

## MM 46: Mechanical Properties III

Time: Friday 10:30–13:15

Location: IFW D

MM 46.1 Fri 10:30 IFW D

**Appearance of dislocation mediated and orientation selective deformation twinning in a bimodally textured FeMnNiCr alloy** — ●DAVID GEISSLER<sup>1,2</sup>, JENS FREUDENBERGER<sup>1</sup>, ALEXANDER KAUFFMANN<sup>1,2</sup>, MARIA KRAUTZ<sup>1,2</sup>, JÖRG EICKEMEYER<sup>1</sup>, and LUDWIG SCHULTZ<sup>1,2</sup> — <sup>1</sup>IFW Dresden, PF 270116, 01171 Dresden, Germany — <sup>2</sup>TU Dresden, 01062 Dresden, Germany

The deformation behaviour of low stacking fault energy (SFE) materials is of great interest to Fe-Mn based austenitic steel research. By comparing the microstructural and texture evolution with tensile stress-strain response of a Fe-24Mn-7Ni-8Cr (mass percent) alloy a slip-dominated deformation process and, at a later stage of deformation, twinning induced plasticity (TWIP) is observed. The annealed starting material exhibits a bimodal fiber texture and the occurrence of TWIP is texture sensitive, i.e. deformation twinning is only observable in grains of one texture component. Based on these experimental results, a model is presented, which reflects an orientational and configurational peculiarity of fcc stacking faults bound by two Shockley partials. With this model the onset point of twinning is reflected by the starting point of stacking fault growth, i.e. movement of the leading partial and stopping of the trailing partial. Calculations based on this model allow to compatibly describe the mechanical behaviour from tensile testing with respect to the microstructural evolution. Furthermore a reasonable SFE of 12.2 mJ per square meter can be extracted from the test data by application of the model assumptions.

MM 46.2 Fri 10:45 IFW D

**Influence of Microstructure on Thermo-Mechanical Fatigue of Al Thin Films on Substrates** — ●WALTHER HEINZ<sup>1</sup> and GERHARD DEHM<sup>1,2</sup> — <sup>1</sup>Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben — <sup>2</sup>Department Materials Physics, Montanuniversität Leoben, Austria

The difference in thermal expansion coefficient between Al and Si can cause interconnect failure by thermo-mechanical fatigue in microelectronic devices subjected to repeated thermal cycling. In this study the influence of grain orientation on damage evolution of 0.2 - 2 $\mu$ m thick Al films on Si and alumina substrates is analyzed by local electron backscattered diffraction in a scanning electron microscope. The films are cycled between 100°C and 450°C up to 10.000 times. The investigations reveal that texture is a route to avoid thermo-mechanical fatigue damage by selecting a sharp (111) fibre texture. This can be explained by orientation dependent plasticity.

MM 46.3 Fri 11:00 IFW D

**Low cycle fatigue of lead free solder joints** — ●LARS SCHEMANN, ANDRE WEDI, DIETMAR BAITHER, and GUIDO SCHMITZ — Institut für Materialphysik, Westf. Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Presently solders containing lead are banned from consumer electronics. Important alternatives are the Sn-Ag-Cu (SAC) solders and solders containing antimony. This work studies the isothermal low cycle fatigue properties of SAC solders and the SnSb(8) solder. For the experiments, model solder joints were produced and used. They consist of two pure copper plates joined together by a circular disk of solder. Low cycle fatigue experiments were done under displacement control. Furthermore hardness was tested by a micro indenter. In order to find an explanation for the different lifetimes of the solders, several micro structural investigations were performed. For this we used transmission and scanning electron microscopy as well as optical microscopy. The measured data showed a strong relation between lifetime and hardness of the solder alloy. We also found, that the type of solder influences the crack propagation.

MM 46.4 Fri 11:15 IFW D

**Brittle-to-ductile transition of the intermetallic compound YCu** — ●ROLF SCHAARSCHUCH<sup>1</sup>, CARL-GEORG OERTEL<sup>1</sup>, GUANGHUI CAO<sup>2</sup>, H.N. TIAN<sup>2</sup>, JENS FREUDENBERGER<sup>3</sup>, HEINZ-GÜNTER BROKMEIER<sup>4</sup>, and WERNER SKROTZKI<sup>1</sup> — <sup>1</sup>Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Department of Materials Engineering, Shanghai University, Shanghai 200072, P.R. China — <sup>3</sup>Institute for Metallic Materials, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — <sup>4</sup>GKSS-

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The temperature dependence of the tensile deformation behaviour of an extruded, polycrystalline YCu intermetallic compound with B2 structure at room temperature was investigated in the temperature range from room temperature down to 77K. The samples were deformed along the extrusion axis characterized by a weak <110>-fibre texture. The brittle-to-ductile transition (BDT) was found around 140K. The BDT is related to the transformation of the cubic B2 to the orthorhombic B27 structure proved by X-ray diffraction.

