

at the interface Ni/Sn by transmission electron microscopy (TEM) in detail. At short times, the growth rate agrees with the flux driven ripening theory for soldering [1] [2], but for longer times, the time exponent deviates significantly. TEM analysis reveals that the general assumption of constant interface area is not fulfilled at any time. We will compare the experimental data with existing soldering models and present an approach for the growth kinetics of Ni<sub>3</sub>Sn<sub>4</sub> in the Ni/Sn system. (supported by DFG)

[1] K.N. Tu et. al., Physical Review B 66, 115403 (2002)

[2] G. Gosh, J. Appl. Phys. Volume 88, Nr. 11 p.6887

MM 28.2 Wed 17:45 H 0107

**Fabrication of CoTiSb and NbNiSb Half-Heusler phases for thermoelectric applications** — **NOTE: This talk has been withdrawn** — •WILFRIED WUNDERLICH, YOSHIKAZI AOKI, KOUSUKE NAKATSUKA, HIDETO UENO, and YUICHIRO MOTOYAMA — Tokai University, Fac. Eng, Materials Science Dept., Hiratsuka-shi, Kanagawa, Japan

Important applications of Half-Heusler phases are as thermoelectric materials. For the cases of CoTiSb, TiNiSn and others, ab-initio simulation using VASP-software could confirm the phase stability against phases with concurrent crystal structures like TiNiSn, ZrCoAl, ZrBeSi, FeSiV and Full Heusler. However, the thermo dynamical driving force for formation as calculated from the difference in lattice energies is

less than 0.1eV/atom. Hence, the fabrication of Half heusler phases is difficult and requires three steps, surface activation of the raw material by ball milling, arc-melting of pressed pellets and finally long-term annealing treatment. For the CoTiSb system, diffusion couple experiments clarified the complicated diffusion mechanism, which can lead in worst cases to Kirkendahl voids and constitutional vacancies. On doped CoTiSb specimens, Seebeck coefficients up to 0.1 mV/K, on NiNbSb 0.3 mV/K were measured.

MM 28.3 Wed 18:00 H 0107

**Influence of microstructure on magnetostriction properties of FePd thin films** — **NOTE: This talk has been withdrawn** — •WILFRIED WUNDERLICH, KEISUKE TAKAHASHI, DAJI KUBO, YOSHITO MATSUMURA, and YOSHITAKE NISHI — Tokai University, Fac. Eng, Materials Science Dept., Hiratsuka-shi, Kanagawa, Japan

FePd-alloys as thin films are potential actuators materials due to their magnetostriction. Experiments and simulations of TEM and XRD diffraction patterns showed, that the L1<sub>0</sub>-ordering has no influence on the lattice parameter ratio c/a=1.37. The degree of long-range order is higher for the sputtering temperature of 573K than of 423K, but the magnetostriction is higher for thin films produced at 423K. The model for explanation is contrary to the usual behavior, where ordering increases the magnetic susceptibility; for achieving a large magnetostriction an initial degree of disorder is more favorable.

## MM 29: Mechanical Properties I

Time: Wednesday 14:00–15:15

Location: H 0111

MM 29.1 Wed 14:00 H 0111

**Molecular Dynamics Simulations of Grain Boundary Plasticity** — •YVONNE RITTER, ALEXANDER STUKOWSKI, and KARSTEN ALBE — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

Dislocation nucleation at grain boundaries (GB) and as well as grain boundary sliding are relevant mechanisms governing the deformation behavior of nanocrystalline metals. By means of molecular dynamics simulations we examine well defined bicrystal geometries under different loads. The simulations are performed for copper and aluminum in order to investigate the influence of various stacking fault (SF) energies. For a  $\Sigma$  7 (111) twist boundary GB sliding occurs by a collective movement of all atoms in the boundary plane, but no dislocation activity can be detected. A  $\Sigma$  33 (225) tilt boundary with a dissociated structure does not deform by GB sliding but reacts by the growth of pre-existing intrinsic stacking fault facets when exposed to a shear deformation. Under tensile deformation partial dislocations nucleate from both GBs. The nucleation mechanism is thermally activated in both cases. In the case of the  $\Sigma$  7 GB the dislocations are statistically emitted from tetrahedral nucleation sites. The partial dislocations, that are emitted from the  $\Sigma$  33 GB, emerge at well defined positions determined by the GB structure.

