MM 50 Grenzflächen II

Zeit: Dienstag 16:30–17:45 Raum: TU H2038

MM 50.1 Di 16:30 TU H2038

Monte Carlo Simulation of Relaxation Processes in Grain Growth — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Materialphysik, PF 4120, D-39016 Magdeburg

A modified Monte Carlo Potts Model algorithm for single-phase normal grain growth is presented, which allows one to simulate the coarsening of the microstructure of very large grain ensembles in two and three dimensions. The temporal development of the simulated 2D and 3D grain structures exhibit, after an initial period of time, a scaling state that is characterized by a self-similar grain size distribution. A modified mean-field theory based on topological grain size correlations is presented, which yields self-similar grain size distributions that are in excellent agreement with the simulated grain structures in the scaling state. The emphasis of the present work lies on the relaxation process to the scaling state. An algorithm is implemented which allows one to construct the spatial grain structure for a given grain size distribution. Different initial grain structures characterized by different initial grain size distributions are subjected to grain growth via the Monte Carlo Potts Model simulation. The relaxation process to the self-similar scaling state is studied by following the time development of quantities like the average grain size, the variance of the grain size distribution and topological correlations. It is tested whether the relaxation process can be described by time laws such as the stretched exponential form

MM 50.2 Di 16:45 TU H2038

Atomistic modelling of interactions between lattice dislocations and grain boundaries in body-centered cubic transition metals — •Matous Mrovec and Christian Elsässer — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstr. 11, 79108 Freiburg

With grain sizes decreasing towards the nanometer scale, the plastic deformability of polycrystalline metals is increasingly controlled by interactions of lattice dislocations and grain boundaries. To elucidate such interactions at the atomic level, computer simulations were carried out for atomistic models of dislocations interacting with boundaries in body-centered cubic (bcc) transition metals. The interatomic interactions were described by bond-order potentials (BOP) derived from tight-binding electronic-structure theory [1]. These recently developed BOP have been applied already to simulate atomistic core structures of individual screw dislocations [2] and twin boundaries [3] in Mo, W and other bcc metals. In this contribution, BOP simulation results will be presented for atomistic structures and mechanical responses of W bicrystal models containing a twin boundary and a screw dislocation.

[1] M. Mrovec, Thesis, University of Pennsylvania (2002). [2] M. Mrovec et al., Phys. Rev. B 69 (2004) 095115. [3] T. Ochs et al., Phil. Mag. A 80, 2405 (2000).

MM 50.3 Di 17:00 TU H2038

Untersuchung der Wechselwirkung Mikrorisse-Grenzflächen zum Zweck des Grain Boundary Engineering — •Michael Marx — Universität des Saarlandes, Institut für Grundlagen der Werkstoffwissenschaft und Methodik, Geb. 43B, 66041 Saarbrücken

Die Ausbreitung kurzer Risse entscheidet über die Lebensdauer zyklisch beanspruchter metallischer Bauteile. Bis zu 90 Prozent der Lebensdauer werden in dem Stadium des Kurzrisswachstums verbraucht. Dabei können kurze Risse an Korngrenzen und Phasengrenzen in ihrem Wachstum behindert werden, bis hin zum völligen Rissstopp. Obwohl einige versetzungsbasierte Modelle zur Wechselwirkung zwischen Rissen und Korngrenzen existieren, fehlen systematische Untersuchungen der Abhängigkeiten der Wechselwirkung von der Art der Korngrenze, dem Orientierungsunterschied der angrenzenden Körner, der Eigenschaften kohärenter oder inkohärenter Phasengrenzen. Mittels Focused Ion Beam (FIB) können erstmals Mikrorisse mit genau vorherbestimmten Parametern wie Risslänge und Abstand der Rissspitze zur Korngrenze an ausgewählten Korn- und Phasengrenzen erzeugt werden und somit systematische Untersuchungen durchgeführt werden. Es werden erste In-Situ-Untersuchungen im Rasterelektronenmikroskop vorgestellt, die die Wechselwirkung FIB-initiierter Mikrorisse mit Korngrenzen zeigen. Ziel ist dabei die physikalischen Mechanismen der Wechselwirkung zu verstehen und somit die Entwicklung ermüdungsresistenter Werkstoffe durch Grain Boundary Engineering zu ermöglichen.

MM 50.4 Di 17:15 TU H2038

Influence of Tensile and Compressive Creep Deformation on Gamma/Gamma Prime Lattice Mismatch in Single Crystal Superalloys — •Weye Chen[1], Nora Darowski[2], Ivo Zizak[2], Gerhard Schumacher[2], Helmut Klingelhöffer[3], and Wofgang Neumann[1] — [1]Humboldt University Berlin, Institute of Physics — [2]Hahn-Meitner-Institute Berlin , Structure and Dynamics — [3]Federal Institute of Materials Research and Testing, Berlin

Gamma/Gamma prime lattice mismatch has been measured in single crystal superalloy SC16 after tensile and compressive creep deformation. The measurements have bean performed at ambient temperature along [001] orientation using X-ray diffraction at BESSY. On both tensile and compressively creep-deformed specimens an orientation-dependence of lattice mismatch was observed. After tensile creep deformation an increase in lattice mismatch in the orientation parallel to the load axis and a decrease in the orientation perpendicular to the load axis were found. In the compressively creep deformed specimens, however, the lattice mismatch in both of the orientations develops in the opposite direction in comparison to that of tensile creep deformation. The relative change in lattice mismatch during compressive creep deformation is clearly smaller than that of the tensile creep-deformed specimens at comparable strains. These experimental observations are discussed on the basis of a dislocation model which involves the details of deformation nature of superalloys under tensile and compressive creep loading.

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MM 50.5 Di 17:30 TU H2038

Determination of adhesion energies by using hydrogen loading. — •Eugen Nikitin, Astrid Pundt, and Reiner Kirchheim — Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen

Hydrogen loading of thin films leads to large mechanical stress that increases with hydrogen concentration. That results in local film detachment and buckling above a critical stress. The critical stress depends on the material as well as on the film thickness. It can be used as a measure for the adhesion energy between the film and the substrate [1]. A simple model will be presented to calculate the adhesion energy from critical stress data [2]. Adhesion energies of different metals are measured for the metal/polycarbonate interface. This work is financially supported by the DFG via grant Ki 230/30-1. [1] A. Pundt, P. Pekarski, Scr. Mat. 48 (2003) 419. [2] A. Pundt, E. Nikitin, P. Pekarsky, R. Kirchheim, Acta Mat. 52 (2004) 1579.