MM 46.5 Fri 11:30 IFW D

**Intermediate temperature embrittlement in high purity nickel and binary nickel-bismuth alloy** — ●LEI ZHENG<sup>1,2</sup>, REDA CHELLALI<sup>2</sup>, DIETMAR BAITER<sup>2</sup>, and GUIDO SCHMITZ<sup>2</sup> — <sup>1</sup>School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing, 10083, China — <sup>2</sup>Institute of Materials physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149, Muenster, Germany

Intermediate temperature embrittlement (ITE) is a general phenomenon in Ni-based superalloys. Comparisons of existing interpretations given by different authors reveal considerable differences in understanding the mechanism of ITE. To clarify this situation, high purity nickel and binary Ni-Bi alloy were selected as the tested alloys and their tensile tests in the temperature range of room temperature to 850 °C were carried out. It was demonstrated clearly that high purity nickel has no ITE while Ni-Bi alloys show evident one. With the elevation in temperature, elongation after fracture decreases gradually to a minimum around 750 °C and then increases again rapidly. According to the experimental results, it must be concluded that the ITE is an impurity effect.

MM 46.6 Fri 11:45 IFW D

**Deformation behaviour of cryo-drawn CuAl-wires** — ●ALEXANDER KAUFFMANN<sup>1,2</sup>, JENS FREUDENBERGER<sup>1</sup>, YIN SONG<sup>1,2</sup>, TOM MARR<sup>1,2</sup>, VADLAMANI SUBRAMANYA SARMA<sup>3</sup>, JÜRGEN ECKERT<sup>1,2</sup>, and LUDWIG SCHULTZ<sup>1,2</sup> — <sup>1</sup>IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — <sup>2</sup>TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — <sup>3</sup>Dept. Metallurgical and Materials Engineering, IIT Madras, Chennai 600036, India

The effect of temperature on the active deformation mechanism is studied. For this purpose cryogenic drawing of several CuAl alloys was performed. Hence, a solid lubrication is needed which remains operating at cryogenic temperatures. We present a comparison of several solid lubricants for the deformation of two Copper alloys.

The comparison cryogenic temperature deformation of several CuAl alloys with conventionally drawn wires shows that the strengthening of these alloys during the deformation process is significantly affected by their stacking fault energy. The deformation at cryogenic temperature is most effective at intermediate stacking fault energies. This is interpreted in terms of a changing deformation mechanism from dislocation slip to deformation twinning. The analysis of the microstructure during the deformation process strengthens these assumptions.

MM 46.7 Fri 12:00 IFW D

**Investigation of the mechanical properties of the 413-MAX phase Ti<sub>4</sub>AlN<sub>3</sub> by perturbed  $\gamma$ - $\gamma$  angular correlation** — ●CHRISTOPH BRÜSEWITZ<sup>1</sup>, DANIEL JÜRGENS<sup>1</sup>, MICHAEL UHRMACHER<sup>1</sup>, HANS HOFSSÄSS<sup>1</sup>, and MICHEL W. BARSOUM<sup>2</sup> — <sup>1</sup>II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — <sup>2</sup>Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

MAX phases are nanolaminated layered carbides and nitrides, which feature an unusual set of the best attributes of both metals and high-performance ceramics. Due to their layered structure these phases are good electric and thermal conductors, superb thermal and mechanical shock resistant and easily machinable. To investigate the microscopic behaviour of these phases under uniaxial load, we selected Ti<sub>4</sub>AlN<sub>3</sub> and performed measurements by using perturbed  $\gamma$ - $\gamma$  angular correlation (PAC). The PAC method uses the oscillating anisotropy in the decay cascade of implanted <sup>111</sup>In, which is influenced via the hyperfine interaction by the local probe environment. The measured electric

field gradient (EFG) and especially the change of the frequency damping show the elasticity under applied and after released pressure in a sub-nanometer around the Al-site. Those measurements were not affected by the already known kink band formation in MAX phases under applied stresses, which are used to describe the high elasticity on the  $\mu\text{m}$  scale, as long as the phase is still stable. Therefore XRD was chosen to prove that the phase did not decompose. This work is supported by the DFG under contract HO 1125/19-1.

