measurement, martensite and austenite phase transformation temperatures change from 900°C to 1150°C with increasing Ru element. Thermal stability is also investigated by applying several thermal cycles, and it is found that this Ru-Ta alloy is very stable between 900°C and 1400°C. Optical microscope as well as X-ray diffraction analysis are performed for characterization of the metallurgical microstructures of the tested Ru-Ta alloys.
[1]R. Fonda et al: Final Program & Absract of ASM-TMS Materials Week '96, p.153 (Oct.1996, Cincinnati, US) [2]Y. Furuya: Proc. 1st Japan-France Intelligent Materials and Structures Seminar (Sendai, '98), p.113-122 (1998)

N5.31
ON THE DUCTILITY OF Nb-Ti-Al ALLOYS AT INTERMEDIATE TEMPERATURES. Sundar Amancherla, Gopal B. Viswanathan, Hamish L. Fraser, Ohio State University, Columbus, OH; Tadeu Carneiro, Reference Metals Company Inc., Bridgeville, PA.

Advanced jet engine design requires new structural materials with improved high temperature capability, lower density, adequate toughness and producibility. A candidate system is the Nb-Ti-Al system, which exhibits good high temperature properties as well as room temperature ductility in certain compositional ranges. However, at intermediate temperatures ($<1000°$C), some alloys in this system show a significant decrease of ductility. Thus, recently research has been conducted on the tensile behavior and discontinuous yield behavior of some alloys in this system. These studies have shown strong evidence for reduction in ductility at intermediate elevated temperatures. This phenomenon may be attributed to the O-phase,

which forms at these intermediate elevated temperatures in these alloys. The O-phase has a stoichiometry of Ti$_2$AlNb with orthorhombic crystal structure. Tensile tests have been performed on the alloy of composition Nb-40Ti-15Al-5Cr. Cr was added to improve the oxidation resistance. Transmission electron microscopy studies on specimens near the fracture surface revealed certain interesting observations, which include preferential slip for.certain variants of O-phase in B2 matrix. Efforts are in progress to study the same phenomenon on Nb-40Ti-15Al alloy samples with different intermediate temperature heat treatments. This would give insight to functional dependence between the undesirable effect of reduction in ductility and the formation of O-phase. The alloy Nb-40Ti-15Al has been reported to have a significant amount of room temperature ductility when compared with the Cr added alloy. Consequently, significant amount of dislocation activity could be accommodated by the specimen during compression tests. In this paper, interesting observations regarding preferential slip in the two above mentioned alloys will be discussed in detail. In addition, some newly emerging observations in the ongoing effort on the characterization of the preferential slip will also be presented.

N5.32
THE FORMATION OF AN ORDERED OMEGA-RELATED PHASE IN THE CENTRAL PORTION OF THE Nb-Ti-Al SYSTEM. D.T. Hoelzer, I.M. Anderson, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN; F. Ebrahimi, Materials Science and Engineering Department, Univ. of Florida, Gainesville, FL.

Transmission electron microscopy (TEM) was used to investigate the formation of an ordered omega-related phase in an alloy containing 33Ti-27Nb-40Al (at.%). The results showed that a single bcc β phase was present at temperatures above 1400°C and that it ordered to the B2 phase upon cooling. However, the B2 phase transformed completely to an omega-related phase during slow cooling from annealing temperatures above 1400°C and also during low temperature annealing at 600°C. Precipitates of the omega-related phase had two size distributions, a coarse size of 0.5 to 1.0μm and a fine size of 10 to 50nm, that depended on the formation conditions. Convergent beam electron diffraction (CBED) showed that the coarse precipitates possessed the P63/mcm space group. The structural analysis indicated that the formation of the coarse precipitates involved additional chemical ordering in the atomic site occupancy that was inherited from the B2 phase and that the atomic site occupancy consisted of Al (2b) and Nb (4d) atoms on single layers and Ti (6g1) and Al (6g2) on double layers in the hexagonal close-packed structure. The transformation of the β phase to the coarse omega phase is proposed using subgroup and symmetry relations. This type of analysis suggests that the fine precipitates have a ordered trigonal structure. Research at the Oak Ridge National Laboratory (ORNL) SHaRE User Facility was sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.

N5.33
FIRST-PRINCIPLES CALCULATIONS OF ELECTRONIC STRUCTURE AND ELASTIC PROPERTIES FOR MoV, MoNb, AND MoNb IN THE B2 PHASE. Romeo de Coss, Gabriel Murrieta, Aaron Aguayo, Department of Applied Physics, CINVESTAV-Merida, MEXICO.

First-principles total-energy electronic structure calculations based on the full-potential linearized augmented plane wave (LAPW) method have been used to study the electronic and elastic properties of MoV, MoNb, and MoTa in the B2 (CsCl) phase. The calculated equilibrium lattice constants are all within 1% of the experimentally determined value. The electronic structure around the Fermi level and the chemical bond are analyzed. From the calculated values of the elastic constants, we have determined the ductility and the melting temperature using empirical correlations for the three ordered alloys. In particular, we found that MoTa present the more covalent bond, while MoNb is the most ductile of these intermetallic compounds. This work was supported by Consejo Nacional de Ciencia y Tecnologia (CONACYT, Mexico) under Grant. No. 34501-E.

N5.34
GROWTH OF COBALT TETRAANTIMONIED BY VERTICAL BRIDGEMAN METHOD AND EFFECTS OF POST ANNEALING ON CRYSTAL QUALITY. M. Akasaka, G. Sakuragi, H. Suzuki, T. Iida, Y. Takanashi, S. Sakuragi[a], Science University of Tokyo, Dept of Materials Science and Technology, Chiba, JAPAN; [a]Union Material Inc, Ibaraki, JAPAN.

Cobalt tetraantimonied (CoSb3) has attracted much attention as a promising thermoelectric material for use in energy conversion, because of its appreciable conversion efficiency even at a high temperature. In growing a single crystal of CoSb3, there exists a

difficulty that such other phases as CoSb and CoSb2 are easily formed. In order to obtain CoSb3 with high crystalline quality (to improve uniformity and reproducibility), CoSb3 Crystal has been grown by a vertical Bridgeman (VB) method. The growth was performed in an electric furnace without seed, with 10 atomic % of Co and 90 atomic % of Sb sources charged in a quartz ampoule crucible. The pulling rate during growth was varied from 0.6 to 2.8 mm/h and the axial temperature profile was approximated by a linear gradient of 70 to 100°C/cm near the melt-solid interface. The composition of grown samples was characterized using electron probe microanalysis (EPMA) and x-ray diffraction (XRD). Seebeck coefficient, electric conductivity, and power factor have been evaluated. For a various growth conditions, polycrystalline CoSb3 has been successfully obtained without forming such other phases as CoSb and CoSb2, but a metal Sb was observed along the CoSb3 grain boundary. An optimum growth-condition of minimizing the introduction of Sb was by reducing the growth speed to 0.6 mm/h and setting the temperature graduation to 80°C/cm obtained, thereby each CoSb3 grain being proximately located. This sample showed the Seebeck coefficient and electric conductivity comparable to those previously reported, in spite of the fact that it involves a slight amount of Sb at the grain boundary. In order to remove Sb, the heat treatment at 800°C for 20 h was carried out in a vacuum, thereby the residual Sb being sufficiently eliminated. The obtained Seebeek coefficient and electric conductivity of the post-processed sample have been improved significantly and this causes much better power factor to be observed.

N5.35
MICROSTRUCTURE AND PLASTIC DEFORMATION IN UNIDIRECTIONALLY SOLIDIFIED $NbSi_2(C40)/MoSi_2(C11_b)$ CRYSTALS. Takayoshi Nakano, Yasuhiro Nakai, Yukichi Umakoshi, Osaka University, Graduate School of Engineering, Department of Materials Science and Engineering, Suita, Osaka, JAPAN.

Microstructure and plastic deformation behavior in duplex silicides composed of C40 and $C11_b$-type phases were examined using pseudo-binary $(Nb, Mo)Si_2$ crystals with a single set of lamellae. Single crystals with a single phase of the C40-type were grown from the master ingot containing different compositions of $(Nb_xMo_{1-x})Si_2$ (x=0.15~0.20) by a floating zone method and subsequently two-phase microstructures containing a single set of lamallae were obtained by heat treatment in the temperature range between 1200°C and 1600°C. During the heat treatment, the $C11_b$ phase was transformed from the C40 matrix by satisfying the crystallographic relationship of $(0001)_{C40}//(110)_{C11b}$ and $[11\overline{2}0]_{C40}//[1\overline{1}1]_{C11b}$ at the lamellar boundary, while the randomly oriented $C11_b$ grains also appeared at the further annealing. As a result, the duplex crystals with a single set of lamellae contain the C40 phase with a single orientation and three variants of the $C11_b$ phase. The lamellar spacing and the volume fractions of their phases depended strongly on alloying composition, annealing temperature and time.
In compression tests, yield stress and fracture strain of the duplex silicide crystals depended strongly on temperature and angle (ϕ) between the laoding axis and lamellar boundaries, similarly to TiAl-PST crystals. At $\phi=0°$, the specimens fractured just after showing high yield stress even at 1400°. In contrast, at $\phi=45°$ where shear deformation occurred parallel to lamellar boundaries, low yield stress and significant plastic strain were acheived at 1400°C.

