Vortrag

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Modelling and simulation of crystalline solids at and across multiple length scales

This talk gives an overview of some modelling approaches and simulation techniques for crystalline solids from the nanoscale up to the macroscale.
First, the main characteristics of a novel variational formulation of the quasicontinuum (QC) method is outlined, that enables a seamless transition from fully atomistic resolution towards continuum length scales at zero temperature. Among concurrent multiscale methods the present framework realizes an upscaling via coarse-graining with adaptive resolution. The second modelling approach of crystal plasticity can be classified as a mesoscale model, that accounts for the discrete nature of plastic glide in discrete slip systems within the realm of continuum mechanics. The third approach is a continuum constitutive model of anisotropic elastoplasticity which describes the effective properties of polycrystalline aggregates with e.g. orthotropic texture. For all modelling approaches, the main assumptions, properties as well as the range of applicability is discussed. Representative simulations of problem sets in materials science and in engineering applications demonstrate the predictive capacity and effectivity of each modelling and simulation framework. More specifically, (i) in nanoindentation, the force-depth curve and the evolution of dislocation microstructure is analyzed by means of the atomistic-based multiscale approach and compared with the results of fully atomistic lattice statics. (ii) The surface deformation pattern of an fcc single crystal subject to microindentation is simulated by means of the crystal plasticity finite element method and compared with experiments. (iii) At the macroscale, the continuum model of anisotropic elastoplasticity is used for the finite element analysis of typical forming processes such as deep-drawing. The simulations correctly predict the so-called 'earing' phenomenon observed at the rim of deep-drawn cups owing to the induced anisotropy in rolled sheet metal.

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gez. Prof. Dr.rer.nat. Hartmaier

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