Discrete dislocation modelling of Nano- and Micro-indentation

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Chapter 9

Conclusion and Recommendations

The indentation simulations presented here using the [1] discrete dislocation model is able to capture many important aspects, such as the indentation size effect, indenter-shape effects, polycrystalline material grain-size effect, *etc.* The most important findings are as follows.

The significance of the indenter shape has been revealed. Despite the difference in their geometrical properties, *i.e.* a wedge indenter is self-similar while circular indenter is not, quite remarkably, both indenters give rise to the usual size-effect "smaller is harder". This, however, requires the use of different measures of "size": indentation depth h for wedge indentation and indenter radius R for circular indenter.

The predicted hardness values strongly depend on the definition of the contact length. The determination of the contact length has several aspects such as elastic and plastic sink-in during indentation and –important yet largely ignored sofar– surface roughness. The nominal contact length gives the lowest hardness, followed by the contact length estimated by using the Oliver-Pharr [2, 3] method. The highest hardness is obtained by using the actual contact definition, which accounts for surface roughness. The predicted nominal hardness for wedge indentation is found to fit well with the $h^{-1/2}$-scaling predicted by Nix and Gao [4] upon consideration of geometrically necessary dislocations. For circular indenters a similar scaling with $R^{-1/2}$ has been found from the simulations.

In two dimensions, the crystal orientation relative to the indentation direction does not have a strong effect on the indentation hardness. Even though there is an effect of orientation on the indentation force and on the contact length, the hardness apparently is rather insensitive to orientation. Apparently, the orientation effects to indentation force and to contact length cancel out. The indentation response has been found, however, to be sensitive to the number of slip systems. In particular what matters is the availability of slip directions close to the indentation direction.

In polycrystalline material subject to indentation, there are two length scales that play an important role: one is the indenter size scale (indentation depth h for wedge indenters, indenter radius R for circular indenters) and the other is grain size d. Although the reason is still unclear, we observe a remarkable relation between the nominal hardness and the square root of grain size, similar to the Nix-Gao square-root relation for single crystals. Further work in the future is needed to scrutinise the complex coupling between these two length scales: indentation depth and grain-size. The grain size dependence is mainly caused by (i) the limited dislocation glide distance determined by the spacing between grain boundaries and (ii) the grain-size controlled length of dislocation pile-ups that cause hardening. Slip incompatibility caused by misorientation of adjacent is likely to be another factor but this is left for future studies.

By construction, discrete dislocation plasticity applies down to lengthscales of several Burgers vectors. Events at atomic scales are not resolved and, instead, their effect on dislocation evolution is incorporated through constitutive rules. One of the mechanisms for which a constitutive rule is not available at this moment, is homogeneous nucleation of dislocations. Other researchers have investigated this type of nucleation, mainly molecular dynamics. On the basis of this, several criteria have been proposed in the literature: (i) a resolved-shear-stress criterion, (ii) a stress-gradient criterion, and (iii) an elastic stability criterion. The implementation of these criteria into the discrete dislocation model would be useful in bridging the gap between the atomistic and the sub-micrometer regime. However, taking into account also other studies of the appropriateness of these criteria, we have not been able to identify which criterion is to be preferred. Further work is also necessary to establish rules for dislocation nucleation from free surfaces.

References

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