



HAL
open science

Edge dislocation impingement on interfaces between dissimilar metals

Robbert-Jan Dikken, Mohsen Khajeh Salehani

► **To cite this version:**

Robbert-Jan Dikken, Mohsen Khajeh Salehani. Edge dislocation impingement on interfaces between dissimilar metals. 2017. hal-01572509

HAL Id: hal-01572509

<https://hal.science/hal-01572509>

Preprint submitted on 7 Aug 2017

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Edge dislocation impingement on interfaces between dissimilar metals

R.J. Dikken* and M. Khajeh Salehani
*Department of Materials Science and Engineering,
Delft University of Technology,
2628CD Delft, the Netherlands*

(Dated: August 7, 2017)

In this work, the effect of material dissimilarity on the impingement behavior of a dislocation on the interface of a bi-crystal is investigated. To this end, impingement of a single edge dislocation on a Ni-Al interface is studied using molecular dynamics simulations. A dislocation is inserted in either aluminum or nickel and forced to impinge on the interface by an applied compressive load on the bi-crystal. We observe that the contact contains defects due to the lattice mismatch between the materials and hence, the dislocation may impinge on an interface defect or between two defects. Our results show that the dislocation is directly absorbed by the contact only if it impinges on an interface defect. Furthermore, it is demonstrated that dislocation transmission occurs only when it is initially in the Ni crystal. This is explained by looking at the energy of the core of a dislocation. Moreover, the importance of atomic vibrations is emphasized by performing the simulations at two temperatures 100 mK and 10 K.

Keywords: dislocation impingement, molecular dynamics, interfaces, defects, aluminum, nickel

I. INTRODUCTION

Plastic deformation of metals is dominantly due to glide of dislocations carrying plastic flow with an intrinsic length scale, the Burgers vector. When dislocations impinge on interfaces, like grain boundaries or contacts, several phenomena/mechanisms can occur, e.g. stagnation resulting in pile-up, absorption, transmission or re-nucleation [1–3]. Due to the large variety of variables involved, e.g. loading, temperature, crystal structure, dislocation type, relative crystal orientations, etc., it is rather difficult to predict which physical variable is dominant and which mechanism will prevail. However, both experimental [4] and computational [5–11] studies have shown that a critical role in the impingement behavior is played by the atomic structure of the interface.

A recent study has introduced a characterization of contacts, the atomic scale contact roughness [12]. This contact roughness depends simply on the ratio of the total number of interface atoms, i.e. atoms with different structure than atoms in the bulk, and the number of contact atoms (interface atoms which are in compressive mode) [13]. Interestingly, a clear correlation between the normal stress at which a dislocation nucleates from the interface and the contact roughness is found for different Al bi-crystals and disordered interfaces, while there is for instance no universal correlation between nucleation stress and interface energy [12, 14]. Moreover, in Ref. [12] dislocation impingement on interfaces of Al bi-crystals is extensively studied and it is concluded that atomic scale contact roughness is pivotal in the impingement behavior.

In this work, the aim is to determine how the difference in material characteristics, i.e. two dissimilar metals, affects the impingement behavior of edge dislocations on interfaces. To this end, a dislocation is inserted in either aluminum or nickel, and forced to impinge on a Ni-Al interface by an applied compressive load on the bi-crystal.

This article is organized as follows. In Section II the computational approach is described. In Section III the results for impingement from both sides of a Ni-Al interface are presented. Section IV summarizes the conclusions of this study.

II. COMPUTATIONAL APPROACH AND PROBLEM FORMULATION

The simulations are performed with LAMMPS [15] using an EAM-potential [16] for nickel and aluminum that gives accurate surface and stacking fault energies, making it especially suitable to study the mechanical behavior of interfaces and dislocations [17]. Aluminum and nickel are very different in their mechanical properties. The Burgers vectors are 2.49 Å and 2.86 Å and the shear moduli are 76 GPa and 26 GPa for nickel and aluminum, respectively.