MM 29.2 Wed 14:15 H 0111

**Micropillars compression test** — •NOUSHA KHERADMAND, AFROOZ BARNOUSH, and HORST VEHOFF — Saarland University Bldg. D22 P.O. Box 151150, Postcode D-66041, Saarbruecken, Germany

In order to investigate the size effect compression test of single crystal micropillars was performed. Micropillars with different crystallographic orientations were fabricated by focused ion beam and the compression test was performed in a nanoindenter utilizing a flat punch tip. As a new approach in order to observe the micropillars in their intermediate deformation conditions, the compression test was performed stepwise. Between each step the micropillars were imaged in a scanning electron microscope. The engineering stress-strain curves of the micropillars show a clear size effect on mechanical properties of the samples. The small samples show a linear elastic-perfectly plastic deformation followed by incremental strain bursts, while the larger samples show a continuously flow curve. This difference could be described by a so called source truncation strengthening model which occurs in samples with small diameter. According to this model a Frank-Read source line during the growth reaches the free surface before it is able to be multiplied. This leaves two single-arm dislocations which are pinned from one end inside the sample and from the other end on the free surface. These dislocations introduce to the samples new yield

stresses.

MM 29.3 Wed 14:30 H 0111

**Determination of intrinsic stresses in thin films by nanoindentation** — •OLENA CHUKHRAI<sup>1</sup>, ANDRE CLAUSNER<sup>1</sup>, NORBERT SCHWARZER<sup>2</sup>, and FRANK RICHTER<sup>1</sup> — <sup>1</sup>Chemnitz University of Technology, Institute of Physics, Chemnitz, Germany — <sup>2</sup>SIO - Saxonian Institute of Surface Mechanics, Eilenburg, Germany

Intrinsic stresses often occur in thin films as a result of the complex formation of the thin film structure. Therefore, simultaneous determination of intrinsic stress and yield strength are necessary. It was shown [1], that intrinsic stresses can be derived from nanoindentation data by combination of "pure normal" and mixed (normal and tangential) loading, in particular, when the concept of the "effectively shaped indenter" is used. A device for creation of biaxial stress in the samples which can be used together with our nanoindentation setup (UNAT, Asmec GmbH) was constructed, tested and utilized for the investigation of a highly elastic Ni/Ti alloy. We found that for the NiTiInol hardness changed by more than 70% when the stress was varied between 0 and 0.9 GPa. Using our theoretical concept [1], the intentionally introduced biaxial stress could be taken into account and the yield strength could be determined. The next step was to apply for the samples with known biaxial stress a combination of "pure normal" and mixed loading with pointed indenter and to determine the intrinsic stress and the yield stress using our theory. The feasibility of the concept of simultaneous determination of intrinsic stresses and yield strength by nanoindentation was shown and it can now be used.

[1] Schwarzer N.: <http://archiv.tu-chemnitz.de/pub/2006/0018/index.html>

MM 29.4 Wed 14:45 H 0111

**In situ tensile testing of nanocrystalline Pd and Pd-Ag alloys** — •KEJING YANG<sup>1</sup>, JULIA IVANISENKO<sup>2</sup>, JÜRGEN MARKMANN<sup>3</sup>, and HANS-JÖRG FECHT<sup>1,2</sup> — <sup>1</sup>Institute of Micro and Nanomaterials, University of Ulm, D-89081 Ulm, Germany — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — <sup>3</sup>Universität des Saarlandes, FR7.3 Technische Physik, Saarbrücken, Germany

Arising from a low strain hardening ability, the limited uniform elongation of nanocrystalline materials (NC) hinders the further improvement of their mechanical properties. In this study we suggest a way to enhance strain hardening by purposefully alloying Pd to reduce its stacking fault energy (SFE). Nanocrystalline Pd and Pd-Ag alloys were prepared by high-pressure torsion. Tensile testing was carried out in situ in a high-resolution SEM to investigate the mesoscopic deforma-

tion process at a strain rate of 10-3 s-1. The NC alloys demonstrated very high values of strength and ductility. The true stress-true strain curves exhibit a larger strain hardening effect and larger uniform deformation in Pd-Ag alloys than in pure Pd. We relate this enhanced behavior to a decreased SFE in the alloys: the lower the SFE, the more difficult is the cross slip and climb of split dislocations, which leads to greater dislocation storage and, ultimately, to increased strain hardening. The dimpled structure of fracture surfaces in the alloys will also be discussed in relationship to these findings.