N5.36
COEFFICIENT OF THERMAL EXPANSION ANISOTROPY IN TRANSITION METAL SILICIDES. M.J. Kramer, M. Akinc, A.J. Thom, J.J. Williams and H.L. Zhao, Dept of Materials Science and Engineering and Ames Laboratory, Iowa State University, Ames, IA.

Coefficient of thermal expansion (CTE) anisotropy is problematic for low symmetry intermetallics. Stresses developed during thermal cycling result in extensive cracking and eventually lead to failure. High temperature powder diffraction using high energy synchrotron radiation in a Debeye-Scherrer transmission geometry provides a practical tool to measure thermal expansion in multi-phased samples and to explore effects of dopants on changing CTE. We have studied CTE in two related systems, $Ti_5Si_3Z_x$ (Z = B, C, O, N) and Mo_5Si_3B. The Ti silicide forms the $D8_8$ structure while the Mo silicide with B forms either the $D8_m$ of $D8_l$ structure, depending on the Si:B ratio. The $D8_8$ and the $D8_m$ both exhibit large CTE anisotropy between the a- and c-lattice directions. The addition of dopants in the Ti silicide and the Si:B ratio in the Mo silicide had only a minor influence on the CTE anisotropy. On the other hand, the CTE for the $D8_l$ structure was nearly isotropic, consistent with theoretical calculations and more recently, neutron diffraction experiments. This work was performed at Ames Laboratory, and was supported by the Director of Energy Research, U.S. Department of Energy, under contract No. W-7405-ENG-82.

N5.37
$C11_b/C40$ LAMELLAR STRUCTURE IN A Ta-ADDED

MOLYBDENUM DISILICIDE.
Fu-Gao Wei, Yoshisato Kimura, Yoshinao Mishima, Department of Materials Science and Engineering, Tokyo Institute of Technology, Yokohama, JAPAN.

The detrimental properties of molybdenum disilicide ($MoSi_2$, $C11_b$ structure) such as poor room temperature ductility and insufficient high temperature strength could be improved by combining it with a C40 phase. Such a composite consisting of equal volume of each phase was obtained by adding only about 5 atomic percent Ta to $MoSi_2$. It was found that the two phases form a lamellar microstructure by homogenizing at 1673K after arc-melting casting. An alloy of the composition formula $(Mo_{0.85}Ta_{0.15})Si_2$ was used to investigate the lamellar structure by means of transmission electron microscope. Results show that the $C11_b$ phase grows from its parent phase on the $(0001)_{C40}$ plane according to the orientation relationship: $(110)_{C11b}//(0001)_{C40}$, $(-110)_{C11b}//(2-1-10)_{C40}$, $(001)_{C11b}//(01-10)_{C40}$. An emphasis was made to charaterize the interface boundary between the two different phases as well as the boundary between the possible $C11_b$ variants. A network of interfacial misfit dislocations was found in the semi-coherent $C11_b/C40$ interface. Three variants of the $C11_b$ phase were observed as expected from the orientation relationship. Boundaries between $C11_b$ variants also exhibit a network of interfacial dislocations. The nature of dislocations both in the C40 phase and in the $C11_b$ phase was analysed to verify whether or not the $C11_b$ phase inherits the dislocations from its parent C40 phase. Interaction between bulk dislocations and the interface boundary was discussed.

N5.38
THE β-$FeSi_2$ FORMATION AND THERMOELECTRIC POWER OF THE $FeSi_2$-Co BASE ALLOYS. Yoshisato Kimura, Yoshinao Mishima, Tokyo Institute of Technology, MS&E Dept, Yokohama, JAPAN; Kentaro Shindo, Grad Student, Mistubishi Heavy Industries Ltd, Nagasaki, JAPAN.

Thermoelectric generation from heat waste would give us a good solution for the conservation of our limited fossil fuel and the global environment. Our interest is focused on the development of thermoelectric materials applying as a component for micro gas turbine engine based co-generators on the distributed electric generation system. Some transition metal disilicides are attractive candidate materials for relatively high temperature application at around 1073 K. Especially, the β-$FeSi_2$ is a promising material not only because of its high thermoelectric power but also of its excellent oxidation resistance, low cost, and easy accessibility to recycle system. It is known that there are two $FeSi_2$ phases: the metallic α-$FeSi_2$ having chemical composition of 30Fe70Si in at%, not corresponding to Fe:Si=1:2, is high temperature phase and the intrinsic semiconductor β-$FeSi_2$, 33.3Fe66.7Si, is low temperature phase. A specific heat treatment is necessary to obtain the β-$FeSi_2$ phase for thermoelectric generation. It has been pointed out that adequate heat treatment requires very long time over 200 hours at 1073 K, which is a main issue having to be overcome. The path from metallic phases to β-$FeSi_2$ is very complicated, involving two major reactions: the peritectoid ϵ-FeSi α-$FeSi_2$=β-$FeSi_2$ and the eutectoid α-$FeSi_2$=β-$FeSi_2$ (Si), and a minor reaction: (Si) ϵ-FeSi=β-$FeSi_2$. In the present work, we have investigated the relationship between microstructure and material's physical constant such as thermoelectric power and electric conductivity of the $FeSi_2$-based cast alloys on which n-type element Co is doped with or without Cu for promoting the β-$FeSi_2$ formation. The formation rate of β-$FeSi_2$ from metallic ϵ and α phases is examined to seek for the desirable heat treatment condition for cast alloys, which is as lower temperature and shorter duration as possible than previously reported.

N5.39
MICROSTRUCTURES AND HIGH-TEMPERATURE STRENGTH OF Nb-BASED ALLOYS REINFORCED WITH IN-SITU SILICIDE. C.L. Ma, Y. Tan, H. Tanaka, A. Kasama, R. Tanaka, Japan Ultra-High Temperature Materials Research Institute, Ube, JAPAN; Y. Mishima, Department of MS&E, Tokyo Institute of Technology, Yokohama, JAPAN; S. Hanada, Institute for Materials Research, Tohoku University, Sendai, JAPAN.

In the recent study of authors, it has become apparent that the Nb-based alloys solid solution strengthening with Mo and W exhibit superior mechanical properties when comparing with the Nb metal. However, the high-temperature strength is still not sufficient to meet the requirement of structural materials for use at ultra-high temperature above 1500°C. Two-phase in-situ composites contained Nb-silicide and (Nb, Mo, W) solid solution (Nb_{ss}) were investigated in order to improve this point. It is reasonable to expect that the silicide phase provides high-temperature strength and the Nb_{ss} room-temperature toughness. In this paper, the microstructural features and mechanical properties of Nb-based alloys with Si contents less than16 at% and various of Mo and W concentrations, which were prepared using arc melting followed by a sufficient

annealing treatment, are described. The as-cast microstructures consisted of primary Nb_{ss} dendrites and interdendritic lamellar-like eutectic Nb_{ss}-$\beta(Nb,Mo,W)_5Si_3$. The interdendritic eutectic coarsened and formed two-phase network-like structure after extensive annealing treatment, while the $\beta(Nb,Mo,W)_5Si_3$ transformed to stable $\alpha(Nb,Mo,W)_5Si_3$ completely. The high-temperature strength increases with increasing the silicide volume fraction and also the Mo and W additions. Nb-16Si-10Mo-15W showed the highest compressive yield strength of 800MPa at 1500°C, and also exhibited excellent creep resistance strength. Indentation tests showed an effective effect of network-shaped Nb_{ss} on restraining the propagation of microcracks in silicide matrix. Fractographic observations revealed that the silicide phase fractured in a brittle cleavage manner; the primary Nb_{ss} particles in a cleavage mold with river pattern; and the eutectic Nb_{ss} in mixed molds of brittle cleavage and plastic stretching.

N5.40
TAILORING THE THERMAL EXPANSION ANISOTROPY OF Mo_5Si_3. Joachim H. Schneibel, Claudia J. Rawn, Chong Long Fu, Oak Ridge National Laboratory, Metals and Ceramics Division, Oak Ridge, TN.

The silicide Mo_5Si_3 with the W_5Si_3 structure exhibits a high anisotropy of its coefficients of thermal expansion (CTE) in the a and c direction, namely, CTE(c)/CTE(a)=2.2. In order to determine whether the CTE anisotropy can be controlled, Molybdenum was partially substituted with elements such as Ti, Zr, Nb, Ta, or W. CTE's were determined by high temperature powder x-ray diffraction. Partial substitution with 44 at.% Nb reduced the value of CTE(c)/CTE(a) to approximately 1. For higher Nb concentrations, CTE(c)/CTE(a) increased again. When nearly all the Mo was replaced by Nb, the crystal structure changed to the Cr_5B_3 structure of Nb_5Si_3. Our thermal expansion results are interpreted in terms of the site occupation of Nb, the increase in the interatomic spacing of the Mo atom chains (by Nb) along the c-direction, and the reduction in the anisotropy of lattice anharmonicity. This work was sponsored by the Division of Materials Sciences, Office of Basic Energy Sciences; the Division of Materials Sciences and Engineering and the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Transportation Technologies, as part of the High Temperature Materials Laboratory User Program, Oak Ridge National Laboratory. ORNL is operated by UT-Battelle, LLC, for the U.S. DOE under contract DE-AC05-00OR22725.

