Discrete dislocation modelling of Nano- and Micro-indentation

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Summary

Since a long time, indentation testing is a commonly used technique to measure the properties of materials such as hardness and Young's modulus. Recently, nano-indentation is increasingly employed to investigate the properties of very small volumes of material as encountered in today's miniature technology. While an indentation experiment is performed relatively easily, the interpretation of the outcome is far from being trivial. The minimum requirement is the availability of a theory for the deformation processes taking place during indentation. As far as the plastic deformation of metals is concerned, this is precisely the scientific challenge because plasticity in volumes of cubic micrometers is size dependent. While the origin and description of this size dependence are subject of intense debate, one thing is certain: classical plasticity theories do not apply at length scales of tens of micrometers and below since these theories do not contain a material length scale and are therefore size independent.

In this thesis, a model is adopted that does have an inherent material length scale and aims at bridging the length scale gap between atomistics and continuum theories: discrete dislocation plasticity (chapter 3), In this theory, plasticity is viewed as originating from the collective motion of dislocations, which are described as line defects in a linear elastic continuum and characterised by their Burgers vector.

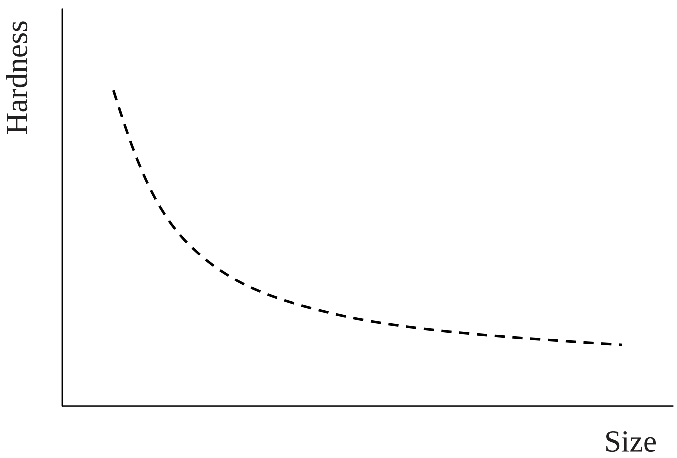

Figure A Indentation size effect: Smaller is harder

Experiments have convincingly demonstrated that indentation at the nano or micro scale also reveal a size effect, as illustrated in Fig. A. For sufficiently large size, the hardness that is measured is size independent (and equal to the value measured macroscopically), but below this one observes that the smaller the indent size, the harder the material is. This indentation size effect cannot be captured by classical continuum models, but this thesis demonstrates that it can be predicted using discrete dislocation plasticity. As one of the salient findings, two-dimensional numerical simulations reveal that the indentation size effect depends on what we use to measure the size. For a wedge indenter, the only length scale is the indentation depth, while for circular indenter the length scales are indentation depth and indenter radius (see chapter 4). By using the proper length scale to measure the size, the usual size effect "smaller is harder" is found.

Apart from several common definitions of indentation hardness, such as Berkovich, Vickers, Brinell, Rockwell, and Knoop (chapter 2), we define hardness simply as indentation force divided by the contact area, *i.e.* $H = F/a$. The estimated indentation hardness strongly depends on the definition of the contact area. Generally the hardness based on the nominal contact area is the smallest, followed by the Oliver-Pharr contact area definition typically used in nano-indentation tests. The highest hardness is based on the contact area that accounts for surface roughness (chapter 5) and on the material's sink-in during indentation, either elastically or plastically.

In chapter 6 we explore the effect of crystal orientation with respect to the indentation direction. In particular, two orientations are considered that differ from each other by 90° are used, with one of them having a slip system parallel to the indentation direction so as to easily accommodate indentation. Despite of the significant orientation effect on the indentation force and the contact length, the hardness is found to be rather insensitive to crystal orientation: apparently the difference in indentation force is cancelled by the difference in contact length.

Indentation of simple model polycrystals is simulated in chapter 7, with one of three types of grain structures: squared, horizontally-layered and vertically-layered. Here, the indentation response is found to be grain-size dependent, caused by: (i) dislocation mobility which corresponds to the distance between grain boundaries on the slip plane, (ii) dislocation pile-ups at the grain boundaries that cause hardening, and (iii) sink-in due to the near-tip plasticity. The predicted nominal hardness of polycrystals with equiaxed grains for deep indentation is found to scale with the inverse-square-root of the grain size, while for small indentation depths there is a complex coupling between the length scales: indentation depth and grain size.

While previous chapters have dealt with the generation of dislocations from sources through the Frank-Read mechanism, there is experimental evidence of homogeneous dislocation nucleation during nano-indentation. In chapter 8, three criteria for homogeneous nucleation are reviewed: (i) resolved shear stress based criterion, (ii) stress gradient based criterion, and (iii) an elastic stability criterion. These criteria were previously evaluated vis-à-vis atomistic simulations, but not yet used in higher length scale dislocation dynamics models. Implementation of these criteria into discrete dislocation plasticity seems possible, but with at least one caveat: the singular stress field close to existing dislocations may cause homogeneous dislocation nucleation according to these criteria, although this is unrealistic. New techniques need to be developed in the future to circumvent this spurious nucleation.