



## Cohesive laws for shearing of iron/precipitate interfaces

A. Elzas\*, T.P.C. Klaver, B.J. Thijsse

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

### ARTICLE INFO

#### Keywords:

Dislocations  
Molecular dynamics  
Shear loading  
Iron/precipitate interface  
Cohesive law

### ABSTRACT

The behaviour of 11 differently oriented iron-precipitate interfaces under a shear load is studied with molecular dynamics simulations. We find that the behaviour depends not only on the interface orientation but also on the shear direction. Furthermore, for many interfaces the presence of a dislocation at the interface triggers a structure change in the interface, and with that completely modifies the shear behaviour. Several interface characteristics are inspected for their possibly decisive influence on the observed loading curves. However, none of these characteristics is found to correlate conclusively with the shear behaviour of the different interfaces. This indicates that actual shear behaviour is rooted in a deeper level of complexity than just depending on the properties of the initial interface. Clearly the time evolution of the interface during shearing is crucial. From the observations a comprehensive cohesive law is derived that represents the shear behaviour for every interface and for both shear directions. This cohesive law can be used in numerical methods at a larger length scale, such as discrete dislocation plasticity.

### 1. Introduction

In everyday use, interfaces in metallic microstructures are routinely subjected to stresses. Deformation and in certain cases mechanical failure are sometimes the ultimate results. Dislocations play an important role in this, but the stress response at interfaces between grains is equally important. Advanced high strength steels show limited ductility due to interface decohesion. To correctly model the material behaviour, so that the limited ductility can be explained, it is crucial to understand the interface behaviour under different loading conditions. This paper sets out to describe interface behaviour under shear loading, using large-scale atomistic simulations as principal method. Dislocation-interface interactions are part of this study. It will be shown that the same crystals but with different orientations on both sides of the interface give rise to widely different mechanical responses to shear. The ultimate purpose of this paper is not only to identify “weak” interfaces and the reasons therefor, but also to derive from the simulation results cohesive laws, which can be used in numerical methods at the next larger length scales beyond atomic, such as discrete dislocation plasticity where interfaces are modelled by cohesive zone models.

The system under study is Fe-X, with X being a material modelling a hard precipitate. Details are given later. In earlier work [1] we derived tensile traction relations  $T_n(u_n)$ , where  $T$  is traction,  $u$  is displacement of two points on opposite sides of the interface and  $n$  is the direction normal to the interface. Tensile loading is just one case.

In the present study we use classical molecular dynamics (MD)

simulations to derive shear traction relations  $T_t(u_t)$ , where  $t$  is a direction parallel to the interface, for the same 11 interfaces as those studied earlier ( $u_n \equiv u_b \equiv 0$ , where  $n$  is the direction normal to the interface and  $b$  is a direction parallel to the interface forming a right-hand coordinate system with  $n$  and  $t$ ). The shear loading is applied in two opposite directions to examine symmetry aspects in the interface behaviour. The simulations are done with and without a dislocation initially present at the interface. The main results of the present work are the cohesive laws that are derived from the observed traction data and a deeper insight in the differences between the various Fe-X interfaces.

Cohesive zone models were introduced by Barenblatt [2] and Dugdale [3], who addressed fracture as a gradual process. They assumed that there is no stress transmission between the fully separated crack surfaces, while a cohesive zone ahead of the crack continues to transmit forces between a pair of virtual surfaces. This behaviour is governed by a traction-crack opening displacement constitutive law.

Cohesive zone models can be either potential-based or non-potential-based. The most commonly implemented cohesive zone model is the potential-based model developed by Xu and Needleman [4]. Here the first derivatives of an interface potential function give the traction-separation relations. The normal and tangential behaviour are coupled, which means that both tractions depend on both the normal and tangential separation. The coupling is controlled by two coupling parameters  $r$  and  $q$ . The ratio between the work of tangential separation and the work of normal separation,  $q = \phi_t/\phi_n$ , determines the relative strength of the interface under mode I and mode II separation. The

\* Corresponding author.

E-mail address: [astridelzas@gmail.com](mailto:astridelzas@gmail.com) (A. Elzas).

coupling parameter  $r$  gives the ratio between the normal separation after complete shear separation without normal traction and a characteristic length for the normal debonding process. Van den Bosch et al. [5] have shown that only for  $r = q$  the required tangential traction increases with increasing normal compression, as it does in friction. Furthermore, physically realistic coupling is obtained only for  $q = 1$ , since only then the required normal traction reduces to zero at complete shear separation. However, that implies that  $\phi_t = \phi_n$  which experimental studies [6] have shown is often not true. Van den Bosch et al. [5] modified the Xu-Needleman cohesive zone model by allowing for  $\phi_n \neq \phi_t$ . This model is no longer potential-based.

Park et al. [7] proposed a potential-based constitutive model where fracture energies are different for the different fracture modes, which they showed is necessary to correctly simulate the mixed-mode fracturing. McGarry et al. [8] analysed various cohesive zone models with respect to over-closure and found that when traction-separation relations are obtained from a potential function, non-physical repulsive normal tractions can result when the work of tangential separation exceeds the work of normal separation. They proposed a number of new potential-based and non-potential-based models to control, respectively eliminate, the problem of repulsive normal tractions. Dimitri et al. [9] checked various models for their thermodynamical consistency and found that most produce inconsistencies at the local level, which may cause undesirable features in the global behaviour. They also proposed a reformulation of the cohesive zone model by Xu and Needleman [4] as modified by van den Bosch et al. [5] within a thermodynamically consistent framework.