N5.41
HIGH TEMPERATURE COMPRESSION STRENGTH OF DIRECTIONALLY SOLIDIFIED Nb-Mo-W-Ti-Si IN-SITU COMPOSITES. Hisatoshi Hirai, Tatsuo Tabaru, Sha Jiangbo, Hidetoshi Ueno, Akira Kitahara, Kyushu National Industrial Research Institute, Tosu, JAPAN; Shuji Hanada, Institute for Materials Research, Tohoku Univ, Sendai, JAPAN.

In order to examine the potential of niobium solid solution (Nb$_{SS}$)/niobium silicide in-$situ$ composites as future high temperature structural materials, directionally solidified Nb-xMo-22Ti-18Si ($x =$ 10, 20 and 30 mol%) and Nb-xMo-yW-10Ti-18Si ($x =$ 10 and 20 mol%; $y =$ 0, 5, 10 and 15 mol%) alloys were prepared. After annealing at 1870 K for 100 h in a vacuum, the microstructures, Vickers hardness (H_V), high-temperature compressive strength and compressive creep behavior were examined. All the samples consisted of Nb$_{SS}$ and (Nb, Mo, (W,) Ti)$_5$Si$_3$ silicide. The H_V increased with increasing the content of molybdenum and tungsten. As for Nb-xMo-22Ti-18Si system, samples with $x =$ 10 had the highest maximum stress at 1670 K, but it showed a sharp stress drop after reaching the maximum stress. Samples with $x =$ 20 and 30 showed lower yield and maximum stresses than that with $x =$ 10, while they showed small stress drop and almost constant flow stress of 330 and 400 MPa, respectively, for large strain range. The sample of Nb-20Mo-22Ti-18Si had the minimum creep rate ($\dot{\varepsilon}_m$) of 9.6×10^{-7} s^{-1} at 1670 K and the initial load of 200 MPa. In general, the samples in Nb-xMo-yW-10Ti-18Si system had higher yield and maximum stress than those in Nb-xMo-22Ti-18Si system, although the stress decreased gradually after reaching the maximum stress and showed no steady state deformation. The $\dot{\varepsilon}_m$ of the sample of Nb-10Mo-15W-10Ti-18Si was 1.4×10^{-7} s^{-1} at 1670 K and the initial load of 200 MPa, which was much slower than that of Nb-20Mo-22Ti-18Si compared at the same testing condition. The acceleration of the creep rate in the third creep regime of Nb-10Mo-15W-10Ti-18Si was slower than that of Nb-20Mo-22Ti-18Si.

N5.42
GROWTH OF THE Mo_5SiB_2 PHASE IN A Mo_5Si_3/Mo_2B DIFFUSION COUPLE. Sungtae Kim, R. Sakidja, Z. Dong, J.H. Perepezko, Dept of Materials Science and Engineering, University of Wisconsin-Madison, Madison, WI; Yeon Wook Kim, Dept of Materials Science and Engineering, Keimyung University, Taegu, KOREA.

The high melting temperature and oxidation resistance of the Mo_5SiB_2 (T2) phase and multiphase microstructures incorporating the T2 phase in the Mo-Si-B system have motivated further studies for applications in very high temperature environments. Since the long term microstructural stability is determined by diffusional processes, a diffusion couple consisting of binary boride and silicide phases has been examined in order to evaluate the kinetics of T2 phase development and the relative diffusivities controlling the kinetics. Long term annealing (500 hrs) of the Mo_5Si_3/Mo_2B diffusion couple yields the phase sequence of Mo_5Si_3/Mo_3Si/T_2/Mo_2B at 1600°C. This indicates that the T_2 phase initiates and grows from the Mo_2B side to a thickness of about 32mm and the Mo_3Si phase initiates and grows from the Mo_5Si_3 side to a thickness of about 15mm. Other annealing treatments allow for an analysis of the diffusion kinetics based upon the layer thickening and composition profile measurements. To identify the crystallographic growth direction of T2 on Mo_2B, a wedge shaped TEM sample with very thin leading edge was prepared. Microstructure images indicate that the growth mode of the T2 phase is columnar. There is a clear tendency for the growth of T2 to be approximately normal to c-axis and for neighboring columnar grain interfaces to be semicoherent. The preferential growth direction of the T2 phase resembles that observed in the T2 grains produced from the solidification reaction. The preferential growth behavior may be considered from the crystal structure of the T2 phase wherein the network of the metalloid components in the c-axis is absent. The support of the AFOSR (F49620-00-1-0077) is gratefully acknowledged.

N5.43
INCOMMENSURATE STRUCTURE IN Al-RICH TiAl ALLOYS. S. Wang, D. Fort, I.P. Jones, J.S. Abell, School of Metallurgy and Materials, The University of Birmingham, Birmingham, UNITED KINGDOM.

The microstructures of Ti-Al alloys in the range 52-62 atomic % Al have been studied. These compounds consist of a basic L10 structure on which is superimposed an irrational modulated structure (Ti$_3$Al$_5$ related). This is incommensurate by occupation (as opposed to strain). It has two-dimensional modulations in which the wave vectors are q1 = α(a* b*) and q2 = α(-a* b*) where a* and b* are the basis of L10 and α is an irrational fraction. α = 0.345-0.26 and decreases with Al concentration up to 60% Al, i.e., the positions of the satellites change continuously with varying Al concentration. A third phase, TiAl2, appears at a composition of 62% Al which means that no Ti$_3$Al$_5$ (62.5% Al) of stoichiometric composition can ever exist in the arc-melted samples. The possible effects of these incommensurate structures on the plastic deformation of L10 are discussed.

N5.44
EFFECT OF SURFACE DEFECTS ON THE FATIGUE BEHAVIOUR OF A CAST TiAl ALLOY. Mohamed Nazmy, Marc Staubli, ABB Alstom Power, Baden, SWITZERLAND; Giovanni Onofrio, Valentino Lupinc, CNR-TEMPE, Milan, ITALY.

The effect of surface defects on the performance of TiAl base alloys is an issue of importance in contemplating their application into engine components. Due to the relatively low ductility and low impact resistance of gamma alloys the validation of models for estimating economic life and for safe-life approaches employed for components becomes of great importance. Surface defects can be attributed to various sources during the manufactoring or handling of the components. In fact little is known about the detrimental effects of surface defects on gamma alloys. In the present study, the effect of artificially introduced surface defects, on the high cycle fatigue of the Ti 47Al 2W 0.5Si, will be investigated and correlated with the crack growth behaviour at temperatures of 700 and 750°C and at different R ratio values. The results are reported in the form of the Kitagawa diagram in which the safe and unsafe zones for the crack advance are defined.

N5.45
THE GENERATION OF STACKING FAULT DIPOLES AND DISLOCATION ACTIVITY IN γ-TiAl. Fabienne Grégori, LPMTM, Institut Galilée, Villetaneuse, FRANCE; Patrick Veyssiére, LEM, CNRS-ONERA, Châtillon, Cedex, FRANCE.

Faulted dipoles (FDs) are a frequent and sometimes dominant feature within microstructures encountered in γ-TiAl deformed at low and intermediate temperatures. The contribution of FDs to deformation has however not been assessed yet by lack of a mechanism that would explain why these defects form so readily. The present model is founded on TEM observations of Al-rich γ-TiAl single crystals oriented so as to activate single <011]{111} slip. Foils sectioned parallel to the slip plane enable full correlation between FDs and operating dislocations. It is shown that a FD nucleates at the tip of a <011] screw lock as the latter is being unzipped by a mobile mixed segment. The reaction is encouraged by the fact that the <011]

dislocation is asymmetrically dissociated into two components with 1/6<121] and 1/6<154] Burgers vectors. A partial with 1/3<112] Burgers vector and zonal core is created at the 1/6<154] partial, as the parent <011] dislocation switches from a 3D non planar configuration at the lock to a fully coplanar core at the connecting mixed segment. The ensuing local core configuration is capable of bordering an extrinsic stacking fault. FDs are thus formed as a by-product of the propensity of <011] dislocations towards forming screw locks. Their presence should therefore be regarded as a direct manifestation of the operation of <011] dislocations during deformation.

N5.46
WEAR RESISTANCE OF TiAl ALLOYS SURFACE NITRIDED WITH AMMONIA. Bin Zhao, Jian Sun, Jiansheng Wu, Fei Wang School of Material Science and Technology, Shanghai Jiao-Tong Univ, Shanghai, PR CHINA, Open Laboratory for High Materials and High Temperature Test, Shanghai Jiao-Tong Univ, Shanghai, PR CHINA.

