MM 28: Nanostructured Materials I

Time: Wednesday 10:15–11:45 Location: H16

MM 28.1 Wed 10:15 H16

Microstructure and thermodynamics of nanocrystalline NiTi alloy processed by high pressure torsion — •Reeti Singh[1], Harald Rösner[1], Ruslan Z. Valiev[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institut für Materialphysik, Westfälische Wihelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149, Münster, Germany — [2]Institute of Physics of Advanced Materials, Ufa State Aviation University, 12 K. Marx Street, 450000 Ufa, Russian Federation

An equiatomic nano-NiTi alloy, deformed by high-pressure torsion (HPT) was investigated. By HPT, almost complete amorphization is obtained in bulk NiTi containing B2 austenite. Crystallization and structural changes during annealing were investigated by differential scanning calorimetry (DSC), X-ray diffraction analysis and transmission electron microscopy (TEM). The DSC signals observed during continuous heating experiments from 323 K to 723 K indicate an unusually large separation between the nucleation and the growth stages. A large variation in the grain size is observed after annealing at 723 K. This behavior is discussed with respect to the nanoscale microstructural heterogeneity after initial deformation processing. The activation energy for grain growth was determined to be 289 kJ/mole. Additional TEM studies reveal amorphous bands sandwiched between crystalline parts after heating at lower temperatures below 623 K, where the atomic mobility is sufficiently low to prevent long-range diffusion. The heat release during annealing in the temperature range from 453 K to 623 K shows an unexpected decrease at 423 K, possibly due to a reverse amorphization, takes place at lower temperatures.

MM 28.2 Wed 10:30 H16

Influence of solutes on the deformation behaviour of nanocrystalline alloys: A molecular dynamics study of PdAu — •Jonathan Schäfer, Alexander Stukowski, and Karsten Albe — FB Materialwissenschaft, TU Darmstadt, Germany

In nanocrystalline (nc) metals various deformation mechanisms like grain boundary sliding and rotation have been identified which are not operational in coarse-grained materials. Moreover, it is well established that the barriers for dislocation emission from grain boundaries are governed by the generalized stacking and twinning fault energies.

While a number of elemental metals have been studied in the past, both in experiment and via computer simulations, little is known on how solutes affect the deformation behaviour of nc-metals.

In this contribution, we present molecular dynamics (MD) simulations of nc PdAu. Model structures are created by the Voronoi tesselation technique and alloyed via a hybrid MD/Monte-Carlo method to determine their structural and chemical equilibrium state. The deformation behavior is analyzed with respect to dislocation activity by employing a novel algorithm for dislocation detection. For comparison, chemically equilibrated and randomly alloyed structures are studied. Our results provide an understanding of the effect of substitutional solutes on the deformation processes in miscible, nanocrystalline alloys.

MM 28.3 Wed 10:45 H16

Absolute concentration of free volumes in nanophase metals prepared by high-pressure torsion — •Bernd Oberdorfer[1], Wolfgang Sprengel[1], Daria Setman[2], Michael Zehetbauer[2], Reinhard Pippan[3], Werner Puff[1], and Roland Würschum[1] — [1]Inst. f. Materialphys., TU Graz, 8010 Graz, Austria — [2]Phys. Nanostrukt. Mater., Fakultät f. Physik, Univ. Wien, Austria — [3]Erich Schmid Institute of Materials Science., Leoben, Austria

This contribution is concerned with the yet unsettled question of absolute concentrations of free volumes in nanocrystalline metals. Despite indications for high concentrations of lattice vacancies and excess volumes in non-equilibrated grain boundaries in these materials, studies by direct and specific methods are scarce. Initial studies to determine the absolute concentration of defects in nanocrystalline metals by time-dependent dilatometry are presented. Bulk nanocrystalline Cu and Fe samples were prepared by high pressure torsion. Length-change measurements with a differential dilatometer show the irreversible annealing of excess free volume $\Delta V/V$ of up to ca. 3×10^{-3} (Fe) or 1×10^{-3} (Cu) upon heating. The annealing behaviour is analyzed by non-isothermal transformation kinetics. The relative contributions of the various types of defects (vacancy agglomerates, dislocations, grain boundaries) with respect to the total excess free volumes are discussed. The dilatometric measurements are compared with studies of positron lifetime spectroscopy and differential scanning calorimetry. Financial support by the FWF Austrian Science Fund is appreciated (project P21009-N20).