Conventionally the parameters for a traction-separation law are obtained empirically, from polycrystalline samples. However, they then reflect the average response of many interfaces. This is therefore inappropriate as a representation of constitutive behaviour of interfacial debonding at the nano-scale. To obtain the parameters of the cohesive law to accurately describe interfacial debonding at the nano-scale atomistic simulations can be used.

Zhou et al. [10,11] derived with MD simulations a cohesive zone law for crack growth at the interface of a brittle material under mixed mode loading. Only one interface was considered. Given the set-up of their simulations, interface sliding and dislocation nucleation and movement were not possible. Spearot et al. [12] performed MD simulations on a copper bi-crystal interface under pure shear and pure tensile loading to extract information as input for a cohesive law. In [13] they showed the effect of the deformation path on the resulting microstructure for a nanoscale copper bi-crystal interface. They conclude that ‘in order to incorporate path-history dependent effects into continuum interface separation potentials, additional parameters must be used to describe dissipative structural rearrangement within the deformation boundary layer’. Dandekar and Shin [14] parametrised, based on molecular dynamics simulations, a cohesive law for pure mode I and mode II decohesion for an Al-SiC interface. Yamakov et al. [15,16] derived a cohesive zone law from molecular dynamics simulations for implementation in a cohesive zone finite element model for simulating fracture in nano-crystalline or ultrafine grained aluminium. Gupta et al. [17] performed MD simulations on an Al(metal)-Cu<sub>50</sub>Zr<sub>50</sub>(metallic glass) interface under mode I and mode II loading conditions to predict the strength of the interface. Paliwal and Cherkaoui [18] developed for a specific symmetric tilt grain boundary in copper an atomistic simulation based cohesive zone law which accounts for the non-planarity of crack propagation.

Although many studies, as can already be seen in the short selection described above, studied interface behaviour, only little information is available on interfaces in steel. In the present study we therefore examine the behaviour of iron-precipitate interfaces, as a model for the interfaces between the matrix and precipitates that can be encountered in advanced high strength steels. Most of the literature in which cohesive zone law parameters are determined from MD simulations focusses on one particular interface for a certain material (combination).

In the present study we derive a cohesive law for 11 different iron-precipitate interfaces under pure shear loading, with and without dislocations interacting with the interface. We show that not just the material combination across the interface, but also the specific orientations of the crystals give a large variety in the response to a shear load. Furthermore, this response is shear direction dependent. Section 2 describes the material, the set-up of the simulations and the analysis methods. The tangential traction relations and the differences in sliding behaviour are described in Section 3.1 for simulations without initial dislocations. The role of the geometrical and structural characteristics of the interfaces is studied in Section 3.1.4. The influence of an initial dislocation is described in Section 3.2. In Section 4 cohesive laws are derived which quantitatively describe the relation between  $T_t$  and  $u_t$  for all interfaces. Finally, conclusions are given in Section 5.

## 2. Method

The response of 11 different iron-precipitate interfaces to a shear load is studied by classical molecular dynamics simulations. The response to a tensile load applied to the same interfaces was already reported in [1]. In the tensile case it was found that stress concentrations may develop which in turn lead to crack nucleation. Here, because of periodic boundaries of the simulation volume, crack nucleation is impossible.

### 2.1. Material description

Iron is described with the EAM potential by Ackland et al. [19]. In the EAM format the potential energy of atom  $i$  is given by

$$U_i = F(\rho_i) + 1/2 \sum_j \phi_{ij}(r), \quad (1)$$

where  $F$  is the embedding energy of atom Fe or atom X as a function of the local electron density  $\rho_i$ , and  $\phi_{ij}$  is the pair interaction between atom  $i$  and the surrounding atoms  $j$  as a function of their distance  $r$ . The local electron density  $\rho_i$  is made up from the contributions  $\psi_j$  to the electron density by the atoms  $j$  surrounding atom  $i$  at distances  $r$ ,

$$\rho_i = m_j \psi_j(r). \quad (2)$$

$F$ ,  $\phi$  and  $\psi$  are relatively simple functions, parametrised for Fe. They can be found in the original paper [19].

The artificial precipitate material X is chosen to be material X<sup>(3)</sup> from [20]. In this work we choose  $\phi_{XX} = 2\phi_{FeFe}$ ,  $a_X = 1.1a_{Fe}$ , and the embedding term  $F(\rho_i)$  is equal for Fe and X atoms. To create material X with lattice constant  $a_X = 1.1a_{Fe}$ , we use

$$\begin{aligned} \phi_{XX}(r) &= \phi_{FeFe}(r/1.1), \\ \psi_X(r) &= \psi_{Fe}(r/1.1). \end{aligned} \quad (3)$$

X has thus a 10% larger lattice constant than Fe and, as a result of the X-X pair interaction being twice as strong as that of Fe-Fe and the X- and Fe-embedding terms being equal, X has a 49% larger Young’s modulus than Fe. Material X is thus stiffer than Fe and, due to the different lattice constant, forms semi- or non-coherent interfaces with Fe. Dislocation transfer into the precipitate material is therefore hindered, just as it is in real precipitate materials found in steel, such as carbides and nitrides of different alloying elements. Similar to [20] the mixed Fe-X pair interaction is a linear combination of the individual Fe-Fe and X-X pair interactions,

$$\phi_{FeX} = q(\phi_{FeFe} + \phi_{XX}), \quad (4)$$

where the factor  $q$  in this study equals 1/3. This Fe-X pair interaction in combination with the orientations of the Fe and X grains on either side of the interface determines the interface strength. However, defects at the interface, initially present but also those developing during loading and grain sliding, may be of significant additional influence.

Download English Version:

<https://daneshyari.com/en/article/7957263>

Download Persian Version:

<https://daneshyari.com/article/7957263>

[Daneshyari.com](https://daneshyari.com)