It is known that the intermetallics compound TiAl has attractive and comprehensive properties, which are useful for applications in aircraft, aerospace structures and automobiles. In recent years, more and more attention has been paid to the investigation on the surface modification of TiAl alloys. However, compared to the other methods, high temperature gas nitridation with ammonia is a competitive one for its simple handling and money saving. In this work, the Ti-47Al-2Nb-2Cr-0.2Si alloy was nitrided according to the different technics with ammonia. The surface knoop hardness and tribological behaviors were systematically investigated. Compared to the non-nitrided samples, the knoop hardness of the corresponding nitrided alloys was greatly increased with increasing nitridation temperature and time. The hardness values of samples nitrided at 1073K, 1133K and 1213K with 50 h were 1008.268 kg/mm^2, 1038.391 kg/mm^2 and 1286.206 kg/mm^2 respectively. The wear behavior of the TiAl alloy with and without nitridation has been studied by the block-on-ring wear test. According to the weight loss and wear trace width of the block wear volume and wear rate were calculated. The results showed that the existence of the nitriding layers significantly enhanced the wear resistance of the TiAl alloy. Furthermore, the wear resistance of the nitrided samples was improved with the increasing of the nitridation temperature and time. Hence it is necessary to raise the nitridation temperature and prolong the nitridation time so as to produce a wear resistant layers on the TiAl alloy. Finally, the tribological mechanism of the TiAl alloys nitrided with ammonia was discussed.

N5.47
DEFORMATION OF Ni$_3$Al POLYCRYSTALS IN A MULTI-ANVIL APPARATUS AT EXTREMELY HIGH STRESSES. J.W. Otto, Joint Research Center for the European Commission (Headquarters, Brussels); J.K. Vassiliou, Dept. of Physics, Villanova University, Villanova, PA; and G. Frommeyer, Max-Planck Institute für Eisenforshung, Dusseldorf, GERMANY.

The compressional behavior in a multi-anvil apparatus of pure NaCl and of a foil of Ni$_3$Al embedded in a pressure medium of NaCl has been studied by energy-dispersive X-ray diffraction. At ambient temperature, the pressure and stresses, determined from line positions of NaCl, were constant throughout the sample chamber. Line positions and line widths of NaCl reflections were reversible on pressure release. A saturation of microstrains observed in NaCl at 2 GPa is thus attributed to brittle fracture setting in at uniaxial stresses of around 0.3 GPa. Ni$_3$Al polycrystals, in contrast, undergo extensive (ductile) plastic deformation above 4 GPa. The compressional behavior of both Ni$_3$Al and NaCl is identical to that previously determined in a diamond anvil cell. While a multi-anvil device has the advantage, compared with a diamond anvil cell, of constant pressure and stress through the sample chamber, microstrains in polycrystalline samples arise in both devices. Samples in a multi-anvil apparatus thus need to be mixed with a pressure medium and to consist of essentially single crystals just as in a diamond anvil cell. Annealing experiments at high pressures confirm that the release of the uniaxial stress component in the pressure medium does not cause a release of microstrains in the embedded sample if the latter has been plastically deformed.

N5.48
MICROSTRUCTURAL STABILITY OF PST-TITANIUM ALUMINUM DURING LOW STRAIN MECHANICAL TESTING AT ELEVATED TEMPERATURE. Abishek Gupta, Jorg M.K. Wiezorek, Dept of MS&E, University of Pittsburgh, Pittsburgh, PA.

The anisotropic mechanical properties associated with lamellar TiAl based intermetallics are very well documented in the literature and so-called "soft" and "hard" deformation modes can be distinguished. Interestingly, the elevated temperature creep resistance of lamellar TiAl appears to be related to the "soft" mode behavior, which in general is unaffected by the presence of the lamellar interfaces, yet

lamellar refinement improves the creep strength. The present systematic study investigates the role of microstructural evolution and interface related deformation processes active during elevated temperature loading on strength retention of lamellar TiAl. The stability of microstructures in PST TiAl alloys with 48 at % Al after mechanical testing, at constant low strain rate (∼10exp-5) along "soft" and "hard" orientations (f = 0°, 45° & 90°), at 750°C was studied by transmission electron microscopy as well as scanning electron microscopy. Furthermore, the deformation modes active in the various lamellae under these different sets of loading conditions have been identified by TEM. The emphasis of the present study was on the change in distribution and morphology of the alpha-2 and gamma phases. Based on the results regarding the defect activity and the microstructural evolution possible instability mechanisms operative at such strain and temperature conditions have been identified. Implications of these experiments are discussed in relation to the elevated temperature creep behavior in these microstructures. Part financial support by the National Science Foundation with Dr. Bruce MacDonald as program manager and from the School of Engineering of the University of Pittsburgh is acknowledged.

N5.49
THE ROLE OF SOLID SOLUTION AND LAMELLAR INTERFACES ON THE CREEP RESISTANCE OF TiAl-BASE ALLOYS. W.-J. Zhang, S.C. Deevi, Research Center, Chrysalis Technologies Incorporated, Richmond, VA; C.T. Liu, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

The objective of this paper is to study the role of lamellar interfaces and solid solution of refractory elements like W and Nb on the creep resistance of TiAl alloys at different stress levels. The creep behavior of TiAl-base alloys containing high Nb and W was evaluated in the stress range 70-500 MPa at 760°C in the form of duplex and fully lamellar microstructures. The deformation substructures of the creep specimens were examined using TEM. The contribution of lamellar interfaces and solid solution at low stress (70-150 MPa) and high stress (200-500 MPa) regimes were discussed and compared with the data on conventional alloys.

N5.50
LONG TERM OXIDATION OF GAMMA TiAl ALLOYS AT 700°C. I.E. Locci, M.P. Brady, J.L. Smialek.

Gamma TiAl alloys are of great interest for high temperature structural applications. Most of the oxidation studies found in the literature have focused on the response of TiAl alloys to the environment at temperatures above 800°C, while near term structural applications will involve service below 800°C. The purpose of this research was to characterize the oxidation behavior of several model (TiAl, TiAl-Nb, TiAl-Cr, TiAl-Cr-Nb) and engineering alloys (XD, K5, Alloy 7, WMS) after long-term isothermal exposure (∼9000 h) at 700°C, and after shorter time exposure (∼1000 h) at 800°C in air. Field Emission and Microprobe Scanning Electron Microscopy was used to characterize the scales formed on these alloys. Similarities and differences observed in the scales are correlated with the various Nb, Cr, W, etc. ternary and quaternary microalloying additions.

N5.51
MICROSTRUCTURAL DEVELOPMENT IN A GRAIN-REFINED CREEP-RESISTANT TITANIUM ALUMINIDE ALLOY. H. Yang, T.T. Cheng and M. Aindow Dept of Metallurgy and Materials Engineering, Univ of Connecticut, Storrs, CT.

In recent work at the University of Birmingham, UK it has been shown that both the properties and the microstructural stability of lamellar TiAl-based alloys can be enhanced by heavy alloying. Alloys with compositions in the range Ti-44Al-8(Nb,Ta,Zr,Hf)-(0-0.2)Si-(0-1)B were investigated and it was shown that the microstructures of these were significantly different from those of binary or 48-2-2 type alloys, with lamellar plus gamma and/or transformed beta regions. These differences led to significant increases in the strength, creep resistance and/or ductility of these alloys depending on composition and thermal history [1,2]. In the present study we have considered the microstructural development in one of these alloys, Ti-44Al-4Nb-4Zr-0.2Si-0.3B, in more detail. This alloy was selected as having the most promising properties of those considered in the previous work. In this paper we will present SEM and TEM data on the character and distribution of the features in the microstructure as a function of thermal history. Particular emphasis will be placed upon the decomposition of the beta phase and the development of the lamellar colonies from prior alpha grains in this alloy. [1] T.T. Cheng and M.H. Loretto, Acta Mater. 46: 4801 (1998). [2] T.T. Cheng, M.R. Willis and I.P. Jones, Intermetallics 7: 89 (1999).

N5.52
SEGREGATIONS OF TERTIARY ELEMENTS TO THE LAMELLAR INTERFACES FOR A TiAl INTERMETALLIC

ALLOY. <u>Wei Zhao</u> and David E. Luzzi, University of Pennsylvania, Department of Materials Sciences and Engineering, Philadelphia, PA.

Polysynthetically-twinned (PST) TiAl is under evaluation for applications in rotary components in the aircraft and automotive industries due to its high specific strength, and a high strength-retention capability at elevated-temperatures. However, the low ductility at room- to mid-high temperatures of the material hinders its scale-up applications. Additions of certain tertiary elements to the binary TiAl system appear to mitigate the embrittlement. In this article, segregation of tertiary elements (W, Ta, Ni, Cu, and Mn) to the lamellar interfaces is investigated. Single crystals of a Ti-Al with 0.6% atomic percent tertiary additions are grown by an ASGAL optical floating-zone furnace. Segregations of these elements to the lamellar interfaces and the microstructure of the interfaces are characterized by a high-resolution JEOL 2010F field emission analytical transmission electron microscope, coupled with an energy dispersive x-ray spectroscopy elemental mapping technique. The mechanical responses of these ternary TiAl systems are studied using microhardness testing. From these results, the correlation between segregation, microstructure and mechanical properties will be established.

N5.53
INTERDIFFUSION AND PHASE BEHAVIOR IN PST TiAl / V AND PST TiAl / Ti DIFFUSION COUPLES. <u>Ling Pan</u>, David E. Luzzi, Univ of Pennsylvania, Dept of Materials Science and Engineering, Philadelphia, PA.