MM 46.8 Fri 12:15 IFW D

**Influence of grain boundaries and crack length on the propagation of microstructurally short cracks in austenitic stainless steel** — •MICHAEL SCHARNWEBER<sup>1</sup>, CARL-GEORG OERTEL<sup>1</sup>, VLADIMIR MIKULICH<sup>2</sup>, WOLFGANG TIRSCHLER<sup>1</sup>, and WERNER SKROTZKI<sup>1</sup> — <sup>1</sup>Institut für Strukturphysik, TU Dresden, 01062 Dresden — <sup>2</sup>Fraunhofer-Institut für Werkzeugmaschinen und Umformtechnik, 09126 Chemnitz

Austenitic stainless steel (X2 CrNiMo 18 14 3) was cyclically deformed at RT in air under plastic strain control with amplitudes of  $5 \times 10^{-4}$  and  $2 \times 10^{-3}$ . Every 30.000 and 3.000 cycles, respectively, the samples were investigated in the scanning electron microscope in order to determine the propagation rate of the existing microstructurally short cracks as well as the corresponding distance between the crack tip and the opposing grain boundary. The results will be discussed with regard to the barrier effect of grain boundaries to crack propagation as well as the correlation between crack length and propagation rate at different strain amplitudes.

MM 46.9 Fri 12:30 IFW D

**A phase-field study of crack propagation** — •DANIEL SCHNEIDER<sup>1</sup>, JAN HÖHN<sup>1</sup>, MICHAEL SELZER<sup>1,2</sup>, ALEXANDER VONDROUS<sup>2</sup>, MARCUS JAINTA<sup>2</sup>, and BRITTA NESTLER<sup>1,2</sup> — <sup>1</sup>Institute for Reliability of Components and Systems, Karlsruhe Institute of Technology — <sup>2</sup>Institute of Materials and Processes, Karlsruhe University of Applied Science

An extension of the phase-field model is formulated incorporating a formulation for elastic and plastic effects on the evolution of microstructure. We show an approach to describe linear elasto-plastic and linear hardening material behavior based on the Prandtl-Reuss model in the context of the phase-field method. Adapted boundary conditions for the different field quantities allow a more accurate modeling of experimental processes. We validate the simulations by a comparison of stress profiles with analytically predicted stress fields of brittle fracture and with the energy criterion according to Griffith theory. Further we present simulations of micro crack propagation induced by external stresses in both, two phase systems as well as polycrystalline structures. The dynamics of the crack formation and the shape of the phase boundaries are analyzed for different processing conditions.

MM 46.10 Fri 12:45 IFW D

**Fracture as Pattern Formation Process** — •ROBERT SPATSCHEK<sup>1</sup>, MICHAEL FLECK<sup>2</sup>, DENIS PILIPENKO<sup>2</sup>, and EFIM BRENER<sup>3</sup> — <sup>1</sup>Max-Planck-Institut für Eisenforschung — <sup>2</sup>Universität Bayreuth — <sup>3</sup>Forschungszentrum Jülich

Fracture is an important process in materials science, that still lacks fundamental understanding. Here we report on a series of theoretical investigations and numerical simulations on crack propagation, which treat this problem in the spirit of an interfacial pattern formation process. This means, that not only the crack velocity, but also the entire shape of the crack with a finite tip radius is self-consistently predicted by the theory. For fast cracks in brittle materials with velocities close to the speed of sound inertial effects become important, and for lower speeds, in particular close to the Griffith point, we consider viscoelastic bulk dissipation as efficient selection mechanism for steady state crack growth. We use phase field simulations to describe also the combined effect of both inertia and bulk damping. Alternatively, multipole expansion methods provide exact solutions for each effect separately, and perturbative approaches are used for the combination of both physical effects. Altogether, this allows to obtain a broad perspective on the predictions of the crack growth models.

MM 46.11 Fri 13:00 IFW D

**Ab-initio calculation of second- and third-order elastic constants** — •ROSTAM GOLESORKHTABAR<sup>1,2</sup>, PASQUALE PAVONE<sup>1,2</sup>, JÜRGEN SPITALER<sup>1,2</sup>, PETER PUSCHNIG<sup>1</sup>, and CLAUDIA AMBROSCH-DRAXL<sup>1</sup> — <sup>1</sup>Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — <sup>2</sup>Materials Center Leoben, Forschung GmbH, Austria

Elastic properties of solids play a key role in materials science and technology. Various mechanical and thermodynamical properties are directly connected to elastic constants of different orders. In particular, the analysis of nonlinear quantities such as the third-order elastic constants (TOEC) gives a direct way of exploring the effect of anharmonicity of the lattice potential. In this work, we present a framework for the first-principles calculation of both second-order elastic constants (SOEC) and TOEC. We have implemented their calculation in the **ElaStic** package. The latter is now able to evaluate the full SOEC and TOEC for any crystal structure from ab-initio total-energy and/or stress calculations. We have applied **ElaStic** to obtain SOEC for one representative crystal of the 9 different symmetry classes. Furthermore, we calculate the TOEC and pressure dependence of the SOEC for diamond, hexagonal Mg, and rhombohedral  $\text{Al}_2\text{O}_3$ . The calculations are performed using total energy and stress data from the FP-LAPW codes WIEN2k and **exciting** and the pseudo-potential code Quantum ESPRESSO. Our results demonstrate the **ElaStic** describes with high precision linear and nonlinear elastic constants for materials characterized by different chemical bonding.