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Editor's Choice

Impingement of edge dislocations on atomically rough contacts

R.J. Dikken, B.J. Thijsse, L. Nicola *

Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628CD Delft, The Netherlands

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ABSTRACT

The impingement of edge dislocations on nano-scale interfaces formed when bringing in contact aluminum crystals is investigated using molecular dynamics simulations. Dislocations, inserted in the bottom crystal, glide towards the contact when the two crystals are pressed together. There, dislocations are absorbed and upon further loading new dislocations are nucleated from the impinging site.

Absorption and nucleation are events that affect the length of dislocation pile-ups and therefore the plastic behavior of crystals under contact loading. While it is possible to track absorption and nucleation at the nano-scale with molecular dynamics simulations, larger scale models, which are suitable to study plasticity, do not have the right resolution and neglect these events. The goal of this work is to gain a better understanding of dislocation impingement and to assess to which extent absorption and re-nucleation would play a role at the larger scale.

The contacts are here characterized by their initial atomic scale roughness for which a simple, novel definition is introduced. Results show for the first time that roughness controls dislocation nucleation from the contact. This is true for both dislocation-free crystals and for crystals containing one or more dislocations before application of contact loading. In dislocation-free crystals nucleation occurs at decreasing load for increasing roughness. When a dislocation impinges on the contact, it affects its local roughness, by that decreasing the load necessary for dislocation nucleation. Only when the initial roughness of the contact is above a given threshold, dislocation impingement does not affect the load required for nucleation.

If instead of a single dislocation, a train of dislocations impinges on the same site, dislocation nucleation is even more facilitated. However, even in this case the contact pressure required to nucleate dislocations is in the order of one GPa, rather high compared with the pressure required to sustain plastic deformation when macro-scale bodies are in contact.

1. Introduction

When dislocations impinge on two-dimensional defects like interfaces, grain boundaries (GBs), or contact areas between crystals, several mechanisms can occur, i.e. absorption, re-nucleation, transmission, or stagnation by pile-up [1–3]. Which of these mechanisms will prevail depends on a large number of variables, e.g. dislocation type, crystal structure, (relative) crystal orientations, loading and temperature. There is both experimental [4] and computational [5–9] evidence that a critical role is played by the atomic structure of the two-dimensional interface. While specific interfaces favor dislocation absorption through local atomic rearrangement [10], others favor dislocation nucleation into one of the two adjacent crystals [11]. Also, depending on the atomic interface structure, nucleation of new dislocations was measured to occur at a wide range of critical nucleation stresses [4].

The molecular dynamics studies that have been performed so far have focused on perfect interfaces [11,10,12,13]. However, real GBs are not perfect and contacts, formed by pressing two crystals together, are even less perfect, because of the presence of adatoms on each of the surfaces [14].

The main aim of this study is to identify, by means of molecular dynamics simulations, the effect of atomic scale roughness on the impingement behavior of dislocations on Al contacts between clean surfaces without native oxide layer. To this end, we characterize two dimensional contacts, also perfect ones (i.e. without adatoms), by their average atomic scale roughness. Interestingly, we find that there is a direct correlation between atomic scale roughness and the applied load required to nucleate a new dislocation from the contact after impingement. Notice that in previous studies, interfaces were characterized by their energy, but no uni-

* Corresponding author.
E-mail address: L.Nicola@tudelft.nl (L. Nicola).

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versal correlation was found between interface energy and nucleation stress [13].

An additional question that we intend to answer is: what is the limit to the number of dislocations that can pile up on the same slip plane against an atomically rough contact? This is of interest to us because of the impact that pile-up length has on the plastic behavior of metal contacts at larger scales. Micro-scale models of the type of discrete dislocation plasticity are used to study the plastic behavior of micro-scale contacts [15–17], but details of the contact and of dislocation nucleation and absorption are below the resolution of the method. The contact is simply described as an impenetrable boundary for dislocations, where dislocations therefore form unbounded pile-ups. Interfaces can certainly be strong barriers for dislocation glide. It is shown, for instance, by Tsure et al. [18] that the interaction energy of an edge dislocation with an energetically stable Al grain boundary is 10^4 times higher than the Peierls potential. This could lead to dislocation pile-up, as for instance experimentally observed in Ref. [19]. Nevertheless, absorption and re-nucleation are phenomena that limit the length of pile-ups on many interfaces, as supported by the experimental observations in Ref. [20] where at certain critical strain a sudden change in the dislocation distribution of the pile-up was found. Our goal in this respect is to extract information from the molecular dynamics simulations to determine what are the conditions that limit the length of a pile-up, and trigger re-nucleation. This information can be used in future discrete dislocation plasticity simulations of contact.

In this work two aluminum crystals with different orientation are pressed into contact. Dislocations are introduced in one of the crystals and their glide towards the contact is enforced by applying a normal load to the bi-crystal. The surface of each crystal is either perfect or contains adatoms.

