Discrete dislocation and nonlocal crystal plasticity modelling

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Chapter 1

Introduction

1.1 Bridging scales in metal plasticity

Beyond the elastic limit a material undergoes plastic deformation. In metals, plastic deformation originates from the motion of a large number of discrete defects: dislocations. Plastic deformation can be observed at various length scales. Relevant processes range from the atomistic scale where the atomic arrangement and individual defect properties of a material are of crucial importance for its deformation properties, up to the macroscopic scale where the actual material microstructure is not resolved and plasticity is described on phenomenological grounds. A schematic of the length scales and associated plasticity models in metals is given in Fig. 1.1, showing the four distinct length scales at which plasticity may be addressed: nanometer scale (atomistic), the microscopic scale, the mesoscopic scale (tens of microns) and the macroscopic scale.

Currently one of the most interesting issues in the computational mechanics of materials community is how to make a smooth and clear connection between plasticity related processes going on at the atomic scale and the plastic material behavior at the macro scale. A solution to this issue would, in principle, lead to a development of a consistent, unified plasticity theory based on a multi-scale strategy.

Yet, each of the four major length scale in plasticity, as depicted in Fig. 1.1, requires its own plasticity model. For example, phenomenological continuum plasticity based models serve well for many problems at the macroscopic scale. Starting from macroscopic engineering mechanics problems, the increasing miniaturization of mechanical devices takes us down to mesoscopic scales, where the material microstructure is of great importance in determining the material response. Crystal plasticity models that do account for the crystalline microstructure by distinguishing between different crystallographic orientations have become popular and successful models for the anisotropic plastic deformation of single crystals. The discrete slip systems that depend on the crystal structure are incorporated into these models, but the plastic part of deformation is still modelled in a continuum sense. One of the fundamental ingredients of such theories, the plastic flow rule, is usually given on purely phenomenological grounds, by e.g. Asaro (1983).

The characteristic length of a deformation microstructure becomes significant in the analysis of the material at a scale where the microstructure characteristic length is no longer negligible with respect to the material size. This triggers an important question, whether and how macro-