Poly-synthetically twinned (PST) TiAl has attracted a large amount of interest in the past decade for its potential as a high temperature structural material. The strongly crystallographic twins and pseudo-twins between the lamellae of the PST TiAl crystal provide an ideal system to study interface diffusion. A PST TiAl (49.3 at.% Al) "single crystal" is grown in an optical floating zone furnace. The as-grown crystal is cut in the $< 110 >$ direction parallel to the lamellar interfaces and then diffusion-bonded with pure V in a high vacuum hot-pressing furnace at $750°C$ for two hours after surface electro-polishing. After bonding the diffusion couple, a cross section through the interface is cut perpendicular to the bonding plane and the lamellar planes. Diffusion anneals are carried out in the same furnace for various times and temperatures. The sample is examined by back-scattered electron imaging in a JEOL6400 SEM at 20kV with quantitative wavelength-dispersive X-ray fluorescence spectroscopy (WDS) measurements of the Ti, Al and V compositions at many points throughout the diffusion couple. Consistently higher V contents are found within the $\alpha2$ phase than in the γ phase indicating faster diffusion of V. Field emission TEM (JEOL 2010F) is used to determine the distribution of V across and along the lamellar interfaces. The results in V are compared with an identical study made using a diffusion couple of PST TiAl and pure Ti.

N5.54
CONTROL OF LAMELLAR ORIENTATION IN γ-TiAl BASED PST CRYSTAL BY USING SEED CRYSTALS. <u>Yukinori Yamamoto</u>, Masao Takeyama, Takashi Matsuo, Tokyo Institute of Technology, Dept of Metallurgy and Ceramics Science, Tokyo, JAPAN; Hiroaki Morishima, Keisuke Koike, Nissan Motor Co., Ltd., Tokyo, JAPAN.

Unidirectional solidification of Ti-48Al binary alloy using γ-TiAl single-phase seed crystals has been carried out by an optical floating zone method. The lamellar orientation of the grown PST crystal succeeds to an orientation of the single crystal seed of Ti-57Al, while it fails to succeed in case of Ti-53Al seed. Microstructure analysis reveals that the single crystal seed of Ti-57Al exhibits a flat liquid/solid interface in melting ($\gamma \rightarrow \gamma$ + L) even after making contact with 48Al alloy to grow, whereas the seed of Ti-53Al shows an cellular interface due to the peritectic reaction in melting ($\gamma \rightarrow \alpha$ + L). At the 57/48 interface, an abrupt change of Al concentration was detected from the seed to the grown crystal, indicating an occurrence of composition travel to skip the pritectic reaction, which is responsible for the control of lamellar orientation of the grown PST crystals. The same attempt has been made by using the 57Al single crystal seed with a different orientation, and the lamellar orientation of the grown PST crystal was confirmed to succeed to the seed orientation. The detailed crystallographic orientation relationship between the 57Al seed the 48Al grown crystals, together with the growth mechanism, will be presented.

SESSION N6: NICKEL ALUMINIDES
Chairs: David G. Morris and Ronald D. Noebe
Wednesday Morning, November 29, 2000
Room 208 (Hynes)

8:30 AM *<u>N6.1</u>
DEFORMATION BEHAVIOR OF SINGLE AND POLYCRYSTALS OF (Fe,Ni)-Al INTERMETALLIC COMPOUNDS WITH THE B2 CRYSTAL STRUCTURE. <u>M.J. Mills</u>, P.S. Brenner, R. Srinivasan, Department of Materials Science and Engineering, The Ohio Sate University, Columbus, OH; T. Lograsso, 111A Metals Development, Ames Laboratory, Ames, IA; R.D. Noebe, NASA Glenn Research Center, Cleveland, OH.

The mechanical properties and the dislocation microstructure of single crystals with a range of compositions within the (Fe,Ni)-Al pseudobinary system have been investigated. This alloy system offers an opportunity to explore the effect of large substitutional solute additions to the properties of these ordered B2 intermetallic compounds, thereby bridging the behavior from FeAl to NiAl. Compression testing at room temperature has been performed on $< 001 >$ oriented single crystals as well as polycrystals with a family of compositions of the form Fex-Ni60-x-Al40. The single crystal experiments are specifically designed to explore the effect of composition on the behavior of a$< 111 >$. The polycrystalline samples have been used to study the transition from a$< 111 >$ dominated slip for Fe-rich compositions, to a$< 100 >$ dominated slip for Ni-rich compositions. In addition, the variation of yield strength and dislocation activity as a function of temperature has been studied in the $< 001 >$ oriented single crystals in order to examine the effect of composition on the transition to non-$< 111 >$ activity at higher temperatures. The results of this investigation will be discussed in light of solute strengthening mechanisms and relevant dislocation-based deformation models for B2 compounds. This research supported by the U.S. Department of Energy under contract no. DE-FG02-96ER45550 (for PSB, RS and MJM).

9:00 AM <u>N6.2</u>
ATOMISTIC MODELING OF TERNARY AND QUATERNARY ORDERED INTERMETALLIC ALLOYS. <u>Guillermo Bozzolo</u>, Ohio Aerospace Institute, Cleveland, OH and NASA Glenn Research Center, Cleveland, OH; Joseph Khalil, Matthew J. Bartow and Ronald D. Noebe, NASA Glenn Research Center, Cleveland, OH.

The phase structure of NiAl- and FeAl-based ternary and quaternary ordered intermetallic alloys is studied using the BFS method for alloys. A simple calculational procedure, based on the determination of atomic configurations containing different defect structures, is introduced. The computational simplicity of the approach, the lack of restrictions on the number and type of elements included, and the universality of the BFS parameters used - determined from first-principles calculations - allow for a detailed atom-by-atom analysis of the energetics, thus helping in the understanding of the driving force behind the behavior observed. The procedure is illustrated with two different examples: 1) the phase structure of ternary Ni-Al-Fe alloys, covering the transformation from B2 NiAl to B2 FeAl, and 2) the change in the solubility limit of Ti in NiAl due to the interaction with small quantities of a fourth element (Hf or Zr). The analysis is supplemented with results of large-scale Monte Carlo simulations and comparison with experimental results, when available.

9:15 AM <u>N6.3</u>
TRANSITION METAL IMPURITY-DISLOCATION INTERACTIONS IN NiAl: DISLOCATION FRICTION AND DISLOCATION LOCKING. <u>O.Yu. Kontsevoi</u>, Yu.N. Gornostyrev, and A.J. Freeman, Northwestern University, Dept of Physics and Astronomy, Evanston, IL.

The energetics of the interaction of a $< 100 > \{010\}$ edge dislocation in NiAl with early 3d transition metal impurities (Ti-Mn) and 4d transition metal impurities (Zr-Mo) was studied using the *ab-initio* real-space tight-binding LMTO-recursion method [1] with 20,000 atom clusters and up to 1,000 non-equivalent atoms in the dislocation core. A quasi-dynamical approach was employed to simulate the dislocation motion by generating a set of dislocation core configurations using the Peierls-Nabarro model with restoring forces determined from full-potential LMTO total energy calculations [2], with substitutional impurities placed in different positions relative to the dislocation core. We found that for most positions studied the interactions between impurities and the dislocation is slightly repulsive (dislocation friction). However, when the impurity is next to the central atom of the dislocation core, the interaction becomes strongly attractive, thus causing chemical dislocation locking. The nature of the locking is found to be due to the formation of the preferred bonding between the electronic states of the impurity atom and the localized electronic states appearing on the central atom of the dislocation core. The results are then discussed in the scope of experimental data on solid solution hardening in NiAl.
Supported by the AFOSR (Grant No. F49620-98-1-0321) and the NSF (Cooperative Agreement ACI-9619019 through the UIUC).
[1]. O.Yu. Kontsevoi, O.N. Mryasov, Yu.N. Gornostyrev, A.J. Freeman, M.I. Katsnelson and A.V. Trefilov, Phil. Mag. Lett., **78**, 427

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(1998).
[2]. N.I. Medvedeva, O.N. Mryasov, Yu.N. Gornostyrev, D.L. Novikov, and A.J. Freeman, Phys. Rev. B, **54**, 13506 (1996).

9:30 AM N6.4
MICROHARDNESS ANISOTROPY AND INDENTATION SIZE EFFECT IN SINGLE CRYSTAL NiAl. Michael E. Stevenson, Richard C. Bradt, Mark L. Weaver, The University of Alabama, Dept of Metallurgical and Materials Engineering, Tuscaloosa, AL.

Beta NiAl base intermetallic compounds are widely used as oxidation resistant coatings in aerospace applications, as seed interlayers in magnetic recording media, and are under consideration for use as structural components in advanced aerospace applications. This study uses Knoop microhardness to provide both a mechanical property evaluation of NiAl as well as to examine some commonly observed microhardness testing phenomena: i) microhardness anisotropy, and ii) the Indentation size effect. The low test load microhardness anisotropy is reported and analyzed for high purity single crystals of NiAl. In addition, the load dependence of the microhardness (known as the indentation size effect or ISE) is also addressed. The ISE is analyzed through a fundamental energy balance model that can be applied to all types of materials. Based on the results ascertained through the model, a load independent Knoop microhardness is determined for single crystal NiAl for the crystallographic planes tested in this study.

10:15 AM N6.5
THE EFFECTS OF MAGNETISM ON SOLID SOLUTION HARDENING IN NiAl ALLOYS WITH Fe AND Co ADDITIONS. C.T. Liu, C L. Fu, and L.M. Pike, Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, TN.

