International Journal of Engineering Science 94 (2015) 195–211

Contents lists available at ScienceDirect

International Journal of Engineering Science

journal homepage: www.elsevier.com/locate/ijengsci

# Dislocation structure during microindentation

M. Baitsch [a], K.C. Le [b,*], T.M. Tran [b]

[a] Bauinformatik und Numerische Verfahren, Hochschule Bochum, D-44801 Bochum, Germany
[b] Lehrstuhl für Mechanik – Materialtheorie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

ARTICLE INFO

*Article history:*
Received 17 April 2015
Accepted 24 May 2015

*Keywords:*
Dislocations
Crystal plasticity
Variational calculus
Finite elements

ABSTRACT

Within the recently proposed continuum dislocation theory, numerical simulations of the displacement controlled wedge indentation for single crystals using the finite elements are provided. Under the assumption of plane strain deformation of the crystal having only one active slip system on each side of the wedge the load–displacement curve as well as the dislocation density are computed for the loading and unloading path in terms of the indentation depth. The results of numerical simulations are compared with those obtained from the experiments which shows qualitative agreement.


## 1. Introduction

In recent years, the micro-indentation test is widely used to measure the hardness and elastic moduli of materials having micron sizes like thin films, sensors and actuators, and electronic micro-devices (see Oliver & Pharr (1992, 2004) and the references therein). When various independent indentation tests are performed for specimens of the same material but at different indentation depths, the striking size effect is observed: the indentation hardness, defined as the applied force divided by the contact area between the indenter and the tested material, increases by a factor of two as the depth of indentation decreases from 10 microns to 1 micron (Ma & Clarke, 1995; Nix, 1989). Thus, opposed to the common believe existed in the material testing community for long time, the hardness is not the characteristics of material of small sizes. The reason for this size effect are dislocations which nucleate when the resolved shear stress (or Schmid stress) on some slip planes exceeds a certain critical threshold. The subsequent pile-ups of nucleated dislocations against the contact area of the indenter as well as the evolution of the dislocation network depend essentially on the indentation depth that leads to the size effect. The latest indentation tests using high-resolution electron backscatter diffraction (EBSD) to measure the lattice rotation and the density of geometrically necessary dislocations provided by Kysar, Saito, Öztop, Lee, and Huh (2010) confirmed the above statement. Thus, to be able to predict the size effect properly, the mechanism of dislocation nucleation and the subsequent dislocation pile-ups causing the hardness of the crystal should be well understood and captured in the mathematical model of indentation.

There were various attempts to describe the dislocation network occurring in plastically deformed crystals within the so-called gradient-plasticity theory initiated by Fleck, Muller, Ashby, and Hutchinson (1994), Fleck and Hutchinson (1997), Gao, Huang, Nix, and Hutchinson (1999), and Nix and Gao (1998). Despite their successful numerical implementation in various indentation problems to describe the size effect, there are two main deficiencies of this kind of gradient theories: (i) the dislocation density is not directly related to the measure of incompatibility of the plastic slip of the active slip systems

* Corresponding author. Tel.: +49 234 3226033; fax: +49 234 3206033.
*E-mail address:* chau.le@rub.de (K.C. Le).

http://dx.doi.org/10.1016/j.ijengsci.2015.05.005
0020-7225/

(Nye–Bilby–Kröner dislocation density tensor), but to some scalar function of the second gradient of the total displacement vector, so it depends on the history of creation of dislocations and cannot be used as state variable in constitutive equations, (ii) it is not clear whether such gradient-plasticity theory can justify the low-energy dislocation structure (LEDS) hypothesis formulated first by Hansen and Kuhlmann-Wilsdorf (1986) and supported by various experimental evidences (see Laird, Charsley, & Mughrabi (1986) and Kuhlmann-Wilsdorf (1989)). A new approach based on the continuum dislocation dynamics has emerged in recent years (see, e.g., Groma, Csikor, & Zaiser (2003), Arsenlis, Parks, Becker, & Bulatov (2004), and Sandfeld, Hochrainer, Gumbsch, & Zaiser (2010, 2011)) that can predict in principle not only the dislocation densities but also the direction and curvature of the dislocation lines. In addition to the high computation cost in applied problems like indentation, the link of such approach to the energetics of crystals and LEDS-hypothesis is also not clear. Let us mention here the first finite element implementation of the approach similar to that of Arsenlis et al. (2004) to the indentation problem realized in Reuber, Eisenlohr, Roters, and Raabe (2014). The results obtained in Reuber et al. (2014) will be compared with the results of this paper.