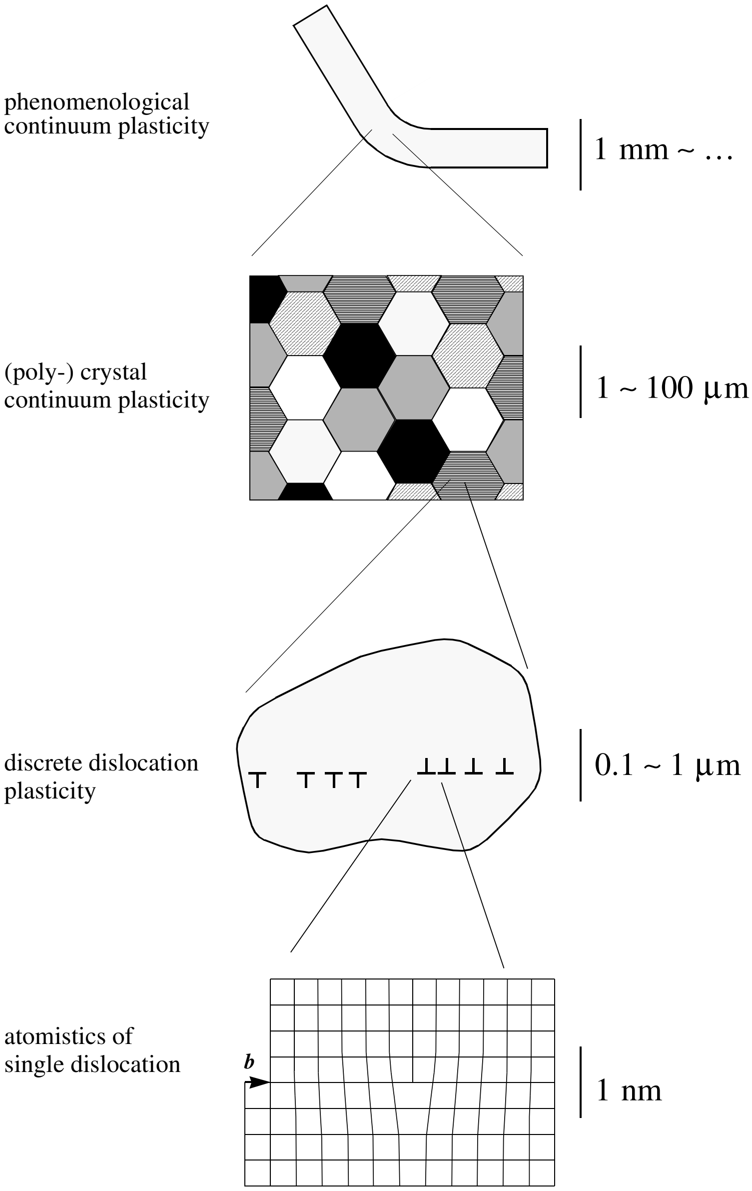

Figure 1.1 Plasticity in metals at various length scales.

scopic overall mechanical properties as strength, hardness etc. depend upon a natural internal length scale related to the characteristic size of the microstructures in the material. To answer this question, a detailed knowledge of the dislocation structure generation and evolution with the applied deformation is required.

Standard continuum plasticity models are local in the sense that the stress at a material point is assumed to be a function of a strain in that point only. Local theories do not make reference to the characteristic length scale for dislocations and, therefore, are not able to resolve dislocation structures. As a consequence, such models exhibit also no size dependence. However, there is a considerable, and growing, body of experimental evidence that shows that the response is in fact size dependent at length scales of the order of tens of microns and smaller. Fleck *et al*. (1994) showed, for example, that in a torsion experiment a wire exhibits a greater strength for smaller diameters. Size effect of the type "smaller is stronger" is common at these scales and has been also observed, for example, by Ma and Clarke (1995), Stölken and Evans (1998) for composites and in bending, respectively. The increase in strength in those experiments is related to strain gradients produced by so-called geometrically necessary dislocations (Ashby, 1970) that are needed to maintain compatibility in the material. Such nonlocal dependence of the response should be incorporated into a plasticity theory to accurately reflect the experimental observations at micron-size scales. Thus, these experimental observations motivate the development of plasticity models different from the standard continuum plasticity ones, which should account for physical properties of the individual dislocations and, therefore, be able to predict size effects.

One such type of plasticity theory, known as discrete dislocation plasticity (DDP), is inherently nonlocal. In DDP, the dislocations are modelled as line discontinuities in a linear elastic continuum. This approach poses a problem in calculating the strains along the dislocation line, i.e. inside the dislocation core. The strains in the core are just too large for linear elasticity theory to hold there. The core is usually only a few lattice spacings wide and its contribution can be estimated either from the atomistic simulation of a dislocation or indirectly from experiments. Outside the core, the strains can be described accurately by classical linear elasticity. From experiments, various mechanisms involving the dislocations such as dislocation glide, generation, annihilation, junction formation and breaking etc. are known. These mechanisms can be directed modelled in atomistic simulations. However, the only possibility to incorporate such dislocation features into DDP is through prescribed 'constitutive rules' mimicking the atomistic scale behaviour. Some of the effects like junction formation, line tension, mixed dislocations require fully three-dimensional discrete dislocation frameworks (e.g. Kubin *et al.*, 1992; Weygand *et al.*, 2002). Such advanced three-dimensional DDP models are usually computationally very costly and, thus, applicable only to rather small systems. However, for a particular class of plasticity problems, two-dimensional dislocation plasticity can be applicable, which is less computationally intensive and allows to handle complex boundary value problems. The range of dislocation related processes which can be simulated is, of course, limited to two-dimensional dislocation interactions defined by the set of constitutive rules.

