Cohesive law describing crack growth at iron/precipitate interfaces

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A B S T R A C T

Single dislocations and dislocation pile-ups at crystalline interfaces cause stress concentrations. This can lead to decohesion of the interfaces under tensile loading. To describe this decohesion quantitatively, a cohesive law for planar crack growth at iron/precipitate interfaces is developed. This cohesive law is based on a universal description of the adhesive energy for different interfaces. Only a single scaling factor c must be applied to convert the prediction based on this universal adhesive energy into the actual traction-separation behaviour during crack growth. This scaling factor takes into account the atomic strain and relaxations. The cohesive law derived here can be implemented in a Discrete Dislocation Plasticity framework to describe crack growth at a larger scale. The method presented in this paper for the derivation of a cohesive law can be applied to other material combinations showing brittle crack growth as well.

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1. Introduction

Interfaces in iron and other metals act as a barrier for dislocation motion. Due to the crystallographic mismatch across an interface and the atomic disorder in an interface, there is a discontinuity of slip planes across the interface, which impedes dislocation motion. When dislocations encounter an interface, they can be stopped, transmitted, reflected, broken up, dissolve or even spawn new dislocations. By reducing the grain size, a material can be made stronger, since dislocations encounter more obstructing interfaces and slip is reduced, as is expressed by the Hall-Petch relation [1]. According to this relation the yield strength of a polycrystalline material is proportional to $d^{-1/2}$, where d is the mean grain size. The mechanical properties of a material, however, can also be negatively influenced by interface effects. Hindered dislocation motion at an interface leads to a pile-up of dislocations at this interface, which, in turn, gives a stress concentration. If this stress concentration becomes high enough, this can lead to decohesion of the interface, which leads to the formation of a void and eventually, by coalescence of multiple voids, can lead to the formation of a macroscopic crack. Advanced high-strength steels and other multiphase alloys show limited ductility due to interface decohesion.

In this work we derive a cohesive law for interface decohesion during crack growth. This cohesive law can be implemented in a cohesive zone model to improve existing larger-scale models such as Discrete Dislocation Plasticity. To derive this cohesive law we study the interaction of single edge dislocations and dislocation pile-ups with interfaces between an α-iron crystal and a precipitate. With Molecular Dynamics simulations (MD) we study for different orientations and different numbers of dislocations how and when interface decohesion occurs under tensile loading. From these simulations the cohesive law for interface decohesion during crack growth is derived. The influence of pure shear loading on dislocation-interface interactions was previously studied [2]. In forthcoming work the combination of tensile and shear loading, mixed-mode loading condition, will be considered, as well as crack nucleation.

Based on effective displacement and effective traction data, various constitutive relationships for interface decohesion, such as cubic polynomial [3], trapezoidal [4], smoothed trapezoidal [5], exponential [6], linear softening [7], and bilinear softening [8] have been defined. Most of these relationships are a phenomenological characterisation of the zone where separation takes place along the interface, and not a description of the true atomic separation process between the interfaces. Only the exponential potential based on the work of Rose et al. [9] is based on information from atomistic calculations.

Gall et al. [10] have fitted their results from MD simulations to three models by Needleman [3,11], Tvergaard and Hutchinson [12] and Tvergaard and Hutchinson [12–14] for an aluminium-silicon interface. For aluminium Yamakov et al. [15,16] developed a cohesive zone representation of intergranular fracture based on results of MD simulations. Zhou et al. [17] determined the traction-separation behaviour for a pre-cracked bimetal with a weak

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interface under mixed mode loading conditions. In [18] the effect of elastic constant mismatch was also included. Using MD simulations on single-crystal aluminium, Krull and Yuan [19] confirmed that steady-state crack growth can be described with the exponential traction-separation relation by Needleman [20], while crack initiation shows a non-uniform traction-separation relation. For a symmetric tilt grain boundary in copper Paliwal and Cherkaoui [21] developed a mixed-mode cohesive zone law for non-planar crack growth.

In all of the above studies the growth of a pre-existing crack in an fcc material is considered, while in the current study we focus on cracks nucleated from stress concentrations due to a dislocation pile-up in a bcc material.

We start our study by determining the adhesive energy as function of separation for different interfaces and interface strengths. In this work the term 'adhesive energy' is used for the separation energy between two crystal halves as rigid blocks, i.e. without any relaxation of the atomic positions. From these different adhesive energy curves we are able to derive a universal adhesive energy curve by scaling. The predicted traction-separation behaviour derived from this energy curve, called 'template curve', is compared with real traction curves from MD simulations. To obtain a match between the template curve and the calculated traction-separation relations from the MD simulations, the template curve is scaled with a scaling factor c. We find that only one universal scaling factor is needed for all iron/precipitate interfaces. In this way we are able to derive a cohesive law for interface decohesion, where the different interfaces are only characterised by a different adhesion energy. The small deviations in behaviour between the calculated curves for different interfaces and different numbers of dislocations in the pile-up and the predicted curve obtained by scaling the template curve show the atomic-scale details. These are no longer important for Discrete Dislocation Plasticity models. We expect the method to be universal and also applicable for other bimetal interfaces. The thus derived cohesive law captures the essence of separation physics.

