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Discrete dislocation simulation of nanoindentation: Indentation size effect and the influence of slip band orientation

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Abstract

Nanoindentation is modelled on the computer by means of a simple two-dimensional discrete dislocation model in order to study the influence of the orientation of predefined slip bands on certain phenomena, which often occur during real indentation experiments, systematically. By assuming single slip, different simulations were performed, which show that the increase of the hardness with decreasing indentation depth, known as the indentation size effect, is significantly influenced by the slip band orientation in such a model. Compared to a case where the slip bands are oriented parallel to the surface, a less pronounced decrease of the hardness with increasing indentation depth is observed for the non-parallel slip band orientation. The value at which the hardness remains constant independent of the indentation depth is also significantly affected by these assumptions. Possible reasons for the origin of the different effects, which can partly be attributed to the discrete nature of plasticity, apparent in the nanometer regime, and Hall–Petch type mechanism, will be discussed.

Keywords: Dislocation dynamics; Dislocations; Computer simulation; Size effects Hall–Petch relation

1. Introduction

It is a well-known fact that in the early stage of plastic deformation the involved length scales play an important role, because the discreteness of the structure of matter is decisive. Certain phenomena, which cannot be explained by conventional continuum mechanics, become apparent in small dimensions. During nano- and microindentation tests, one observes an increase in the hardness with decreasing indentation depth, called indentation size effect (ISE) [1,2]. This effect is commonly explained by an application of the theory of strain gradient plasticity (SGP) [3–7] on an idealised nanoindentation process, as described by Nix and Gao [1]. Their model is based on the presumption that during indentation, the amount of dislocation loops necessary to accommodate for the shape of the indent (i.e. geometrically necessary dislocations) scales linearly with the contact area, whereas the volume in which the dislocations are stored, which is assumed to have a hemispherical shape, scales with the power of 3 of the contact width. The varying density of the geometrically necessary dislocations thus accounts for a size dependence of the plastic strain gradient; i.e. a smaller indent causes a larger gradient. Their considerations are followed by the necessity to introduce a representative material length scale which is capable of describing the qualitative and quantitative behaviour of the ISE. However, as the physical interpretation of the length scale is more or less hidden or remains indistinct, the discrete nature of plasticity is taken into account in this theory only in a secondary way. Discrete dislocation modelling in comparison, provides a good methodology to study certain phenomena, such as the ISE, in a direct manner. It implies the generation and movement of dislocations and their interactions, triggered by the local shear stresses, on a simple physical basis. Nevertheless, during the indentation process the number of dislocations and interaction mechanisms can become very large, so that in such simulations the computational effort strongly depends on the chosen level of complexity (e.g. two- or three-dimensional

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simulations, number of allowed slip systems, character of dislocations such as edge- or screw-type, cross-slip). As a consequence, it is not surprising that, up to now, such studies can describe the qualitative behaviour of such effects as the ISE only.

In our previous two-dimensional simulations of nanoindentation with a wedge-shaped indenter [8,9] we observed the occurrence of an ISE, even in the drastically simplified case of only one slip system, oriented parallel to the free surface. Those investigations showed that the characteristic of the ISE is mainly influenced by the assumed density of dislocation sources and by the value of the lattice friction stress (moving conditions for the dislocations); thereby, a higher source density and/or a higher lattice friction stress causes a less pronounced decrease of the hardness with increasing indentation depth. Furthermore, the continuum mechanics value of the nominal hardness (the value at which the hardness remains constant independent of indentation depth) is affected mainly by the critical stress for the emission of a dislocation dipole (the source strength) in our model. It is noteworthy that such an effect of the source density cannot be explained by SGP theory. This interesting point, together with recent observations of similar size effects in uniaxial compression experiments [10,11], where obviously no strain gradients can occur, are reasons for further investigations by means of our simple model. Therefore, in the present paper an attempt is made to study the influence of the orientation of the chosen slip system in relation to the free surface, and to illuminate further reasons for the occurrence of size effects during nanoindentation based on dislocation simulations.

2. Simulation procedure

A schematic representation of the simulation is shown in Fig. 1. In principle, this model is based on a linear elastic description of stress and strain fields induced by an indenter and by parallel edge dislocations in a model material. The nonlinear, i.e. plastic, material behaviour is taken into account by the motion of discrete dislocations, which is governed by the assumed lattice friction stress, σ_f, in the simulations. The material itself is thereby idealised by an infinite half space, where one parallel slip system with an arbitrary orientation to the free surface is arranged (single slip). On each slip band, point-type Frank Read sources are placed at random positions, which produce dislocation dipoles by multiplication. In each simulation step, the indenter is pressed into the specimen by a very small amount, typically in the order of the absolute value of the Burgers vector, b. From the displacement of the surface induced by the indenter and by the dislocations (plastic displacement), the local shear stresses are calculated by means of a collocation method. This technique is in principle based upon a discretisation of the interval of contact into small contact elements of constant width, followed by an iterative procedure, in order to obtain the correct contact stress distribution. Whenever the local shear stress at the position of a dislocation source exceeds the critical value for the emission, σ_{em}, a dipole is generated. During the procedure, the emitted dislocations are moved to the equilibrium positions under the influence of the stress field caused by the indenter and by all other dislocations. After each loading step, the nominal hardness, H_{nom}, which is defined as the sum of the contact stresses caused by the compression contact elements, divided by the contact width, is plotted versus the x_2-displacement of the indenter tip. Unloading is performed by decreasing the indentation depth in small steps of one b. Two dislocations with opposite Burgers vectors on the same slip plane will be removed from the arrangement if their mutual distance becomes less than a predefined annihilation distance, d_{ann}. A more detailed description of our computer program for the simulation of nanoindentation by means of a discrete dislocation is presented in Ref. [12].

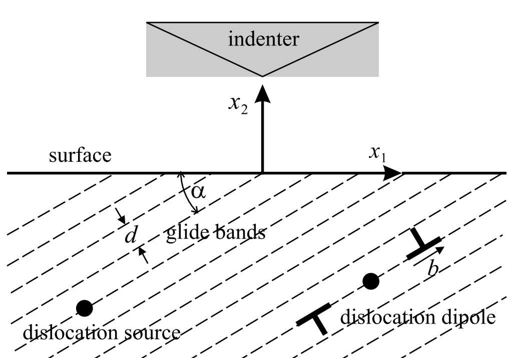

Fig. 1. Schematic of the simulation and coordinate system.

Beyond controversy, this is far from real nanoindentation, but, as highlighted above, our computer program provides a method to systematically investigate and understand certain occurring effects on the basis of a discrete dislocation model, with a large number of dislocations involved. Nevertheless, with an extension of our program, it would also be possible to investigate the effect of more than one type of slip system in one single simulation pass, such as intersecting slip bands, in order to study certain hardening mechanisms or dislocation multiplication from dynamically generated dislocation sources [13] etc. Aside from the increasing complexity of the program in such a case, one has to be resigned to the fact that all necessary modifications would be made, at least at the expense of computation time and effort. Furthermore, one should note that such improvements often go hand in hand with the growing difficulty of clearly separating different influence factors in the simulations.

3. Parameters and assumptions

The material parameters, common to all simulations in the present investigations, are the shear modulus $\mu = 80$ GPa, the Poisson ratio $\nu = 0.3$ and the absolute value of the Burgers vector $b = 2.5 \times 10^{-10}$ m. The geometry of the indenter is a wedge with an opening angle of