# MM 34 Symposium Materials Modelling III

Time: Thursday 17:00–18:45 Room: IFW A

MM 34.1 Thu 17:00 IFW A

**Material Modelling and Mathematical Simulation of Steel Carbonitriding** — •Nicolas Bontems[1], Taláat Al-Kassab[1], Jürgen Gegner[2], Reiner Kirchheim[1], and Peter-J. Wilbrandt[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]SKF GmbH, Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Carbonitriding of low-alloyed steels is performed in the austenitic region in gas mixtures offering high carbon and nitrogen potential at temperatures of about 850 °C. Inward diffusing nitrogen leads to a varying microstructure from the surface to the bulk. Such process is often applied to standard bearing steel 100Cr6. Since nitrogen increases the carbon activity, carbon will be released by carbide dissolution and chromium nitride precipitates will be formed. Carbon diffuses in the steel according to the activity gradient, which is acting as driving force. Two basic models have been developed to treat these two complex diffusion problems. The first model for nitrogen diffusion distinguishes atoms dissolved in the lattice and trapped in precipitates or at phase boundaries. The second model for carbon diffusion considers the varying gradient of the carbon activity. A numerical scheme enables the solution of Fick second laws. First results show the applicability of the models, which deliver a numerical evaluation of the variations of the carbon activity with the amount of nitrogen and support a special kinetic mechanism for nitrogen in-diffusion in presence of CrN precipitates.

MM 34.2 Thu 17:15 IFW A

**A parallel 3D simulator for solidification microstructures with fluid flow** — •Britta Nestler, Michael Selzer, and Frank Wendler — University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe

The effect of fluid flow on three-dimensional crystal growth structures is studied by numerical simulations. It is a phenomenon with particular effects in three dimensions where solute is transported in the spatial domain and around the growing crystals. From experiments, it is well known that fluid flow dramatically alters the solidification structure during a casting process. The presence of flow admits the possibility of instabilities due to the flow itself, in addition to the well known morphological instabilities found in crystal growth. Hence, flow has an important influence on the process conditions and on the resulting material properties during the solidification from a melt. We first present a new model for an arbitrary number of phases with fluid flow, which is thermodynamically consistent. Then we introduce our parallel 3D simulator optimized for solving the coupled set of the phase-field model equations and the Navier-Stokes equations for fluid flow. The phase-field equations contain partial differential equations describing the transport of mass and heat and the corresponding temporal evolution of the phase states (order parameters) in the system. Examples of applying the simulator to the solidification of alloy microstructures under the influence of forced and convective flow are considered, and the interaction between diffusion and convection is discussed. In particular, we show simulation results of growing grains and of eutectic microstructures in a flow field.

MM 34.3 Thu 17:30 IFW A

**Using the phase-field method to treat large scale grain growth problems** — •Frank Wendler and Britta Nestler — University of Applied Sciences Karlsruhe, Moltkestr. 30, 76133 Karlsruhe

A multi-phase-field model formerly introduced allows the treatment of free boundary problems with complex interface morphologies, where the phase-fields (order parameters) define diffuse interfaces between adjacent phases. Anisotropy in surface energies and kinetic coefficients of the crystalline phases enable the modelling of polycrystals where each grain is represented by a different phase. In the talk special attention is given to grain structures and polycrystals, with applications in alloy solidification as well as geology. Correctly choosen thermophysical and numerical parameters for the binary Ni-Cu alloy system allow for quantitative simulations, initiated with a high number of differently oriented seed crystals growing into an undercooled melt. When starting from a domain wall, selection processes depending on undercooling and distribution of crystal orientations were found and compared for 2D and 3D simulations. Secondly, the seeds are randomly distributed in the simulation domain to mimic homogeneous nucleation. In each case after a complete solidification the resulting polycrystal shows characteristic morphologies, directed by selection processes and grain orientation relationships. Additionally, the influence of a convective melt flow is shown. As a final processing step, grain coarsening at increased temperature is simulated and characteristic relations for grain size and orientational evolution were found.

