MM 50: Materials Design I

Time: Friday 10:15–11:15 Location: H 0111

MM 50.1 Fri 10:15 H 0111

An adaptive grid algorithm for solving multi-scale solidification processes on large domains — •Sebastian Waniorek, Michael Selzer, and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences

To gain insight into interdiffusion microstructures occurring between two contact alloys is critical for the design of new materials and surface coatings. In ternary and more generally multicomponent systems, the so-called Kirkendall effect is accompanied by a phase interface migration, both influencing the material properties. The simulation of interdendritic eutectic growth in one domain is, due to the multiple scales involved, a major challenge in computational engineering. We use a phase-field model coupled with multicomponent diffusion equations to simulate the outlined solidification processes. To numerically solve the phase-field equations with high accuracy, a small physical distance between computation points in the interface is needed. Thus a large computational domain is required to resolve the whole effect. These problems are hardly solvable on a uniform grid due to the vast memory and computation time requirements. However most approaches solve the mentioned equations this way. Since a computation with high resolution is only required in areas of steep gradients, we adapt the computation grid to the accuracy affordances. By this approach, the computation effort in the bulk solid phase and in liquid regions is minimized. We apply the method of adaptive mesh refinement to a finite difference solver and enable computations of multicomponent diffusion processes even on personal computers.

MM 50.2 Fri 10:30 H 0111

Post-Machining Thermal Treatment after Surface Finishing of Hardened Steels: Kinetics of XRD Line Width Reduction and Improvement in Rolling Contact Lifetime under Mixed Friction Conditions — •Jürgen Gegner — SKF GmbH, Department of Material Physics, Ernst-Sachs-Str. 5, D-97424 Schweinfurt, Germany

Hard surface finishing represents the final manufacturing step for functional areas of machine elements in state-of-the-art production. Raceways of rolling bearing rings are ground and honed to the required low roughness. Plastic deformation is restricted to a narrow edge zone of the hardened steel. Reheating of the machined components below the martensite tempering or bainite transformation temperature results in a marked decrease of the XRD line width on the surface. The investigated samples are made of through-hardened standard bearing steel 100Cr6 (international denotation: SAE 52100). On the basis of a material model that explains the effect as a complex diffusion process of dislocational carbon segregation, i.e. static strain aging, the measured kinetics of the XRD line width reduction is simulated by an Arrhenius-type equation, which describes the rate-controlling reaction step of temper carbide dissolution. The formation of a small white-etching surface layer of around 1 um thickness by post-machining thermal treatment (PMTT) strongly supports this assumption. First rig tests suggest a considerable increase of the lifetime of Hertzian loaded elements that operate under heavy surface loading. PMTT performed in air leads to a beneficial nanoscaled oxide layer.

MM 50.3 Fri 10:45 H 0111

Long-life Bismuth Liquid Metal Ion Source for Micromachining Application. — •Paul Mazarov, Alexander Melnikov, Rolf Wernhardt, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum 44780, Germany

Liquid metal ion sources (LMIS) are widely used in focused ion beam (FIB) technology for micromachining and surface treatment, and thus LMIS have been broadly developed. Key features of a LMIS for 3D-microfabrication of materials are long life-time, high brightness, stable ion current and a highly effective milling ability for the material to be modified. The most widely used LMIS with such properties is the Ga LMIS, being the working horse of FIB today. A very successful approach to increase the material removal rate, according to sputter theory, is the use of heavier ions and their clusters. We have produced a new long-life (about 1000 h) Bi LMIS with a good beam performance. The investigation of the sputtering rate of NiTi shape memory alloys using Ga and Bi LMIS shows that, for the same experimental conditions, the material removal rate with using of Bi ions without a mass separator is about 5 times larger compared to Ga ions. The sputter threshold dose is nearly one magnitude lower than that of Ga. For many applications this means a drastical reduction of working time. This sputter enhancement is particularly pronounced for target materials with large atomic masses. Furthermore, the roughness induced by the cluster projectile impact is much less pronounced than that generated by the atomic projectiles and the penetration depth is smaller, leading to less contamination of the target.

MM 50.4 Fri 11:00 H 0111

SRμCT in Materials Science at the Beamline HARWI II — •Julia Herzen, Felix Beckmann, Astrid Haibel, Tilman Donath, Funda S. Bayraktar, Stefan Riekehr, Mustafa Kocak, and Andreas Schreyer — GKSS Research Centre, Max-Planck-Str.1, 21502 Geesthacht

The synchrotron radiation based micro tomography is a powerful imaging tool in the wide range of materials science. Compared to laboratory X-ray sources the micro tomography at a synchrotron allows to visualize non-destructively high and low absorbing materials without any beam hardening effect and with a very high density resolution.

The beamline HARWI II operated by the GKSS Research Centre in cooperation with Deutsches Elektronen-Synchrotron DESY, Hamburg is designed for materials science experiments using hard X-rays. A fixed-exit monochromator provides a highly intense, monochromatic X-ray beam in the energy range between 15 and 200 keV. This large range of photon energies, the spatial resolution down to 3 μm and the high density resolution are important for microtomographic applications. The advantages of the beamline are demonstrated for absorption contrast tomography study of crack propagation within laser welded Al-Alloy T-Joints.