The materials studied in this work, nickel and aluminum, are chosen based on their relatively large stacking fault energy. The length of the stacking fault ribbon d_{SF} that separates the partial dislocations of a dislocation in a FCC metal with shear modulus G and Burgers vector magnitude b is approximately proportional to the inverse of the stacking fault energy γ :

$$d_{\text{SF}} \approx \frac{Gb^2}{4\pi\gamma}. \quad (1)$$

Therefore, the larger the stacking fault energy, the smaller the stacking fault ribbon length. This limits the

* R.J.Dikken@tudelft.nl

required dimensions of the system that is modeled, which is computationally beneficial.

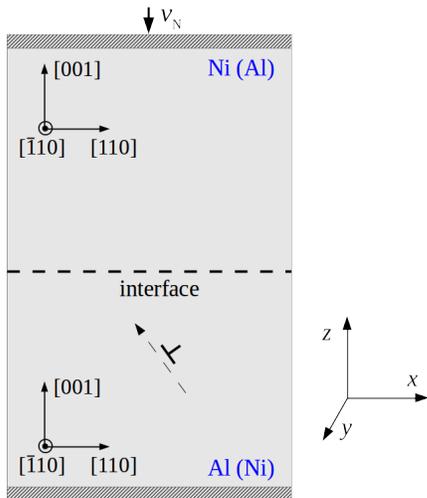


FIG. 1. Schematic representation of the system.

The system is periodic in the x- and y-direction (see Fig. 1). Both the nickel and aluminum crystals have the same crystal orientation, as shown in Fig. 1. The crystal orientation is chosen such that the system has symmetric slip systems with the (dislocation) slip line along the short periodic y-axis. The angle of the slip planes of the two slip systems with the x-axis is $\pm 54.7^\circ$. The y-direction, the direction parallel to the dislocation line, is taken short ($L_y = 2$ nm), to model a pure edge dislocation which does not bow out. Hence, spurious image forces due to line bowing are avoided [18]. The simulation box dimensions are $L_x = 32$ nm, $L_y = 2$ nm and $L_z = 64$ nm.

A dislocation is inserted, in either Ni or Al, through a prescribed displacement to atoms in the dark grey (hatched) region in Fig. 2. The value of displacement is b where the dislocation is inserted and zero at the bottom. This creates a surface step at the bottom of the crystal. Upon relaxation, a dislocation emerges that splits into two partial dislocations.

The dislocation is forced to move towards the interface by applying a compressive load to the bi-crystal. Eight atomic (x,y) planes at the top of the bi-crystal are displaced in the negative z-direction, while keeping eight atomic (x,y) planes at the bottom of the bi-crystal fixed in the z-direction. The loading is uniformly applied with a strain rate of 5×10^7 s $^{-1}$. The velocity of the load is about three orders of magnitude lower than the speed of sound in aluminum, so that setting off shock waves is avoided.

The pressure on the periodic boundaries is kept zero and the full system is thermalized to 100 mK (unless otherwise specified) using a Nosé-Hoover thermostat through a NPT ensemble in LAMMPS.

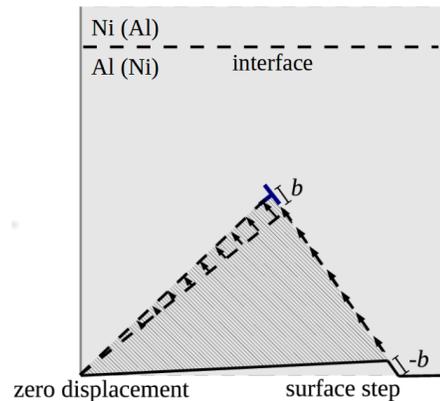


FIG. 2. Schematic representation of the dislocation insertion in either nickel or aluminum.

III. RESULTS

Because of the mismatch of the lattice parameter in aluminum and nickel the contact contains interface defects as shown in Fig. 3. The spacing of these defects is approximately five times the lattice parameter of aluminum. A dislocation can either impinge on an interface defect, or between two interface defects where the interface has a perfect FCC environment.

