Discrete dislocation modelling of Nano- and Micro-indentation

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Chapter 1

Introduction

As mechanical systems in today's technology tend to decrease in size down to micro- and nanometers, it is becoming necessary to develop experimental and theoretical tools to investigate and characterise material properties at these scales. Among the most popular tools to probe material properties on a small scale is micro- or nano-indentation. It is almost a century that people perform indentation experiments on the macroscale to get material properties. After down-scaling by orders of magnitude, nano- and micro-indentation have now become increasingly used tools to investigate the mechanical properties of the material in small volumes. In particular it is a useful tool for studying the onset of plastic flow in small volumes, a phenomenon that plays a significant role in large scale deformation processes such as fracture, adhesion and friction.

While indentation is a relatively simple experiment, its interpretation in terms of material parameters suffers from the fact that the induced deformation is highly nonuniform. Hence, in general, a three-dimensional material model is needed with which the indentation experiment can be simulated in order to extract the material parameters through inverse modelling. When the indentation-induced plastic zone is sufficiently large, standard continuum plasticity can be used, the yield stress can be estimated by the well-known Tabor [1] relation between hardness and macroscopic Von Mises yield stress, see also [2, 3]. When the plastic zone size is smaller, two effects complicate the situation. First, the (poly-)crystalline microstructure of the material requires the use of (continuum) crystal plasticity in order to take the plastic anisotropy into account; this has been accomplished in e.g. [4]. A more difficult effect is the presence of strain gradients under the indenter; strain gradients which are known from various experiments to give rise to size effects with, generally, smaller being harder. In the context of indentation, this is known as the Indentation Size Effect (ISE). Classical crystal plasticity theories are not able to capture this size dependence. Enhanced continuum theories have been and are being developed to attempt accounting for strain gradients; applications to submicron and nano-indentation can be found, for instance, in [5, 6]. However, there is no consensus yet on the ingredients or even the structure of such strain gradient theories.

Experimental and smaller-scale modelling studies of plasticity in small volumes are being carried out to validate proposed theories and/or to aid improvements. In terms of modelling, atomistic studies per se are not feasible in this respect as the behaviour of many dislocations needs to be simulated in order for the transition to continuum plasticity to be meaningful. Discrete dislocation plasticity fills the gap between atomistics and continuum plasticity by treating dislocations as individual entities but having averaged the atoms out to an elastic continuum. Not only the Burgers vector, but also the density of dislocations and the density of sources for dislocations etc. induce material length scales into a discrete dislocation model, which henceforth is able to predict size dependent behaviour. Although the essential idea dates back the the 1960's, discrete dislocation plasticity has become a feasible tool only due to the availability of fast computers as well as the formulation of methods to solve boundary value problems, e.g. [7]. Since then it has been used in a range of studies to explore the validity of various strain gradient theories, e.g. [8, 9, 10]. Only a few discrete dislocation analyses had been published in the literature at the start of this Ph.D. project, e.g. [11, 12], albeit with debatable treatment of contact between indenter and the indented material. At very small scales, the atomic structure obviously does become important and molecular dynamics (with phenomenological potentials) is the preferred method of analysis. Atomistic studies of (nano-)indentation can be found for instance in [13, 14, 15].