The material model proposed in this paper is based on the continuum dislocation theory (CDT) developed in Berdichevsky (2006a, 2006b), Berdichevsky and Le (2007), Kaluza and Le (2011), Kochmann and Le (2008, 2009a, 2009b), Le and Sembiring (2008a, 2008b, 2009), Le and Nguyen (2010), Le and Nguyen (2012, 2013) (see also the finite strain CDT proposed by Le & Günther (2014), Koster, Le, & Nguyen (2015)). We apply this material model to the two-dimensional plane strain problem of wedge indentation for single crystals having one active slip system on each side of the wedge. In case the dissipation can be neglected, the displacements and the plastic slip satisfying the contact conditions on the contact area between the crystal and the indenter should minimize the energy of crystal in the *final* equilibrium state. This contact variational problem is discretized by the finite elements and the Newton–Raphson solution procedure is applied to obtain the minimizer numerically. To the best of our knowledge, such finite element discretization of the contact problem within CDT is implemented here for the first time, so we discuss in details several numerical difficulties associated with the specific form of the dislocation density and of the energy density, and then propose the modifications and integration algorithm required to overcome these difficulties. Based on the obtained numerical solution the load–displacement curve, the dislocation density distribution, the lattice rotation, and the plastic slip are analyzed in terms of the wedge displacement for the loading/unloading processes. If the dissipation cannot be neglected, the simplest rate-independent dissipation will be taken into account leading to the incremental minimization of "relaxed" energy functional at each time step. We compare the results of our numerical simulations with experimental data obtained in Kysar et al. (2010) and Dahlberg, Saito, Öztop, and Kysar (2014), with the numerical simulations within the conventional crystal plasticity performed by Saito, Öztop, and Kysar (2012), and with the numerical simulations based on the approach of Reuber et al. (2014). The qualitative agreement of the load–displacement curve as well as the lattice rotation and the dislocation density with experiments supports the proposed continuum dislocation theory.

The outline of the paper is as follows. In the next Section the plane strain wedge indentation problem within CDT for a single crystal having one active slip system on each side of the wedge is formulated. Sections 3 and 4 are devoted to the finite element discretization and the Newton–Raphson solution procedure, respectively. Section 5 reports the results of the numerical simulations and the comparison with experiments. Finally, Section 6 concludes the paper.

## 2. Plane strain wedge indentation

Consider a single crystal subjected to indentation by a rigid cylindrical wedge (see Fig. 1). The depth of the crystal in the $z$-direction (which is equal to the length of the rigid indenter) is taken large enough to guarantee the plane strain state having two component of displacements $u_x = u(x, y)$ and $u_y = v(x, y)$. Besides, the sizes of the crystal's cross-section are much

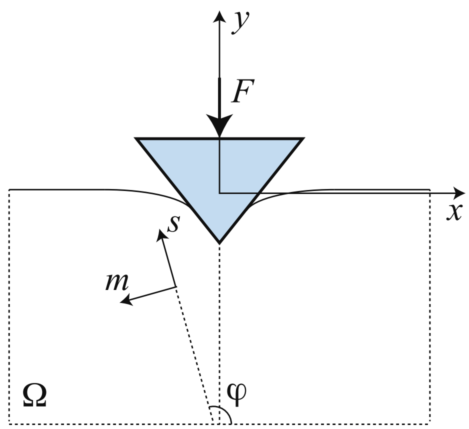


**Fig. 1.** Wedge indentation.