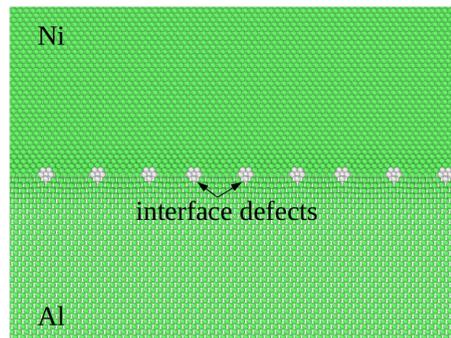


FIG. 3. The contact between Al and Ni showing interface defects.

Figure 4 shows the distance of the leading partial dislocation to the contact as a function of strain for both impingement on and in between defects, when the dislocation comes from the Al side of the contact. It is found that when the dislocation impinges on the defect, the distance to the contact becomes zero, indicating that the dislocation is absorbed by the contact. However, when the dislocation impinges in between defects, the dislocation stops at approximately 11 Å from the contact. Hence, only in the first case a step of size b emerges in the contact. Consequently, the additional step in the contact can have a large impact on the frictional behavior when the bi-crystal is sheared [19].

The number of atoms with HCP structure is a measure of dislocation in the crystal, since the atoms in the

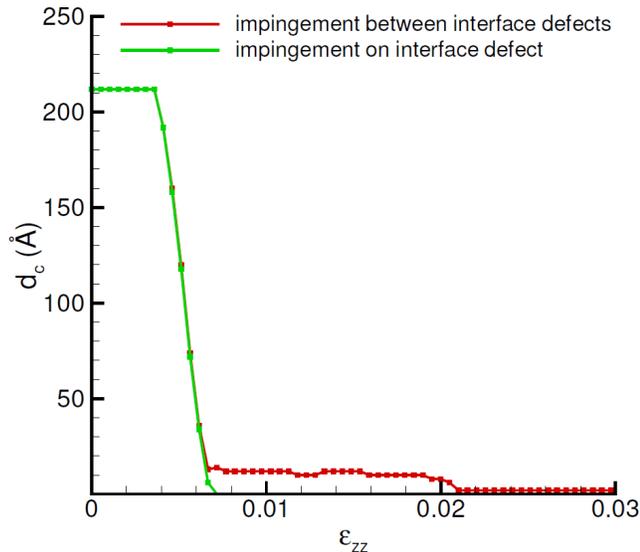


FIG. 4. Distance of the dislocation from the contact for the impingement of a dislocation coming from the Al side of the contact on and in between interface defects (Al \rightarrow Ni).

stacking fault ribbon are of HCP structure. In Fig. 5, the evolution of the number of HCP atoms as a function of strain, when the dislocation impinges on the contact from the Al side, is shown for both impingement on and in between interface defects. When the dislocation im-

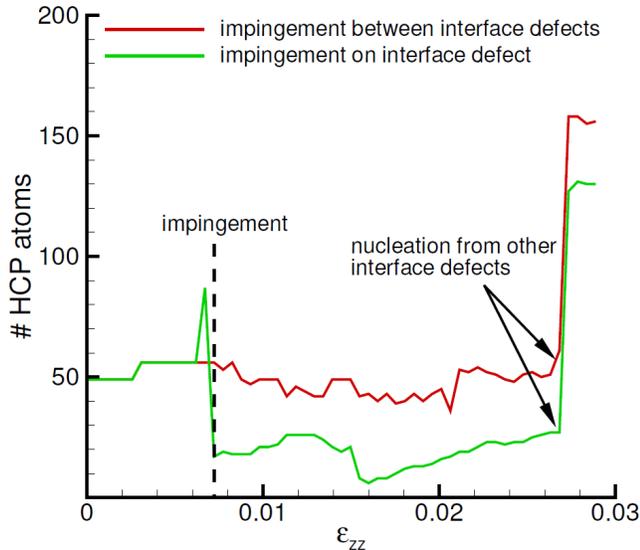


FIG. 5. The number of HCP atoms for the impingement of a dislocation coming from the Al side of the contact on and in between interface defects (Al \rightarrow Ni).

