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Discrete dislocation and nonlocal crystal plasticity modelling

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Summary

The increasing miniaturization of mechanical devices triggers a growing interest in modelling of plastic deformation at micrometer scales and smaller. A general conclusion from various experimental observations is that when dimensions of crystalline materials get smaller at these scales they become harder, i.e. the stresses become higher. This may have major implications for reliability of the devices and therefore has triggered a large research interest in the plasticity at small scales.

The starting point for much theoretical work is that standard continuum plasticity models fail to predict any size dependence of mechanical response due to the lack of any material length scale. There are, however, two alternative approaches that resolve this: discrete dislocation plasticity (DDP) and strain gradient (or nonlocal) continuum crystal plasticity models which are relevant at these scales and can capture such size dependence. The main advantage of DDP is that it is inherently nonlocal but at the same time it is also computationally very demanding on scales where a large number of dislocations need to be simulated. The so-called nonlocal continuum crystal plasticity models aim to incorporate the size dependence of dislocation plasticity usually by extending classical, local continuum descriptions with nonlocal or strain gradient terms based on phenomenological grounds. Irrespective of the precise formulation, such theories introduce a constant material length scale that needs to be fitted to experimental results or to results of numerical DDP simulations.

In this thesis a novel two-dimensional nonlocal plasticity theory is proposed that has strong dislocation grounds. The theory comprises a continuum description of dislocation dynamics and standard small-strain crystal continuum kinematics. The dislocation dynamics is derived by statistically averaging the equations of motion of an ensemble of interacting edge dislocations. Contrary to phenomenological strain-gradient theories the proposed theory is inherently nonlocal with the length scale being determined by the evolving dislocation densities.

After a brief introduction to the problem of plasticity in metals at different length scales in chapter 1, an overview of a few recent phenomenological nonlocal continuum crystal plasticity theories is given in chapter 2. Different methodologies of embedding the length scale in the theories are discussed. Emphasis is also given to additional (higher-order) boundary conditions required by some theories and the physical interpretation of such boundary conditions.

Chapter 3 presents a step-by-step derivation of the novel two-dimensional nonlocal plasticity model in single slip. It is distinctly different from existing phenomenological theories in that it involves two coupled diffusion-convection equations for two dislocation densities, one of which represents the density of geometrically necessary dislocations. Moreover, these transport equations comprise a source term for dislocation generation and annihilation. These are

well-established physical mechanisms that are absent in all currently existing continuum plasticity models, which, instead, presume that dislocations are available whenever and wherever they are needed for plastic flow.

Subsequently, the analysis of the problem of simple shearing of a model composite material is compared to the DDP simulations of the same problem to validate the novel approach in single slip. A numerical solution of the problem is obtained using a finite element method. The free parameters in the nonlocal theory are fitted to the corresponding DDP solution. The continuum theory is shown capable of distinguishing between the responses of two different particle morphologies (with the same area fraction), one involving unblocked slip in veins of unreinforced matrix material, the other relying on particle rotations induced by plastic slip gradients and geometrically necessary dislocations. During unloading the nonlocal theory predicts a pronounced Bauschinger effect that is also consistent with the DDP results. Comparison with the predictions of other strain gradient theories emphasizes that they cannot deal with source-limited plasticity in small-scale structures.

A necessary condition for a constitutive model to have predictive power is that, once fitted to a particular problem, it is able to predict other boundary value problems for the same material. Therefore, in chapter 4 the theory is applied to another boundary value problem with different boundary conditions, namely bending of a single-crystal strip. Rather than no-slip conditions, this problem involves traction-free boundary conditions. The parameter values used are identical to those obtained in chapter 3. The bending moment versus rotation angle and the evolution of the dislocation structure are analyzed for different orientations and specimen sizes with due consideration of the role of geometrically necessary dislocations. The results are compared to those of DDP simulations of the same problem. It is shown that without any additional fitting of the parameters, the continuum theory is able to describe the dependence on slip plane orientation and on specimen size.

In chapter 5 the problem of extending the nonlocal crystal plasticity theory from single slip to multiple slip is addressed. Continuum dislocation dynamics in multiple slip is proposed based on the dynamics derived for single slip, and coupled to the small-strain framework of conventional continuum single crystal plasticity. The key in multiple slip is to incorporate the nonlocal interactions between the dislocations of different slip systems. Awaiting a rigorous derivation, a few interaction laws are considered on phenomenological grounds.

To investigate the capabilities of the theory in multiple slip, it is applied to two boundary value problems. One problem is the simple shearing of a crystalline strip constrained between two rigid and impenetrable walls. Key features like the formation of boundary layers and the associated size dependence of the material response are addressed for crystals in symmetric double slip orientations. The other problem is bending of a single-crystalline strip under double slip (contrary to the single slip results in chapter 4). Again, the overall response and the evolution of the dislocation structure are analyzed for different slip orientations and specimen sizes. After identification of the most proper interaction law, the results of both problems are shown to be in a qualitative and quantitative agreement with those of DDP simulations for the same problems.

Chapter 6, finally, deals with the nonlocal plasticity simulations of the stress relaxation in single crystalline thin films on substrates subjected to thermal loading. Symmetric double slip is considered. The stress versus temperature and the evolution of the dislocation structure are analyzed for different orientations and film thickness. The effect of film size is associated with the formation of a boundary layer of piled-up dislocations at the film-substrate interface, the thickness of which does not scale with the film thickness. The thickness of the boundary layer itself, however, is shown to be dependent on the slip system orientation.