We report the first observation of the effect of magnetism on solid solution hardening in intermetallics. Solutes of Co and Fe at levels up to 12 at % were added to replace Ni in NiAl (60 at % Ni) alloys homogenized at $1250°C$ and quenched from $1000°C$. The selection of Co and Fe is based on the consideration of both atomic size and magnetic effects. Alloying with Fe results in substantial solid solution softening (instead of hardening) whereas additional Co causes essentially no change in hardness of NiAl alloys. These results can not be simply explained in terms of atomic size difference because the Goldschmidt radii of Ni, Co and Fe atoms are similar. First-principles calculations indicate that large magnetic moments are induced at Fe sites (but not in Co sites) when Fe atoms substitute for Ni in Al sublattices. The measurement of lattice parameters confirms the theoretical prediction that Fe additions significantly expand the lattice parameter of NiAl. The solid solution softening observed in NiAl Fe alloys is thus interpreted as a replacement of Ni anti-sites (which have a large hardening effect) with Fe anti-sites (which have a small hardening effect due to the formation of local magnetic moment) on Al-sublattices. This research is sponsored by the Division of Materials Sciences and Engineering, U.S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle, LLC.

10:30 AM N6.6
MEASURING THE ENERGETICS OF BULK THERMAL DEFECTS IN NiAl USING SURFACE MICROSCOPY. K.F. McCarty, N.C. Bartelt, J.A. Nobel, Sandia National Laboratories, Livermore, CA.

We report a new way to characterize the bulk properties of intermetallic alloys by observing the surface morphology in real time. We use a low-energy electron microscope (LEEM) to image the unit-cell-high steps at the (110) surface of NiAl as well as the screw component of dislocations that terminate at the surface. When the temperature of the NiAl crystal is increased, the surface steps advance. With a temperature decrease, the reverse happens – the surface steps recess. These motions result from how the concentrations of the bulk thermal defects change with temperature. That is, when the temperature is changed, the bulk defect concentration is no longer in equilibrium. To restore equilibrium, vacancies are either created or annihilated at the surface steps. This causes the surface steps to move and results in a net mass flux into or out of the bulk that equilibrates the crystal. Thus our surface microscopy technique can unambiguously determine whether the thermal vacancy concentration in a material increases (as for our Ni-rich crystal) or decreases with increasing temperature. At a given temperature, we oscillate the temperature at a rate that is slow enough to ensure that the surface and bulk are in equilibrium. In this manner, we determine an effective formation energy of the thermal defects, which, for our Ni-rich crystal, is exactly one half that of the stoichiometry-preserving "triple-defect." Our value agrees reasonably well with other experimental results but is less than literature calculations. We will also show the various types of dislocation motion and reactions that occur at the NiAl surface. This work was performed under the U.S. Department of Energy contract DE-AC04-94AL85000 and supported by the Office of Basic Energy Sciences-Division of Materials Sciences.

10:45 AM N6.7
MOLECULAR DYNAMICS SIMULATIONS OF DIFFUSION MECHANISMS IN NiAl. Diana Farkas and Benjamin Soulé de Bas, Dept. of MS&E, Virginia Polytechnic Institute and State University, Blacksburg, VA.

Molecular dynamics simulations of the diffusion process in ordered B2 NiAl at high temperature were performed using an embedded atom interatomic potential. Diffusion occurs through a variety of cyclic mechanisms that accomplish the motion of the vacancy through nearest neighbor jumps restoring order to the alloy at the end of the cycle. The traditionally postulated six-jump cycle is only one of the various cycles observed and some of these are quite complex. The results are analyzed in terms of the activation energies for individual jumps calculated using molecular statics simulations.

11:00 AM N6.8
LONG TERM CREEP AND OXIDATION BEHAVIOR OF A LAVES PHASE STRENGTHENED NiAl-Ta-Cr ALLOY FOR GAS TURBINE APPLICATIONS. Martin Palm, Gerhard Sauthoff, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, GERMANY.

A Laves phase strengthened NiAl-Ta-Cr alloy (IP 75) has been developed for structural applications in gas turbines as well as in heat exchangers. It has a lower density and a higher thermal conductivity as well as a higher melting point than conventional superalloys. Different methods for alloy production have been established including investment casting (FG) and a powder metallurgical method (PM). The alloy has been tested extensively to meet the demanding requirements for those applications, i.e. sufficient resistance to creep at $1250°C$ and corrosive attack.
Creep properties have been determined in compression and tension. Tension tests up to 10000 hours were performed at $900°C$ and $1000°C$ for PM and FG material. In compression secondary creep rates as a function of stress were studied between $900°C$ and $1300°C$.
The oxidation behavior of the PM and FG material was studied for up to 1000 hours by thermogravimetry in air at constant temperature between $600°C$ and $1300°C$. The results are compared with results obtained from long term isothermal and cyclic oxidation experiments in air at $1200°C$ for 17900 hours. Microstructures and scales were examined by light optical and scanning microscopy, X-ray powder diffraction and electron probe microanalysis.

11:15 AM N6.9
1300 K COMPRESSIVE PROPERTIES OF DIRECTIONALLY SOLIDIFIED Ni-33Al-33Cr-1Mo. J. Daniel Whittenberger, S.V. Raj, NASA-Glenn Research Center, Cleveland, OH; Ivan E. Locci, Case Western Reserve University at the NASA-Glenn Research Center, Cleveland, OH.

Directional solidification (DS) of NiAl-X systems has shown promise for the simultaneous improvement of elevated temperature strength and room temperature toughness. In general it was believed that such benefits could only be possible when the structure was perfectly aligned and fault free. Unfortunately such ideal microstructures tend to demand very slow grow rates which would be impracticable for commercialization. To determine if faster growth rates could produce materials with acceptable properties, the eutectic system Ni-33Al-33Cr-1Mo (at %) has been directionally solidified over a wide range of rates: 7.6 to 508 mm/h. To date the alloy chemistry, microstructure and 1300 K slow strain rate compressive properties of as-grown and as-cast samples have been determined. Chemical analysis revealed agreement between as-cast and DS'ed compositions, where all the alloys lie in the band (maximum/minimum) of Ni-33.7/31.2Al-34.9/32.9Cr-1.05/0.99Mo. Directional solidification at or below 12.7 mm/h produced lamellar (Cr,Mo) plus NiAl eutectic grains, while faster rates up to 254 mm/h lead to cells containing radial eutectic lamellae or cells with (Cr,Mo) fibers in a NiAl matrix at 508 mm/h. Constant velocity and constant load creep testing in compression revealed that all materials DS'ed at rates ranging from 25.4 to 254 mm/h possessed equivalent strength levels which were significantly above that measured for as-cast alloy and somewhat improved over those exhibited by faster or slower growth rates. Future effort will be concentrated on low temperature fracture toughness measurements as well as the 1200 and 1400 K compressive properties.

11:30 AM N6.10
FRACTURE STRENGTH OF GRAIN BOUNDARIES IN Ni_3Al. Jian-Qing Su, M. Demura and T. Hirano, National Research Institute for Metals, Tsukuba, JAPAN.

It is well known that grain boundaries of boron-free NI_3AL are brittle. Previous works suggested that low angle and $\Sigma3$ boundaries are crack-resistant, and others are much less crack-resistant. However, results were very qualitative. The objective of this study is to make clear experimentally this point, i. e. to establish a relation between

fracture strength and grain boundary types. We prepared miniature bicrystal tensile specimens having single boundaries with various Σ-values for stoichiometric NI_3AL and measured the fracture strength of grain boundaries at room temperature. Low angle, $\Sigma 3$ and $\Sigma 9$ specimens showed high fracture strengthes over 524 MPa with transgranular fracture. The elongations to fracture were large, $52\sim74\%$. Other Σ-value specimens fractured intergranularly, and the fracture strengthes depended on the Σ value. $\Sigma 11$ and $\Sigma 13$ specimens fractured at the stress level of $360\sim370$ MPa with $10\sim40\%$ elongations. Compared to these boundaries, $\Sigma 5$ and $\Sigma 7$ boundaries were weak and fractured below 135 MPa showing less than 10% strain. Most random boundaries were also weak similar to the $\Sigma 5$ and $\Sigma 7$ boundaries with some exceptions. Thus, a relationship between fracture mode, fracture strength and Σ-value boundaries has been established.

11:45 AM <u>N6.11</u>
NONSTOICHIOMETRY AND DEFECT MECHANISM IN INTERMETALLICS WITH L1$_2$-STRUCTURE. <u>Herbert Ipser</u>, Olga P. Semenova, Regina Krachler, Inst of Inorganic Chemistry, Univ of Vienna, AUSTRIA.

Some of the intermetallic compounds with L1$_2$-structure like Ni_3Al, Ni_3Ga, or Pt_3Ga show considerable ranges of homogeneity. This is usually caused by different types of point defects, i.e. anti-structure atoms or vacancies, whereas interstitials play a negligible role in this type of ordered compounds. Of course, the types of defects that are present and their compositions are closely connected to a number of physical properties. A statistical-thermodynamic model was derived which describes the compositional variation of the partial thermo-dynamic properties in these compounds based on either the defect formation energies or so-called disorder parameters (which are the concentrations of thermal defects at the exactly stoichiometric composition) as variable parameters. The model was applied to Ni_3Al using literature data for the aluminum activities, as well as to Ni_3Ga and Pt_3Ga using gallium activity values obtained by emf-measurements in our laboratory. In this way it was possible to estimate values for the energies of formation of the four different types of point defects (anti-structure atoms and vacancies on the two sublattices) as well as for the disorder parameters. It turned out that the deviation from stoichiometry is in principle caused by anti-structure atoms whereas the concentration of vacancies on the two sublattices are negligibly small.