pinges on a defect, the stacking fault ribbon increases right before impingement, indicating an attractive interaction, and then decreases fast once it gets absorbed by the contact. On the other hand, when the dislocation impinges between defects, the sudden increase in number of HCP atoms is not found and as the dislocation

impinges on the contact, the number of HCP atoms stays approximately constant. Eventually, the number of HCP atoms increases fast for both cases. This is due to the fact that dislocation nucleation occurs from other interface defects, at a normal stress of 3.4 GPa. A compressive test simulation without dislocation initially present in the bi-crystal shows that the nucleation stress for the same system without impingement is 3.5 GPa, only slightly higher than for the case with impingement. Hence, the nucleation stress is only minorly affected by the impingement of a single dislocation. This is in line with the observation for relatively rough contacts in Ref. [12].

The difference in the behavior of impingement on or in between defects can be explained by looking at the local normal stress σ_{zz} , as shown in Fig. 6 and 7. When a dislocation impinges on an interface defect, the normal stress field of the dislocation and the defect partially cancel each other. Inversely, when a dislocation impinges between defects the normal stress fields augment each other, which is not favorable.

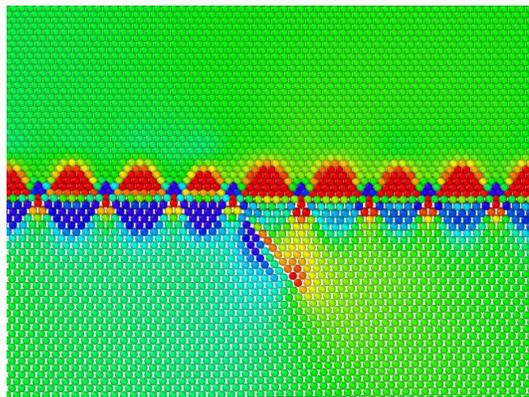


FIG. 6. The normal stress σ_{zz} contour right before impingement on an interface defect.

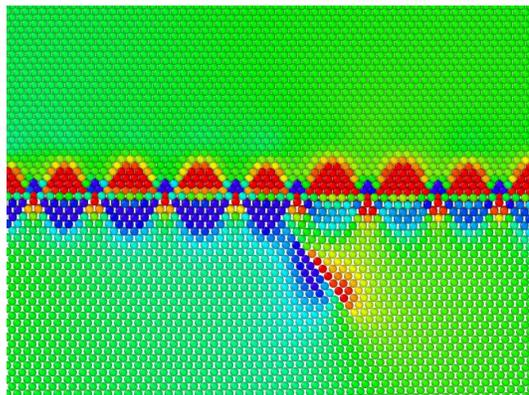


FIG. 7. The normal stress σ_{zz} contour right before impingement in between defects.

A different behavior is found when looking at the impingement behavior of a dislocation coming from the Ni side. Figures 8 and 9 show the distance of the leading

partial to the contact and the number of HCP atoms, respectively. The results show that when the dislocation impinges on or in between defects the leading partial dislocation is directly nucleated into the aluminum (red and blue curve). However, once the leading partial is nucleated, the dislocation is pinned by the contact. Only for the case in which the dislocation impinges on a defect, the dislocation is eventually depinned and moves away in the Al from the contact. To assess how realistic this is, we increase the temperature to 10 K. It is observed that the full extended dislocation is directly transmitted into the aluminum [20]. This emphasizes the importance of atomic vibrations for plasticity and also shows that quantum effects, like zero point fluctuations, are expected to be important for plasticity at low temperatures as shown in Ref. [21]. Proville *et al.* [21] show that for approximately $T < 0.5T_D$, where T_D is the Debye temperature, quantum corrections have to be applied to classical calculations to account for zero point fluctuations. This means that results of classical molecular dynamics at low temperature in the context of plasticity have to be treated with care.