MM 29.5 Wed 15:00 H 0111

**New approach to design the strain hardening ability in nanostructured materials. (exchanged with MM 30.1)** —

•LILIA KURMANAEVA<sup>1</sup>, YULIA IVANISENKO<sup>1</sup>, JÜRGEN MARKMANN<sup>2</sup>, JÖRG WEISSMÜLLER<sup>1,2</sup>, RUSLAN Z. VALIEV<sup>3</sup>, and HANS-JÖRG FECHT<sup>4</sup> — <sup>1</sup>Institute für Nanotechnologie, Forschungszentrum Karlsruhe, Karlsruhe, Germany — <sup>2</sup>Universität des Saarlandes, Saarbrücken, Germany — <sup>3</sup>Institute of Physics of Advanced Materials, Ufa, Russia — <sup>4</sup>Institute of Micro and Nanomaterials, University of Ulm, Ulm, Ger-

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The recent past has seen an increasing interest in studies of mechanical properties of nanostructured materials (NSM), since new methods of continuous processing of bulk NSM using severe plastic deformation were developed. NSM demonstrate superior hardness and strength, but often a limited ductility due to poor strain hardening (SH) ability. In present paper we suggest a simple method to increase the SH ability of NSM by decreasing the stacking fault energy (SFE). The microstructure and mechanical properties of nanocrystalline Pd and Pd-x%Ag (x=5,10,20,40) alloys were investigated. Additions of Ag strongly decrease the SFE of Pd. The initially coarse grained samples were processed by high pressure torsion, which resulted in formation of homogeneous ultrafine-grained structure. The increase of Ag contents led to the decrease of the resulted grain size. Consequently, the samples with larger Ag contents demonstrated the higher values of strength properties. The uniform elongation had also increased, and tensile curves exhibited larger SH. Thus we have obtained a combination of high strength and good ductility in nanostructured Pd-Ag alloy.

## MM 30: Mechanical Properties II

Time: Wednesday 15:45–17:00

Location: H 0111

MM 30.1 Wed 15:45 H 0111

**Tensile tests of magnetron sputtered nanocrystalline palladium (exchanged with MM 29.5)** — •ANNA CASTRUP<sup>1,2</sup>, SEBASTIAN GOTTSCHALK<sup>1</sup>, HORST HAHN<sup>1,2</sup>, RUDOLF BAUMBUSCH<sup>3</sup>, PATRIC GRUBER<sup>3</sup>, and OLIVER KRAFT<sup>3</sup> — <sup>1</sup>Institute of Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany — <sup>2</sup>Institute for Materials Science, Thin Films Division, Darmstadt University of Technology, Petersenstr. 23, D-64287 Darmstadt, Germany — <sup>3</sup>IZBS, University of Karlsruhe, Kaiserstr. 12, 76131 Karlsruhe, Germany

Nanocrystalline Pd films of 1  $\mu\text{m}$  thickness were prepared by rf magnetron sputtering on Kapton substrates. The films were sputtered by use of nanoscale multilayer technology with individual deposition layer thicknesses ranging between 1 and 20 nm at various sputter conditions.

The resulting grain size and texture were characterized using TEM and conventional XRD measurements. Tensile tests were performed ex-situ as well as in-situ in a synchrotron diffractometer. Peak form analysis reveals intrinsic and extrinsic stacking fault density and twin density, which depend on the applied strain rate. Considered deformation mechanisms are: grain boundary sliding, grain rotation and the formation of stacking faults. It is investigated whether the formation of these defects is reversible after relaxation.

MM 30.2 Wed 16:00 H 0111

**Fe-based composite materials with improved mechanical properties** — •KATARZYNA WERNIEWICZ<sup>1,2</sup>, UTA KÜHN<sup>1</sup>, NORBERT MATTERN<sup>1</sup>, JÜRGEN ECKERT<sup>1</sup>, LUDWIG SCHULTZ<sup>1</sup>, and TADEUSZ KULIK<sup>2</sup> — <sup>1</sup>IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — <sup>2</sup>Warsaw University of Technology, Faculty of Materials Science and Engineering, Warsaw, Poland

