

MM 11 Symposium Complex Metallic Alloys III

Zeit: Freitag 17:30–18:45

Raum: TU H1058

MM 11.1 Fr 17:30 TU H1058

Crack propagation in complex metallic alloys — ●FROHMUT RÖSCH¹, PETER GUMBSCH^{2,3}, and HANS-RAINER TREBIN¹ — ¹Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart — ²Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, 76131 Karlsruhe — ³Fraunhofer Institut für Werkstoffmechanik, 79108 Freiburg

Intermetallic compounds frequently combine interesting properties like high melting point, high-temperature strength, and low density. However, possible applications are then often limited by extreme brittleness at low or ambient temperatures. To develop new materials it is essential to understand crack behaviour on an atomistic level. As experiments on this length scale are difficult, computer simulations are the method of choice to reveal the fundamentals of fracture.

We investigate crack propagation by molecular dynamics simulations with model potentials in an icosahedral model quasicrystal and in a C15 Laves phase. In the quasicrystal the roughness of the fracture surfaces is determined by clusters, whereas in the Laves phase the cleavage planes are rough only on an atomic scale. In both materials the crack path cannot be determined by a simple energy criterion. As a step towards realistic simulations of complex metallic alloys, we also present first results with Embedded Atom Method potentials for C15-NbCr₂.

MM 11.2 Fr 17:45 TU H1058

The phasonic degree of freedom in the Ξ -Al-Pd-Mn phases: Metadislocations and phasonic phase boundaries — ●MICHAEL ENGEL and HANS-RAINER TREBIN — Universität Stuttgart, Institut für Theoretische und Angewandte Physik, 70550 Stuttgart

One of the properties which distinguishes complex metallic alloys from ordinary metallic alloys is the possibility of spatial rearrangements of the cluster substructure resulting in new unit cells. Such rearrangements are discrete degrees of freedom, well known for another class of complex metallic compounds, quasicrystals, which can be seen as CMA's with infinite unit cells. By adopting quasicrystal terminology, the degrees of freedom are called phasonic degrees of freedom.

We demonstrate that the Ξ -(AlPdMn)-phases ξ , ξ' , and ξ'_n can be modelled by a simple projection formalism in three-dimensional hyperspace. It follows that in the ξ'_n -phases there is one phasonic degree of freedom, whose excitation results in a movement of structural defects, so-called phason-planes. Furthermore we describe phasonic phase boundaries between different Ξ -phases and metadislocations, which are special textures of partial dislocations. Both are modelled geometrically in the hyperspace and compared to HREM images from the literature. We determine the metadislocations of lowest energy and relate them uniquely to experimentally observed ones. Since moving metadislocations in the ξ' -phase create new phason-planes, we suggest a dislocation induced phase transition from ξ' to ξ'_n .

MM 11.3 Fr 18:00 TU H1058

Plastic behaviour of polycrystalline β -Al-Mg — ●MICHAEL FEUERBACHER and MARC HEGGEN — Institut für Festkörperforschung Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

β -Al₃Mg₂ is a cubic complex metallic alloy phase with particularly large lattice constants of 28.2 Å and 1168 atoms per unit cell. The main structural elements are Friauf polyhedra arranged in fivefold coordinations. The material is potentially interesting for technological applications since it is a lightweight alloy (2.2 g/cm³) and it congruently solidifies from the melt.

We have performed uniaxial plastic deformation experiments on polycrystalline β -Al-Mg in the temperature range from 300 to 400 °C at strain rates of 10⁻⁴ and 10⁻⁵ s⁻¹. The material is highly ductile and shows strong continuous work softening after the upper yield point. We have performed stress-relaxation and temperature-cycling tests to determine the thermodynamic activation parameters of the deformation process. Strongly stress dependent activation volumes in the range of 0.3 to 2.2 nm³ and a stress exponent of about 3.5 were found. The activation enthalpy assumes rather high values of 3 to 5 eV. After deformation the samples show strong shear bands oriented at 45° with respect to the compression axis.

MM 11.4 Fr 18:15 TU H1058

Structural defects in orthorhombic Al₁₃Co₄ — ●DEWEI DENG, MARC HEGGEN, and MICHAEL FEUERBACHER — Institut für Festkörperforschung Forschungszentrum Jülich GmbH

Orthorhombic Al₁₃Co₄ is a complex metallic alloy phase with 101 atoms per unit cell. The lattice constants are $a = 0.8165(1)\text{nm}$, $b = 1.2352(1)\text{nm}$, $c = 1.4451(1)\text{nm}$ and it has a of $Pmn2_1$ space group. It is structurally isomorphic to the well investigated phase ξ' -Al-Pd-Mn in the sense that the [1 0 0] lattice direction of orthorhombic Al₁₃Co₄ can be described using similar types of hexagon-tiling arrangements as for the [0 1 0] direction of ξ' -Al-Pd-Mn. We have grown single crystals of orthorhombic Al₁₃Co₄ using the Bridgman technique. In the as grown material defect analyses were performed by means of transmission electron microscopy.

The material contains planar defects terminated by dislocations. The planar defects were identified as stacking faults. By means of tilting series in the transmission electron microscope the plane normal of the faults was determined as parallel to the [0 0 1] lattice direction. We have performed two beam Bragg-contrast exit nction experiments and determined the strain-field direction of the planar faults and the terminating dislocations as parallel to the [3 2 0] direction. Hence we can conclude that partial-dislocation motion on (0 0 1) lattice planes by pure glide takes place in orthorhombic Al₁₃Co₄

MM 11.5 Fr 18:30 TU H1058

Plastic deformation behaviour of Al₁₃Co₄ single crystals — ●MARC HEGGEN, DEWEI DENG, and MICHAEL FEUERBACHER — Institut für Festkörperforschung Forschungszentrum Jülich GmbH, par 52425 Jülich, Germany

Al₁₃Co₄ is an orthorhombic phase with lattice parameters $a = 0.82\text{ nm}$, $b = 1.24\text{ nm}$, and $c = 1.45\text{ nm}$. It is a structurally complex alloy phase with 101 atoms per unit cell. The structural key feature of this material are pair-connected pentagonal prismatic channels along the b direction. Around these, the structure can be matched by alternately oriented flattened hexagons. Al₁₃Co₄ is a particularly interesting phase due to its structural relationship to ξ' -Al-Pd-Mn, in which the Metadislocation-mediated deformation process was discovered.

We have performed uniaxial deformation tests in compression on Al₁₃Co₄ single crystals, which were grown by means of the Bridgman technique. The material was deformed in a temperature range between 650 and 900 °C at strain rates of 10⁻⁵ and 10⁻⁴ s⁻¹. It shows pronounced yielding and continuous hardening after the lower yield point. Stress-relaxation tests, strain-rate changes and temperature-cycling tests were performed in order to determine thermodynamic activation parameters. The deformed samples show a number of slip lines on the surface oriented 45° with respect to the compression direction.