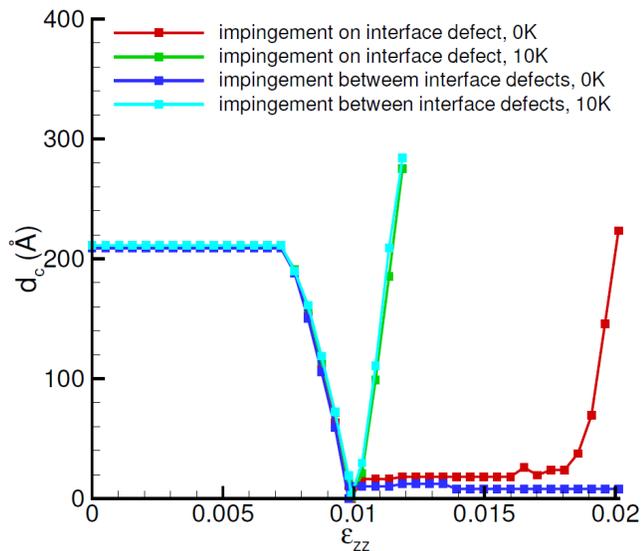


FIG. 8. Distance of the dislocation from the contact for the impingement of a dislocation coming from the Ni side of the contact on and in between interface defects (Ni \rightarrow Al).

In conclusion, it is observed that if a dislocation impinges on the contact coming from the aluminum crystal, the Burgers vector is not transmitted into the nickel crystal. However, if the dislocation impinges on the contact coming from the nickel crystal, the Burgers vector is transmitted into the aluminum crystal. Since the Burgers vector of nickel is smaller than the Burgers vector of aluminum, there is a residual Burgers vector in the contact of 13 % of the Burgers vector in aluminum. In general, the residual Burgers vector should be small in order to have slip transmission [1]. However, a residual Burgers vector of $0.13b_{Al}$ is significant and still slip trans-

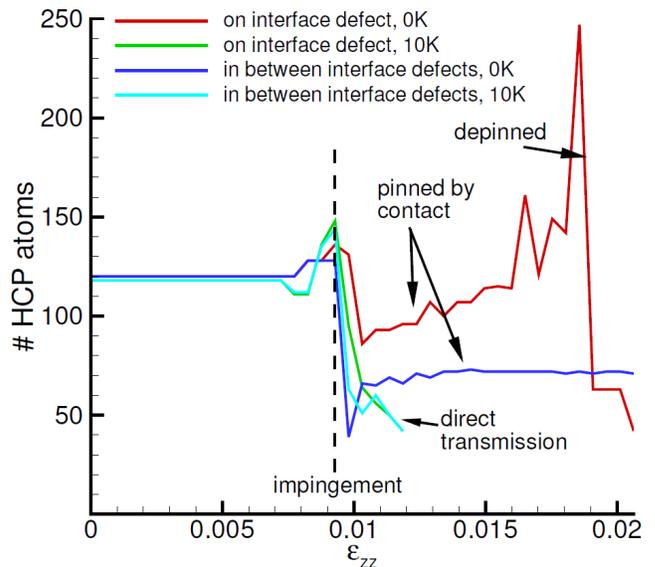


FIG. 9. The number of HCP atoms for the impingement of a dislocation coming from the Ni side of the contact on and in between interface defects (Ni \rightarrow Al).

mission is observed. This can be explained by looking at the energetics of a dislocation. The energy of the core of a dislocation is proportional to the shear modulus and the Burgers vector squared,

$$E_d \propto Gb^2. \quad (2)$$

Substituting the values for shear modulus and Burgers vector in Eq. 2 shows that the energy of a dislocation is more than 2 times higher in nickel compared to aluminum and thus the total energy of the system is lower when the dislocation is in the Al crystal instead of the Ni crystal.