This paper is organised as follows. In Section 2 we describe the choice of the materials (Section 2.1), the set-up of our simulations (Section 2.2), and the calculation method for interfacial traction and separation (Section 2.3). The derivation of the traction versus separation relation from the adhesion energy is given in Section 3 and this relation is compared with the results from tensile simulations in Section 4, which leads to the formulation of a cohesive law. The results are discussed in Section 5 and conclusions are presented in Section 6.

2. Method

For different iron/precipitate interfaces we derive a cohesive law describing the traction-separation relation upon decohesion of the interface under the influence of a tensile load. In order to capture the effects of atomic relaxation, the results are then compared with MD simulations under tensile loading for different interface orientations and different numbers of dislocations interacting with the interface.

2.1. Material description

To describe iron in our simulations a potential had to be chosen that accurately describes both edge dislocations in iron and the structures far from equilibrium resulting from dislocation pile-up/interface interactions. To describe a single edge dislocation in iron, the potential developed by Malerba et al. [22], optimised to describe interstitials and vacancy defects, is a reliable choice. However, since in the present study not just single edge dislocations

but pile-ups of dislocations interacting with interfaces are studied, structures far from equilibrium are expected for which this potential is less appropriate [23]. Studies of crack tips [23,24] have shown that both 'potential 2' developed by Mendelev et al. [25] and the potential developed by Ackland et al. [26] are reliable potentials for this type of study. Although they are both derived from nearly the same input data and predict nearly the same material properties, this does not result in a qualitatively same description of material behaviour at a crack tip [24]. In this study iron is described with the EAM-potential by Ackland et al. [26].

In the EAM-format the potential energy per atom i is given by

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

where F is the embedding energy as function of the local electron density ρ_i and ϕ_{ij} gives the pair interaction between the atom and the surrounding atoms j as function of their distance r. The local electron density is made up of the contributions ψ to the electron density by the atoms j surrounding atom i,

$$\rho_i = \sum_j \psi_j(r). \tag{2}$$

F, ϕ and ψ are relatively simple functions, parametrised for Fe.

In general practice, precipitates in iron are stiffer than the matrix, which hinders dislocation transfer. They also form semi- or non-coherent interfaces with the matrix, depending on their different lattice constant and/or crystal structure. As a model material for a precipitate we create an artificial material X, which is stiffer and has a different lattice constant than iron. Furthermore, we vary the orientations of both the Fe and the X grains, which gives rise to different interface structures. The potential to describe the precipitate material, material X, is based on the Fe-potential. In this study, X is chosen to be material $X^{(3)}$ from [2]. This precipitate material has a 10% larger lattice constant than Fe and a 49% larger Young's modulus.

Similar to [2] the pair interaction between Fe and X is a linear combination of the individual pair interactions in Fe and X, as defined by

$$\phi_{Fe-X} = q(\phi_{Fe} + \phi_X), \tag{3}$$

where the factor q is varied between 1/6 and 1 to obtain different pair interaction strengths. The combination of a given Fe–X pair interaction and a given orientation of the two grains determines the interface strength, in the absence of additional defects at the interface.

2.2. Setup

The Fe/X system is schematically shown in Fig. 1. The system size is dependent on the orientation but on average equals $165 \times 4.4 \times 110$ nm. The system is periodic in x and y. To determine the adhesive energy of the interface as function of normal separation, one crystal is rigidly displaced with respect to the other crystal and the energy is determined as function of separation.

Different interfaces are studied. In iron the $(1\,0\,0)$ plane is the typical cleavage plane. Similarly to the orientations chosen by Rice [27], we here study this $(1\,0\,0)$ crack plane, with the crack front direction in the $[0\,1\,1]$ direction and the crack growth direction in the $[0\,1\,\bar{1}]$ direction, as well as the $(1\,1\,0)$ crack plane, with the crack front direction along $[1\,\bar{1}\,0]$ and the crack growth direction along $[0\,0\,1]$. Either the iron grain, or the precipitate grain, or both are oriented along these directions. To obtain different interfaces and study their influence on dislocation-interface interactions, we rotate one of the grains around the crack front direction. Table 1 shows the different orientations of the Fe and X grains. A tensile