The paper is organized as follows: in Section 2 the method and problem formulation are presented. In Section 3 the contact is characterized and the atomic scale contact roughness is defined. In Section 4 the effect of atomic roughness on the impingement of single dislocations is investigated, while Section 5 is devoted to the impingement of multiple dislocations (up to 4) on contacts of various roughness. The roughening due to impingement and roughness dependent ability to absorb dislocations is studied in Section 6. Section 7 provides a discussion and guidelines for the implementation of constitutive rules in larger scale models.

2. Computational approach

Molecular dynamics (MD) simulations are performed using the embedded atom method. The total energy of the system is given by

$$U = \frac{1}{2}\sum_{i,j(j\neq i)} V(r_{ij}) + \sum_i F(\bar{\rho}_i) \tag{1}$$

where the first term represents pair interactions between atom i and j, and the second term represents the embedding energies of atom i in an electron density $\bar{\rho}_i$ due to the other atoms. The electron density is given by

$$\bar{\rho}_i = \sum_{j\neq i} \rho(r_{ij}), \tag{2}$$

representing the contributions from all neighboring atoms j. This method is especially useful for metals, as the embedding form using the electron density is capable of mimicking the metallic bond [21].

The MD simulations are performed using LAMMPS [22] with a potential developed by Purja Pun and Mishin [23–25] which has shown to give accurate surface and stacking fault energies and is especially suitable for studying mechanical behavior of contacts, interfaces and dislocations.

2.1. Material choice and problem description

In the present study the impingement of edge dislocations on contacts is investigated. In FCC metals it is often energetically favorable for dislocations to exist as partial dislocations separated by a stacking fault ribbon. The width of the stacking fault ribbon d_{SF} is inversely related to the stacking fault energy γ

$$d_{SF} \approx \frac{Gb^2}{4\pi\gamma}, \tag{3}$$

where G is the shear modulus and b is the magnitude of the Burgers vector [26]. The material chosen in this study is aluminum because it has a small stacking fault ribbon, and therefore allows for a relatively small simulation box. The stacking fault ribbon width that results from the potential used in this study is $d_{SF} = 1.3$ nm, which is in close agreement with the experimental value, ranging from 1.1 to 1.6 nm [24].

The contact is established between two Al crystals with different orientation, constituting a bi-crystal. Fig. 1 shows a schematic representation of the model. Two bi-crystals, A and B, are chosen with slip plane orientations that are either favorable or unfavorable for dislocation transmission. The difference between the two bi-crystals is only in the orientation of the upper crystal. The lower crystal is chosen such that the [1 1 0]-direction aligns with the x-axis, the [$\bar{1}$ 1 0]-direction aligns with y-axis and the [0 0 1]-direction aligns with the z-axis. For this orientation we have slip planes for which the dislocation line lies along the y-axis. The angle of the slip planes of two slip systems with the x-axis is ±54.7°.

For the upper half of the bi-crystal, two orientations are used: for bi-crystal A, the [1 0 0]-direction aligns with the x-axis, the [0 1 0]-direction aligns with the y-axis and [0 0 1]-direction aligns with the z-axis. Dislocation transmission is not expected to occur, because this crystal has no slip planes for which the dislocation line lies along the y-axis.

For bi-crystal B, the [0 0 1]-direction aligns with the x-axis, the [1 $\bar{1}$ 0]-directions aligns with the y-axis and the [1 1 0]-direction aligns with the z-axis. This crystal has, like the lower half of the bi-crystal, slip planes for which the dislocation line lies along the y-axis. The crystal is a 90° rotation of the first crystal, which means that the angle of the slip planes of two slip systems with the x-axis is ±35.3°. This means that for bi-crystal B, dislocation transmission is possible.

The dimension in the y-direction is taken to be small, only five times the lattice constant, so that the dislocations are of edge character. Because the periodic box is small in this direction, the dislocation line cannot bow out, so that spurious image forces due to line bowing are avoided [27].

The simulation box contains the bi-crystal and is periodic in the x- and y-direction. The box size is chosen large enough to not influence the dislocation behavior in terms of the onset of dislocation motion and the stress at which nucleation occurs from the contact. For the material studied here the size is $L_x = 445$ Å, $L_y = 20$ Å and $L_z = 810$ Å. Dislocations are inserted in the bottom crystal by prescribing displacement to the atoms in the dark grey (hatched) domain in Fig. 2, where the insertion of the dislocation is schematically depicted. The displacement applied ranges from zero for the atom at the bottom left hand side of the hatched region to b for the atoms at the right hand side of the hatched region. This creates a displacement step of size b at the bottom of the crystal. A relaxation run is then performed. During relaxation, a dislocation emerges at the top corner of the hatched region (see Fig. 3). If the dislocation is inserted close to the contact, the dislocation moves by itself into the contact during relaxation. This is referred to as 'directly inserting the dislocation into the contact' later in this