IV. CONCLUSION

This work provides additional insight into the impingement behavior of a dislocation on interfaces between dissimilar metals. Specifically, the impingement behavior of a single edge dislocation on a Ni-Al interface is studied using molecular dynamics simulations. Due to the lattice mismatch between the two materials, two cases arise, one where a dislocation impinges on an interface defect and one where a dislocation impinges between interface defects.

Dislocation transmission is only observed when the dislocation is initially in the material with higher elastic moduli, Ni in our case. The elastic strain energy decreases when the dislocation enters the material with lower elastic moduli, which makes the transmission energetically favorable. At realistic temperatures, a dislocation is always expected to be transmitted if the elastic moduli of the second body are lower and there is an appropriate slip system available. On the other hand, when

the dislocation impinges while coming from the material with lower elastic moduli, transmission does not occur and the dislocation is directly absorbed if it impinges on an interface defect. However, if it impinges between defects, it is observed that the augmentation of the stress fields of the interface and the dislocation prevents direct absorption. The absorption of the impinged dislocation

is expected to have a large impact on the frictional behavior of the contact in a subsequent sliding process.

Although this work gives a fundamental idea about dislocation impingement behavior on interface between dissimilar metals, a full and comprehensive study involving multiple materials, crystal orientations and temperatures is essential for further development and design of high-end material systems.

-
- [1] T.C. Lee, I.M. Robertson, H.K. Birnbaum, *Scr. Metall.* **23** (1989) 799-803.
- [2] T.C. Lee, I.M. Robertson, H.K. Birnbaum, *Phil. Mag. A* **62** (1990) 131-153.
- [3] T.C. Lee, I.M. Robertson, H.K. Birnbaum, *Metall. Trans. A* **21** (1990) 2437-2447.
- [4] Z. Shen, R.H. Wagoner, W.A.T. Clark, *Acta metall.* **36** (1987) 3231-3242.
- [5] M. Dewald, W.A. Curtin, *Model. Simul. Mater. Sci. Eng.* **15** (2007) S193-S215.
- [6] M. Dewald, W.A. Curtin, *Phil. Mag.* **87**(30) (2007) 4615-4641.
- [7] M. Dewald, W.A. Curtin, *Model. Simul. Mater. Sci. Eng.* **19** (2011) 055002.
- [8] M. de Koning, R.J. Kurtz, V.V. Bulatov, C.H. Henager, R.G. Hoagland, W. Cai, M. Nomura, *J. Nucl. Mater.* **323** (2003) 281-289.
- [9] M. de Koning, R. Miller, V.V. Bulatov, F.F. Abrahams, *Phil. Mag. A* **82** (2003) 25112527.
- [10] T. Shimokawa, T. Kinari, S. Shintaku, *Phys. Rev. B* **75** (2007) 144108.
- [11] T. Shimokawa, *Phys. Rev. B* **82** (2010) 174122.
- [12] R.J. Dikken, B.J. Thijsse, L. Nicola, *Comput. Mater. Sci.* **128** (2017) 310-319.
- [13] Y. Mo, K.T. Turner, I. Szlufarska, *Nature* **457** (2009) 1116-1119.
- [14] D.H. Warner, F. Sansoz, J.F. Molinari, *Int. J. Plasticity* **22** (2006) 754-774.
- [15] S.J. Plimpton, *J. Comp. Phys.* **117** (1995) 1-19.
- [16] M.S. Daw, M.I. Baskes, *Phys. Rev. B* **29**, 6443 (1984).
- [17] G.P. Purja Pun, Y. Mishin, *Phil. Mag.* **89** (2009) 3245-3267.
- [18] B.A. Szajewski, W.A. Curtin, *Model. Simul. Mater. Sci. Eng.* **23** (2015) 025008.
- [19] R.J. Dikken, B.J. Thijsse, L. Nicola, *Phys. Rev. B* **95**(10) (2017) 104106.
- [20] 10 K simulations for the case Al \rightarrow Ni show no difference from the 100 mK simulations.
- [21] L. Proville, D. Rodney, M.C. Marinica, *Nat. Mater.* **11** (2012) 845-849.