SESSION N7: TITANIUM ALUMINIDES III
Chairs: Dennis M. Dimiduk and Kevin J. Hemker
Wednesday Afternoon, November 29, 2000
Room 208 (Hynes)

1:30 PM <u>N7.1</u>
STATIC AND DYNAMIC STRAIN AGEING IN TWO-PHASE GAMMA TITANIUM ALUMINIDES. <u>Ulrich Christoph</u>, Fritz Appel, GKSS-Research Centre, Geesthacht, GERMANY.

The deformation behaviour of two-phase titanium aluminides was investigated in the intermediate temperature interval 450-750 K. The observed deformation characteristics include discontinuous yielding and negative strain rate sensitivity, which are indicative of the operation of the Portevin-LeChatelier effect. The pinning processes occuring at the dislocations and associated with these phenomena were studied by static strain ageing experiments. A wide range of alloy compositions and microstructures were investigated in order to identify the relevant defect species. Accordingly, dislocation pinning occurs with fast kinetics and is characterized by a relatively small activation energy of 0.7 eV, which is not cosistent with a conventional diffusion process. Furthermore, the strain ageing phenomena are most pronounced in Ti-rich alloys. This gives rise to speculation that antisite defects are involved in the pinning process. The implications of the ageing processes on the deformation and fracture behaviour of two-phase titanium aluminide alloys will be discussed.

1:45 PM <u>N7.2</u>
MECHANICAL PROPERTIES OF γ-TiAl AND α_2-Ti$_3$Al SINGLE PHASE ALLOYS WITH Zr ATOMS IN SOLUTE SOLUTION. A. Ponchel[1], S. Margueron[1], <u>G. Hug</u>[1], M. Jaouen[2], S. Brochard[2], J. Grilhé[2], J. Woicik[3] and P.E. Petit[4]; [1]Laboratoire d'Études des Microstructures, UMR 104 CNRS-ONERA, Châtillon Cedex, FRANCE; [2]Laboratoire de Métallurgie Physique, UMR 6630 du CNRS-Université de Poitiers, Futuroscope Chasseneuil Cedex, FRANCE; [3]National Institute of Standards and Technology, Gaithersburg, MD; [4]ESRF, Grenoble Cedex, FRANCE.

Mechanical properties of ternary $(\gamma$-Ti$_{46}$Al$_{54})_{97}$Zr$_3$ and $(\alpha_2$-Ti$_{65}$Al$_{35})_{97}$Zr$_3$ alloys have been studied by compression tests in a wide temperature range $(100 - 1000$ K). These compositions were chosen to mimic the compositions in the two phased alloys which are currently developed for application. By comparison to binary alloys, it was found that the Zr induces a strengthening of the γ-TiAl alloys whereas it tends to soften the α_2-Ti$_3$Al. In order to explain the origin of this behavior, the alloys have been characterized by X-ray Absorption Spectroscopy (XAS) to determine the site occupancy and local structure around Zr solute atoms and the fine structure of dislocation is investigated by Weak-Beam Transmission Electron Microscopy. From the analysis of X-ray Absorption Near Edge Structure (XANES) and X-ray Extended Fine Structure (EXAFS) recorded at the Zr K edge, it was found that the substitution site for Zr solute atoms was the Ti site. The displacement field around Zr atoms has been mapped out up to the fourth coordination shell of near neighbors determined experimentally from a multiple scattering analysis of the EXAFS spectrum. The strain field is compared to ab initio calculation using Full Potential Linear Augmented Plane Wave (FLAPW) method. A preliminary study of the interaction between elastic strain around Zr solute atoms and the dislocation strain field was performed.

2:00 PM <u>N7.3</u>
MICROSTRUCTURE AND PROPERTY CHANGE OF Ti-49Al ALLOY INDUCED BY HYDROGEN-CHARGING. K.W. Gao, <u>E. Abe</u> and M. Nakamura; National Research Institute for Metals, Tsukuba, JAPAN.

We have investigated an effect of hydrogen gas-charging on the microstructure and the mechanical property of a Ti-49at.%Al alloy. For Ti-49Al alloy, both the γ-single phase and γ-α_2 two-phase microstructures are obtainable by a simple heat treatment, and thus the alloy is a good candidate to study a role of the α_2 phase on the property change. The fine α_2-γ lamellae-lath containing microstructure was selected as a two-phase Ti-49Al, which is known to show a good ductility. Before and after hydrogen-charging, performed under an atmospheric pressure of hydrogen gas at 1023K for 3 hours, the γ-single phase alloy has become significantly brittle, while this hydrogen-induced embrittlement is suppressed for the two-phase alloy. For the γ-single phase alloy, no apparent microstructural change was observed after hydrogen-charging (approximately 230ppm hydrogen in the alloy); no hydrides even at the grain boundaries, implying an intrinsic embrittlement of the γ-phase due to hydrogen in solution. On the other hand, a significant microstructural change took place for hydrogen-charging two-phase alloy (approximately 340ppm hydrogen in the alloy); a thin amorphous layers with a few nm thickness appear at the pre-existing γ/α_2 interfaces after charging. In situ TEM observation has confirmed that the amorphous phase transforms to a nano-crystalline state after heating to 1000K at which the hydrogen could be removed (degassed), indicating that the amorphous phase exists not as a binary Ti-Al phase but as a ternary Ti-Al-H one. The present results suggest that the near γ/α_2 interface in the lath packets act as the most preferential sites for hydrogen storage. Therefore, the scavenging is expected to occur effectively for the microstructure composed of α_2-γ fine lamellae in which a large number of γ/α_2 interfaces exist. It is worthwhile mentioning that the fine-scale of the lamellae makes it possible to have a large number of interfaces for a given volume of the α_2 phase.

2:15 PM <u>N7.4</u>
EFFECTS OF PRIOR ANNEALING TREATMENTS ON THE MECHANICAL RESPONSE OF Al-RICH γ-TiAl. Fabienne Grégori, LPMTM, Institut Galilée, Villetaneuse, FRANCE; <u>Patrick Veyssiére</u>, LEM, CNRS-ONERA, Châtillon Cedex, FRANCE.

In γ-TiAl, the occurrence of a yield stress anomaly is independent of the operative slip system. There is documented evidence though that the temperature at which the yield stress peaks and the peak stress are both influenced by factors such as alloy composition and load orientation. The present contribution is aimed at showing that, to a very large extent, these values can be effected by transformations that may or may not take place in the alloy depending on thermal treatments prior to deformation. Typically, the peak is lifted to larger stresses and shifted by 200-300°C towards higher temperatures when samples are deformed in the as-grown state or else after being pre-annealed beyond approximately 1100°C. What occurs then is that during deformation within the 600-1100°C range, interstitial atoms of C, N and/or precipitate to form a H-phase or a P-phase and that this precipitation occurs preferentially on dislocations. In adequately annealed samples, interstitial atoms are fully precipitated in the form of large and distant particles which do not strengthen the alloy. This view is generally supported by available experimental and dedicated deformation experiments are presented to analyse the conditions under which precipitation influences the yield stress anomaly. These experiments also provide indication that ordering of the Ti$_3$Al$_5$ phase may take part to the strength of Al-rich γ-TiAl at intermediate temperatures.

2:30 PM N7.5
DEFORMATION OF NANO AND MICROCRYSTALLINE INTERMETALLIC MATERIAL. V. Garibay-Febles, O. Coreno-Alonso, J.G. Cabanas-Moreno, H.A. Calderon, Depto Ciencia de Materiales, ESFM-IPN, MEXICO; M. Umemoto, Toyohashi Univ of Technology, JAPAN.

Mechanical milling and sintering are used to produce intermetallic materials with nano and micro sized grains. TiAl-X, Al_3Ti-X and NiAl have been successfully obtained from mixtures of elemental powders. X represents Mn, Cr and Fe in different amounts. Sintering was performed by a spark plasma assisted technique that allows retention of fine grain sizes depending on the processing temperature. The finest grain sizes were obtained by applying relatively high pressures (100 Mpa) and lower temperatures (1173 K). Materials based on TiAl-X develop a two phase microstructure (α_2 and γ) while Al_3%Ti-X and NiAl have single phase microstructures ($L1_2$ and B2 structures, respectively). Only Al_3Ti-Cr contains a second phase. The mechanical properties have been measured as a function of temperature (up to 873 K) and grain size. High yield stresses above 1 GPa are observed for most alloys. TiAl-X alloys show a large ductility owing to their relatively larger grain sizes. Al_3Ti-X materials show a poor ductility in the as-sintered condition (d around 30 nm) but a considerable increase as the grain sizes is varied by heat treatment (between 70 and 150 nm). Serrated flow curves and a slightly positive dependence of the yield stress with temperature, characterize the deformation of these materials. NiAl alloys show some ductility above 573 K. The present results allow discussion of the mechanism of deformation and its relationship to the nature of the tested specimens.