There is also another class of approaches, which are aiming to incorporate the size dependence of dislocation plasticity by extending classical, local continuum descriptions with nonlocal or strain gradient terms, e.g. Hutchinson (2000). The development of such nonlocal theories is a very active field currently, with a variety of different kinds of theories which differ in the way the nonlocality is incorporated. A subset of them is based on the idea that the geometrically necessary dislocations associated with strain gradients give rise to additional hardening. Most of these employ Nye's (1953) geometrical concept of a dislocation density tensor, but in a variety of ways. Irrespective of the precise formulation, a constant material length scale that enters in such theories needs to be fitted to experimental results (see, e.g., Fleck *et al.*,1994; Fleck and Hutchinson, 1997) or to results of numerical DDP simulations, e.g. Bassani *et al.* (2001), Bittencourt *et al.* (2002). Another very important and still unresolved issue in the formulation of phenomenological strain gradient theories is the necessity or not of additional boundary conditions, e.g. Aifantis (1984), Acharya and Bassani (2000), Bassani *et al.* (2001), Gao and Huang (2003); Gurtin (2002), Van der Giessen and Needleman (2003). Parallel to these developments there is work by, for instance, Arsenlis and Parks (2002) and Evers *et al.* (2002) where a more direct physical connection is sought between dislocation density and hardening.

Coming back to the problem of linking plasticity theories at neighboring scales, one can say that bridging the discrete and continuum plasticity methods would be a significant contribution in understanding plastic deformation phenomena across the scales.

1.2 Scope and outline of the thesis

This work is a contribution in bridging the gap between the discrete dislocation description of a crystal that contains a large number of dislocations and crystal plasticity theory by means of a novel nonlocal continuum crystal plasticity model.

In the derivation of the theory we start from a statistical description of the motion of an ensemble of parallel edge dislocations by Groma and co-workers (1997, 1999, 2003). Averaging leads to two kinds of dislocation density for single slip: the standard total dislocation density and the net-Burgers vector density, which can also be interpreted as the density of geometrically necessary dislocations. The analysis leads to a continuum dislocation dynamics defined by two coupled transport equations for these densities, which form the nonlocal extension of a standard continuum slip model. Dislocation nucleation, the material resistance to dislocation glide and dislocation annihilation are included in the formulation. Thus, the proposed theory has strong dislocation background.

A necessary condition for a constitutive model to have predictive power, is that, once fitted to a particular boundary value problem, it is able to predict other boundary value problems for the same material. Therefore, to assess the validity of the approach, the theory is applied to a number of two dimensional boundary value problems. For each of them a quantitative and qualitative comparison with the corresponding results obtained by DDP is presented.

First of all, in chapter 2 an overview of a few recent nonlocal continuum crystal plasticity theories is given. 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 deals with a step-by-step derivation of the novel dislocation based nonlocal plasticity model in single slip. Subsequently, the analysis of the problem of simple shearing of a model composite material is compared to the discrete dislocation simulations of the same problem by Cleveringa *et al.* (1997, 1998, 1999a). The free parameters in the nonlocal theory are fitted to the corresponding discrete dislocation results of the same problem. 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 discrete dislocation results.

We continue to explore the nonlocal plasticity theory in single slip in chapter 4. After the free parameters of the theory have been fitted in the previous chapter, we aim at studying the abilities of the theory when applied to another boundary value problem with different boundary conditions. This time the theory is applied to bending of a single-crystal strip, using parameter values 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 discrete dislocation 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.

Chapter 5 concerns the problem of extending the nonlocal crystal plasticity theory developed in chapter 3 for single slip to multiple slip. Continuum dislocation dynamics in multiple slip is proposed and coupled to the small-strain framework of conventional continuum single crystal plasticity. Nonlocal interactions between the dislocations of different slip systems are also taken into account. Various interaction laws are considered on phenomenological grounds.

To validate the theory in multiple slip we compare with the results of discrete dislocation simulations of two boundary value problems. One problem is the simple shearing of a crystalline strip constrained between two rigid and impenetrable walls. Key features are the formation of boundary layers and the size dependence of the material response in the case of symmetric double slip. The other problem concerns the bending of a single-crystal strip with double slip. The bending moment versus rotation angle and the evolution of the dislocation structure are analyzed for different slip orientations and specimen sizes.

In chapter 6 we continue to test the nonlocal theory in multiple slip. This time we address the problem of thermal expansion of a single crystal thin films perfectly bounded to an elastic substrate. 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 the dislocations at the film-substrate interface which does not scale with the film thickness. The thickness of the boundary layer itself is shown to be dependent on the slip system orientation.