MM 28.4 Wed 11:00 H16

Mechanical spectroscopy of nanoparticle-reinforced, electrodeposited ultrafine-grained nickel — •Hans-Rainer Sinning[1], Gabriele Vidrich[2], and Werner Riehemann[2] — [1]Institut für Werkstoffe, Technische Universität Braunschweig — [2]Institut für Werkstoffkunde und Werkstofftechnik, Technische Universität Clausthal

The grain size of electrodeposited ultrafine-grained nickel can be reduced down to the nanocrystalline range by adding ceramic nanoparticles like Al_2O_3 or SiO_2. Mechanical spectroscopy (vibrating-reed technique at 200–800 Hz) reveals several different elastic and anelastic phenomena, all sensitive to annealing, which can be used to characterise the microstructural state, defects, and thermal stability of these nanocomposites. Preliminary results are shown on recovery effects (structural relaxation: increase of Young's modulus and decrease of elastic energy dissipation in wide ranges of temperature), low-temperature mechanical loss peaks, and on the gradual development of amplitude-dependent damping components and of the magnetoelastic "ΔE effect" during grain coarsening. Differences in the annealing characteristics between these quantities, as well as between Ni samples with and without Al_2O_3 or SiO_2 nanoparticles, respectively, are discussed with respect to underlying relaxation mechanisms and related processes of recovery and grain growth. In particular, in case of Al_2O_3 nanoparticles, two separate anelastic relaxation peaks near 170 and 120 K indicate, respectively, both the incorporation of hydrogen and the thermal generation of dislocations at the Ni/Al_2O_3 interfaces.

MM 28.5 Wed 11:15 H16

Thermal stability and reaction of nanocrystalline Fe/Cr multylayers — •Patrick Stender and Guido Schmitz — Institut für Materialphysik, Münster

Thermal stability and reaction of iron/chromium multilayers are analyzed using 3D atom probe technique. For this purpose, stacks of up to 50 layers of pure iron and pure chromium with a single layer thickness of 12 nm were deposited on blunted tungsten tips by ion beam sputtering. Subsequent isothermal and isochronal annealing sequences were carried out in an UHV furnace to investigate the thermal behaviour of the system. In a last processing step, samples were sharpened to 50 nm radius of curvature by annular milling using the focused ion beam technique. Although a miscibility gap exists between a chromium rich phase and an iron rich phase up to 820 °C, nevertheless a short-ranged mixing at the layer interfaces on the length scale below 2 nanometers is observed, which is interpreted by the Cahn Hilliard thermodynamics of inhomogeneous systems. Most remarkable, in suitable temperature-time windows above 550 °C, atomic transport across the metallic layers appears along 1D pipe geometries. This observation is interpreted by triple line transport in the nanocrystalline microstructure. Segregation and transport properties of the triple lines are determined.

MM 28.6 Wed 11:30 H16

Trouble at the boundary surface: modeling field distortions and atom trajectories in 3D-AP — •Christian Oberdorfer and Guido Schmitz — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

Within the last years atom probe tomography (3D-AP) has seen an impressive progress. Instruments utilizing femtosecond laser pulses to trigger the fundamental field evaporation process and a wide angle detector alignment are state of the art. The progress in instrumentation draws focus to more sophisticated methods for data analysis and interpretation, since it is now possible to analyse materials of poor conductivity (ceramics, glasses and semiconductors).

Measurements of these materials will reveal strong artefacts which originate from their heterogeneous electronic properties. In order to address this problem, a simulation of the field evaporation of such specimens is carried out. The electric field at the surface of a modeled specimen is computed using finite elements. A single surface atom then

gets field evaporated and subsequently the trajectory onto a detector like counter-electrode is computed. The described procedure is repeated atom by atom until a certain termination condition is reached. Afterwards the collected data of all of the detector positions is used to carry out a common 3D-AP volume reconstruction. This way a detailed analysis of apparent artefacts is enabled.

Results of this approach for different geometric setups of heterogeneous dielectric/metallic structures (layers, precipitates) will be presented and allow estimation of possible measurement artefacts.