3:15 PM *N7.6
STRENGTHENING MECHANISMS IN TITANIUM ALUMINIDE. Peter M. Hazzledine Air Force Research Laboratory, Materials and Manufacturing Directorate, Dayton, OH.

This paper is a review of the mechanisms which contribute to the yield strength of alloys with compositions close to TiAl. In single crystal monolithic TiAl, unit dislocations, super dislocations and twinning dislocations have individual Peierls stresses which define the base level for yield strength. This strength may be enhanced by solid solution interactions between solute atoms and glissile dislocations. Screw unit dislocations are known to cross slip profusely (whether intrinsically or at second-phase particles is controversial) thereby collecting jogs which exert drag forces on the dislocations. Any second-phase particles may also impede dislocations of any character by a similar process but without cross slip. in polycrystalline TiAl. grain boundaries contribute further barriers to dislocations thereby strengthening the material. In lamellar TiAl, polysynthetically twinned specimens gain further strength from the profusion of interfaces in them. One important parameter is the volume fraction of alpha-2 lamellae within a gamma colony and a related parameter is the ratio of gamma/alpha-2 interfaces to gamma/gamma interfaces. One view is that the strength is derived from the incompatibility of deformation between neighboring lamellae and another view is that the interfaces provide barriers of varying strength to dislocations crossing the interfaces. Finally, polycrystalline lamellar TiAl is further strengthened by the presence of grain boundaries. An attempt is made to estimate the relative importance of the many contributions to strength in TiAl alloys.

3:45 PM N7.7
MECHANICAL PROPERTIES OF INTERMETALLIC GAMMA-TiAl BASED ALLOYS AT ELEVATED TEMPERATURES. Manfred Weller, Anita Chatterjee, Max-Planck-Institut fuer Metallforschung, Stuttgart, GERMANY; Gregory Haneczok, Institut of Physics and Chemistry of Metals, Silesian University, Katowice, POLAND; Helmut Clemens, Institut fuer Metallkunde, der Universitaet Stuttgart, GERMANY.

The high temperature strength of materials is largely determined by the creep properties which are closely related to diffusion processes. Mechanical loss (internal friction) experiments give another access for the study of the mechanical properties at elevated temperatures. Specimens of a Ti-46.5at.%Al-4at.%(Cr,Nb,Ta, B) alloy with fully lamellar microstructures exhibiting different interface spacing but a comparable colony size were examined both by mechanical loss and creep experiments. The mechanical loss measurements were carried out with a low-frequency (0.01Hz-10Hz) subresonance apparatus in the temperature range from 300K up to 1300K. The mechanical spectra show two phenomena: (i) A loss peak at about 900K (0.01Hz) which is controlled by an activation enthalpy of 290 kJ/mol. The loss peak it is assigned to thermally activated (reversible) glide of dislocations which are pinned at the lamellae interfaces and within gamma lamellae up to 900K. A minimum dislocation density of E8 to E9 (1/cm.cm) which depends on the mean lamellar spacing could be estimated from the peak height. (ii) A high temperature damping background above 1000 K. The activation enthalpy, determined from

the frequency shift, is 370 ± 20 kJ /mol. This value agrees well with the activation enthalpy of 350 kJ /mol determined by creep experiments conducted on identical samples (970K, 1070K and 200 MPa). These results are discussed in terms of diffusion controlled climb and glide of dislocations.

4:00 PM N7.8
PHASE STABILITY AND HIGH TEMPERATURE TENSILE PROPERTIES OF W DOPED γ-TiAl. Keizo Hashimoto, Hirohiko Hirata, Teikyo Univ., Dept of MS&E, Utsunomiya, JAPAN; Youji Mizuhara, Nippon Steel Corp., Advanced Technology Research Labs., Hikari, JAPAN.

Tungsten(W) doped γ-TiAl is one of the promising alloy compositions among many proposed alloys for elevated temperature structural application. Ingots of W doped γ-TiAl are produced by plasma arc remelting technique, followed by the isothermal forging to control microstructures. Phase stability of W doped γ-TiAl have been studied quantitatively, using the quenched specimens from 1273 and 1473K, by means of EDS analysis of TEM. Isothermal cross section at 1273 and 1473K of Ti-Al-W ternary phase diagrams have been proposed based on the experimental observations. Small amount of W ($<$1at%) addition to Ti-46at%Al binary composition cause the phase shift from α γ two phases to α β γ three phases, which suggests that W is the strongest β stabilizer among transition metals, such as V, Cr, Mn, Nb, Mo and Ta. Mechanical properties of W doped γ-TiAl show that the tensile strength at 1273K have been significantly improved by the W addition. Relationships between the microstructure and the mechanical properties of W doped γ-TiAl have been discussed.

4:15 PM N7.9
MEASUREMENT, CHARACTERIZATION AND MODELING OF THE TENSION / COMPRESSION ASYMMETRY OF SINGLE CRYSTAL GAMMA Ti-55.5AT%AL. Marc Zupan, G.F. Dirras[1] and K.J. Hemker, Johns Hopkins University, Department of Mechanical Engineering, Baltimore, MD. [1]On leave from LPMTM-CNRS, Universite Paris XIII, FRANCE.

Single crystal microsample test specimens of gamma Ti-55.5at%Al oriented along the [001], [010] and [-110] crystal axes have been deformed in tension, compression, fully reversed compression-tension and fully reversed tension-compression tests at temperatures ranging from 500K to 1273K. From these experiments measurements of the Young's modulus, coefficient of thermal expansion and 0.2% offset flow stress have been made as a function of temperature, crystal orientation and sense of the applied load. Microsample measurements of the Young's modulus and coefficient of thermal expansion are in very good agreement with literature values. A measurable violation of Schmid's law was observed and a significant tension/compression asymmetry has been found in the anomalous yielding temperature region. TEM observations of the dislocation fine structure will be presented to characterize the active microscopic deformation mechanisms. The asymmetric superdislocation dissociation for TiAl and its effect on cross-slip and dislocation mobility will be used to explain the yielding asymmetry that was observed for the three orientations tested.

4:30 PM N7.10
ON THE STRESS ANOMALY OF GAMMA-TiAl. Marc C. Fivel, INP Grenoble, St. Martin d'Hëres, FRANCE, Francois Louchet, INP Grenoble, St. Martin d'Hëres, FRANCE, Bernard Viguier, INP Toulouse, Toulouse, FRANCE.

It is generally recognised that ordinary dislocations are responsible for stress anomalies in gamma-TiAl. Two models recently proposed for strength anomalies in this material are based on different supposed behaviours of jogs: in the first one, jogs generated by collisions between primary and cross-slipped kinks are supposed to 'unzip' through conservative motion along the screw direction (pinning-unzipping mechanism); in the other one, screw dislocation motion is supposed to be controlled by either jog or dipole dragging. In the present work, flow stresses are computed analytically in all these cases. At intermediate temperatures, both kink unzipping and dipole dragging lead to an anomalous stress behaviour, but the former mechanism, operating for significantly lower stresses, is favoured. At higher temperatures, jog dragging, which is shown to have a normal (negative) stress - temperature dependence, becomes dominant. We therefore conclude that the stress peak in the yield stress vs temperature plot results from a transition between an anomalous behaviour ascribed to jog unzipping and a normal behaviour due to jog dragging. On the other hand, a 3-d mesoscopic simulation of dislocation behaviour, previously designed for FCC metals, is adapted and run in the L10 case, in order to validate these conclusions.

4:45 PM N7.11
MECHANISMS CONTRIBUTING TO THE PINNING OF ORDINARY DISLOCATIONS IN γ-TiAl. Fabienne Grégori,

LPMTM, Institut Galilée, Villetaneuse, FRANCE; Patrick Veyssière,
LEM, CNRS-ONERA, Châtillon cedex, FRANCE.

The fact that ordinary dislocations (b = 1/2<110]) exhibit a strong
tendency towards being elongated in the screw direction is a
well-documented microstructural property of γ-TiAl alloys. Ordinary
dislocations are in addition known to take a number of pinning points
along their locks. Explanations of the flow stress anomaly all rely on
the presence of these pinning points and some models are founded on
the assumption that local pinning forms dynamically during
dislocation motion, supposedly by cross-slip. Within this frame, the
presence of elongated loops either isolated or else connected to
ordinary dislocations is regarded as a strong evidence in support of a
jog-trailing mechanism. The present work is intended to offer a
different interpretation for the presence of these loops as well as for
the pinning mechanism. It is shown that a significant fraction of the
loops forms by cross-slip annihilation of threading dipoles, forming
loop arrays with specific orientation relationships. These arrays act as
obstacles onto which a new dislocation can be trapped giving rise to
local trailing-like configurations. The process of cross-slip annihilation
may repeat itself when a dislocation with opposite sign encounters an
ordinary dislocation already arrested by loops, thus increasing the
loop density locally. As deformation proceeds, the process of
dislocation gettering by loops operates repetitively forming schools of
loops in places. Evidence is provided in favour of screw locks being
formed prior to pinning and cusping. It is shown in addition that
mixed segments exhibit a tendency towards pinning that is entirely
similar to that already documented on screw locks.