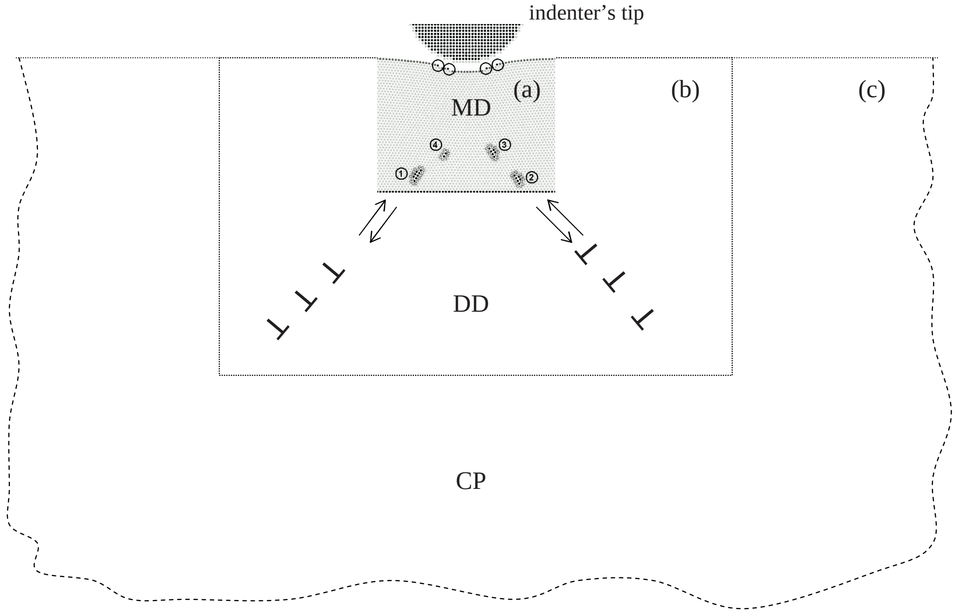

Figure 1.1 Multiple scales of indentation-induced plasticity: from (a) atomistic scale (MD: Molecular Dynamics) to (c) a larger scale (CP: Continuum Plasticity). (b) Discrete Dislocation plasticity (DD) bridges the gap between MD and CP.

All types of modelling mentioned above have a targeted range of size scales, so that many applications have their own preferred approach. Indentation, however, is one of the problems where all length scales matter. As illustrated in Fig. 1.1, one can identify an atomistic region right below the indenter for which molecular dynamics could be applied; on a somewhat larger length scale, discrete dislocation plasticity would be preferred, while at larger distance continuum plasticity would suffice to pick up the field variations. While a purely atomistic study is useful for nano-indentation, and continuum plasticity applies to macroscopic indentation, for the intermediate regime of micro- and submicron indentation discrete dislocation plasticity appears to be the appropriate approach. This, therefore, is the topic of this thesis.

Fundamentally, indentation is a complex problem. It involves mixed displacement and traction boundary conditions, which, moreover, dynamically change during indentation process, following indentation depth and indenter shape. Therefore the solution to the indentation problem is not trivial and it requires quite complex computational technique. This thesis discusses this technique and applies it to study the indentation size effect and the role of indenter shape, crystal orientations, contact length definitions and grain size.

Outline of the thesis

In chapter 2, background information is presented on indentation testing. It includes several common definitions of indentation hardness and contact area determination method in experiment. Also a brief review of contact mechanics related to indentation is given. Some experimental evidence of the indentation size effect is also presented.

The discrete dislocation plasticity model used in this thesis is discussed in chapter 3. It includes the discussion of the technique proposed by Van der Giessen and Needleman [7] , together with the constitutive rules and ingredients of the model. The computational algorithm of the model for the application to the indentation problem is also presented.

Chapter 4 discusses the effect of the indenter shape during two-dimensional indentation of a single crystal. It analyses various indenter shapes (wedge and circular) in relation to the size dependence of the indentation response.

In chapter 5 various measures of indentation hardness are investigated based on different definitions of contact length. Here we use four definitions of contact length: nominal, Oliver-Pharr based, end-to-end contact and actual contact. The roughness of the contact surface, which is related to the contact length determination, is emphasised.

The sensitivity of the indentation response to crystal orientation of a single crystal is studied in chapter 6. In this chapter we investigate the role of slip plane orientations in the crystal related to the hardness trend. The investigation involves comparisons between indentation response of two slip-system crystals and three slip-system crystals for various orientations.

While previous chapters have dealt with single crystal indentation, polycrystalline materials are the topic of chapter 7. The study here emphasises the coupling between the grain size dependence of plasticity and the indentation size effect.

In chapter 8, we review the homogeneous nucleation of dislocations. Three criteria from the literature are discussed, including the possibility of implementation of homogeneous nucleation into discrete dislocation plasticity using these criteria.

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