Following a previous study by the authors two new compositions ( $\text{Fe}_{89.0}\text{Cr}_{5.5}\text{Mo}_{5.5}$ )<sub>91\text{C}9</sub> and ( $\text{Fe}_{89.0}\text{Cr}_{5.5}\text{Mo}_{5.5}$ )<sub>83\text{C}17</sub> have been developed with the aim of improving the ductility of  $\text{Fe}_{65.5}\text{Cr}_4\text{Mo}_4\text{Ga}_4\text{P}_{12}\text{C}_5\text{B}_{5.5}$  bulk metallic glass (BMG). In contrast to the alloys in that study, the recently prepared Fe-based materials are Ga-free. It was expected that the variations in the composition will lead to the changes in the phase formation and, hence, in the mechanical response of the investigated alloys. It was recognized that in-situ formed Fe-based composites show superior plasticity ( $\epsilon_{pl} \approx 37\%$ ) for the alloy with lower C content and ( $\epsilon_{pl} \approx 4\%$ ) for the alloy with higher C content compared to monolithic glass ( $\epsilon_{pl} \approx 0.2\%$ ). Furthermore, on the basis of present as well as previous investigations it has been shown that the Ga addition is beneficial for the plasticity of these Fe-based alloys. It was observed that the ( $\text{Fe}_{89.0}\text{Cr}_{5.5}\text{Mo}_{5.5}$ )<sub>83\text{C}17</sub> alloy exhibits a significantly smaller fracture strain ( $\epsilon_f \approx 5\%$ ) compared to its Ga-containing counterpart ( $\epsilon_f \approx 16\%$ ). Therefore, it can be concluded that appropriate alloying additions are crucial in enhancing the mechanical properties of the complex Fe-based materials developed here.

MM 30.3 Wed 16:15 H 0111

**Mechanical Characterisation of a human tooth with a structured filling material** — •FERENC MOLNAR<sup>1</sup>, FRANK RICHTER<sup>1</sup>, and NORBERT SCHWARZER<sup>2</sup> — <sup>1</sup>Chemnitz University of Technology, Solid State Physics, 09107 Chemnitz, Germany — <sup>2</sup>Saxonian Institute of Surface Mechanics, Lieschow 26, 18569 Ummantz, Germany

New materials for dental use must have mechanical properties comparable to those of the surrounding biological material. To investigate a structured filling material consisting of hard nanometer-sized grains in a tough matrix with high local resolution we have applied the method of nanoindentation. Therefore a cross-section of the tooth has been prepared and depth sensing indentation measurements were performed. Using the UNAT device (Universal Nanomechanical Tester, Asmec GmbH) with a Berkovich indenter an array of totally about 3200 measuring points with a spacing of 75 microns were created covering the essential parts of the tooth including filling, dentine and dental enamel regions. Young's modulus and hardness have been determined for each point of this array to obtain laterally resolved data of these mechanical properties. In addition, we have evaluated the yield strength of the filling material applying the effective indenter approach of Schwarzer [J. Phys. D: Appl. Phys., 37 (2004) 2761-2772]. The filling shows quite homogeneous behaviour to the external load but at smaller scales the microstructure gains more influence. Values of hardness and Young's modulus for particular measuring points being by a factor of two or three bigger than the average could be correlated by optical microscopy to single extraordinary large grains in the matrix.

MM 30.4 Wed 16:30 H 0111

**Simulation der ersten Phasen der Materialermüdung durch ein granulares Modell** — •JUDITH FINGERHUTH<sup>1</sup>, MATZ HAAKS<sup>1</sup>, GUNTER SCHÜTZ<sup>2</sup> und KARL MAIER<sup>1</sup> — <sup>1</sup>Helmholtz-Institut für Strahlen- und Kernphysik, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 14-16, D-53115 Bonn — <sup>2</sup>Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

Basierend auf der Idee des zellulären Automaten werden die ersten Phasen der Ermüdung eines Metalls vor der Initiierung von Mikrorissen mit einem mesoskopischen Modell simuliert. Der Kristall wird dabei als regelmäßige Anordnung von Kristallkörnern betrachtet, deren komplexe, individuelle Eigenschaften durch die skalaren Parameter Korngröße, Orientierung und Schädigung (mittlere Versetzungsdichte pro Korn) repräsentiert werden. Die Schädigung eines Kornes wird aus der plastischen Verformung, der pro Verformungszyklus dissipierten Energie und Schädigung der Nachbarkörner berechnet. In einer eindimensionalen Implementierung wurde das Verhalten von Nickel im einachsigen Zug-Druck-Versuch teilweise wiedergegeben. Es werden nun die Ergebnisse einer realistischeren 2D-Implementierung vorgestellt.

MM 30.5 Wed 16:45 H 0111

**Vorhersage des Ermüdungsbruchs an vordeformiertem Karb-**