MM 34.4 Thu 17:45 IFW A

**Three dimensional investigation of the texture and microstructure below a nanoindent in a Cu single crystal using 3D EBSD and crystal plasticity finite element simulations** — •Nader Zaafarani[1], Dierk Raabe[1], RamNiwas Singh[2], Franz Roters[1], and Stefan Zaefferer[1] — [1]Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Deutschland — [2]Materials Science Division, Bhabha Atomic Research Centre, Mumbai-400085, India

This is a 3D study on the microstructure and texture below a conical nanoindent in a [111] Cu single crystal at a nanometer-scale resolution. The experiments are conducted by using a joint high-resolution field emission SEM-EBSD set-up coupled with serial sectioning in a focused ion beam (FIB) system in the form of a cross-beam 3D crystal orientation microscope (3D EBSD). The experiments (conducted in sets of subsequent (11-2) cross section planes) reveal a pronounced deformation-induced 3D patterning of the lattice rotations below the indent. In the cross section planes perpendicular to the (111) surface plane below the indenter tip the observed deformation-induced rotation pattern is characterized by an outer tangent zone with large absolute values of the rotations and an inner zone closer to the indenter axis with small rotations. The 3D crystal plasticity simulations compared with the experiments have predicted a similar pattern for the absolute orientation changes but they fail to predict the fine details of the rotation patterning with the frequent changes in sign observed in the experiment. Also the simulations over-emphasize the magnitude of the rotation field tangent to the indenter relative to that directly below the indenter tip.

MM 34.5 Thu 18:00 IFW A

**Discrete Dislocation dynamics simulation: plasticity in $\mu$ meter sized pillars** — •Daniel Weygand and Magali Poignat — IZBS, Kaiserstr. 12, University of Karlsruhe, 76133 Karlsruhe

The mechanical behaviour of monocrystalline $\mu$-meter sized pillars is investigated using the three dimensional discrete dislocation dynamics methodology. The dependence of the plastic response of the pillars on the dislocation microstructure initially present and on the loading/boundary conditions is investigated. The analysis of the plasticity is performed in terms of the time evolution of individual dislocation densities on the different slip directions. These density evolutions are discussed in the context of the observed hardening. The study shows furthermore the influence of the grain orientation on the plastic flow. The simulation results are compared to the small strain regime of experimental stress strain curves obtained from compression experiments of such pillars.

MM 34.6 Thu 18:15 IFW A

**A refined statistical strain hardening and recovery model** — •Volker Mohles, Prasad Gurla, and Günter Gottstein — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52056 Aachen, Germany

Statistical models of dislocation density evolution are a means to quickly predict flow stress curves of metal alloys. They involve a relatively large number of parameters to be adjusted, but they can be utilized for instance in Finite Element simulations of plastic deformation for their low calculation effort. One such model actually applied for this purpose is the 3-Internal-Variables-Model 3IVM. This model has been improved recently in several aspects, especially so in respect of recovery kinetics: climb and cross slip are both allowed for, and an additional recovery mechanism has been added which is proportional to the strain rate. With this recovery model, 3IVM can now be fitted quite well to flow curves of Al-polycrystals (almost pure) at various strain rates and temperatures T in the range $20°C < T < 450°C$ with a single set of parameters. In addition, for improved coverage of alloys, the strengthening effect of solutes has been revised such that thermally activated dislocation glide is regarded accurately.

MM 34.7 Thu 18:30 IFW A

**A grain boundary mechanism for nonlocal constitutive laws in crystal plasticity finite element simulations** — •Anxin Ma, Franz Roters, and Dierk Raabe — Max Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf, Germany

When the simulation scale in crystal plasticity becomes small such as in studies focused on the grain boundary region, nonuniform plastic deformations occur commonly which can cause non ignorable orientation gradients for a bulk material point in an infinite small neighborhood, and furthermore a certain number of additional dislocations have to be introduced to preserve the lattice continuity. Furthermore if studies are focused on the grain boundary zone, interactions between mobile dislocations and grain or phase boundaries have to be introduced into constitutive models to reflect the constraint relation between a grain or phase boundary material point with its neighborhood. Based on experimental findings, a grain boundary constitutive mechanism is proposed to consider interactions between two abutting crystals. In this mechanism an additional energy barrier coming from slip transmissions at grain boundaries is added to the general activation energy of dislocation slips in the bulk crystal to capture the thermal activated penetration event in the grain boundary zone. The approach is based on a conservation law for the Burgers vector loop around the interface affected. Furthermore a special grain boundary finite element is introduced in numerical simulations of three bicrystals with small, middle and large angle flat grain boundaries. The hardening effect of grain boundaries, strain distribution and texture evolution of bicrystals are discused carefully.