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Atomistic modeling of the crack–void interaction in α-Fe

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ABSTRACT

The analysis of the crack–void interaction at the nanoscale in α-Fe using molecular statics (MS) and molecular dynamics (MD) in the framework of the embedded atom method (EAM) potential is presented. To this end, following three crack–void specimens are considered: (i) void positioned at a varying distance normal to the crack tip, (ii) void inserted at a varying distance along the initial crack direction in front of the crack tip, and (iii) void placed at a varying distance in the emission direction of the dislocations after the dislocation nucleation. A parametric study involving the crack–void specimen, the strain rate, and the temperature is performed and presented. Depending on different specimens, elastic shielding or anti-shielding on the crack growth is observed as a function of the temperature and strain rate. The increase of the temperature results in the decrease of the dislocation nucleation stress. At a temperature of 0 K, the simulation results reveal that the crack growth rate is independent to the void location with respect to the crack tip. At a temperature of 300 K, when the crack–void distance is $d=5a$ (a being the lattice parameter), the initiation of the crack growth occurs earlier than that of the same specimen at 0 K and the crack growth is blunted after the deflection. When increasing the crack–void distance, the crack growth rate is independent of the temperature.

1. Introduction

The fracture properties of materials are strongly influenced by second-phase inclusions. On one hand, second-phase inclusions can be viewed as a major source of the driving force in the whole failure process, while on the other hand, they can improve the fracture properties through a toughening mechanism [1]. This interaction between the crack and the second-phase inclusions is, however, complicated and depends on such factors as, inclusion geometry and strength, volume fraction of the inclusion, the strength of the interface between the inclusion and the matrix [2], the orientation and location of the inclusion, crack length as well as the crack–inclusion separation distance [3]. Among the aforementioned factors, the crack length and the inclusion size are two characteristic lengths that can lead to size effects while the crack–inclusion separation distance is a coupling distance. Such a system that involves two defects, each of them carrying an associated length scale, is multiscale in nature. Over the years, the consequences of these defects, taken separately, on the macroscopic behavior were investigated from the nanoscale up to the macroscale. However, the interaction between the two defects was mainly investigated at the macroscale, and to the authors' best knowledge, only little work to characterize the interaction between the crack and the inclusion has been performed at the nanoscale.

Insertion of a second-phase inclusion in a pre-cracked matrix leads to an interaction between the crack tip and the inclusion. Several investigations have been carried out in the past, exploiting various experimental, analytical, and numerical techniques, to address the problem of crack–void interaction. On one hand, some researchers solved the crack–inclusion problems by extracting the stress field around the crack tip according to a complex potential. Then, they solved the resulting formulation either numerically or analytically [4–6]. On the other hand, other researchers used numerical techniques such as the finite element or the boundary element methods to investigate the similar problem [2,3,7,8]. Adopting different approaches, some other researchers consequently presented an integral representation of the problem and solved the resulting integral equations by using numerical techniques [1,9,10].

One consequence of the crack–inclusion interaction is the alteration of the stress field around the crack tip. Depending on the location and the separation distance, such an inclusion can reduce or amplify the effective stress intensity factor in the close proximity of the crack tip [3]. The reduction and amplification of the near crack tip stress field are termed in the literature as crack tip "shielding" and "anti-shielding", respectively. In these works,

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shielding of the crack tip by an elastic particle was reported in the case of the soft inclusion, while anti-shielding of the crack tip was concluded as the result of the insertion of the stiff inclusion [7,10].

Apart from the change in the stress intensity factor, inclusions in the vicinity of the crack tip can influence the crack growth direction. This was studied by analyzing the energy release rate as the crack propagated [1,2,7,10]. While stiff inclusions lead to the swirl of the crack path between the matrix and the inclusion, soft inclusions result in the deflection of the crack away from the inclusion [10].

Overall, previous works on the crack–inclusion interaction demonstrated that the strength of the crack–void interaction is usually measured by using the stress intensity factor and the energy release rate. While the former is used to measure the previously described shielding and anti-shielding effects, the latter is utilized to characterize the crack deflection. Most of these studies have been concerned with the mode-I crack loading and have considered the plane strain conditions. Only a few studies were reported to consider the mode-II [6] and mode-III of fracture [11].

However, until today, the comprehensive understanding of the atomistic characteristic of the crack–inclusion interaction has not been widely addressed in the literature and is limited to a few studies. For instance, by using MD simulations, Mattoni et al. [12] suggested a possible increase in the macroscopic fracture toughness by the introduction of stiff inclusions as fibers in the SiC matrix. Rafii-Tabar et al. [13] used MD simulations to model the crack–inclusion problem and observed the crack-tip shielding in metals containing impurities under mode-I loading. Musazadeh et al. [14] studied the effect of the type and the shape of the second-phase inclusions on the crack propagation in Ni nanocrystals. Their study demonstrated that the shape of the inclusion has an appreciable effect on the crack propagation, while the material type of the inclusion shows no significant effect on the crack growth. Recently, Bitzek and Gumbsch [15] investigated the relationship between the propagating crack and the dislocation density in Ni alloys by using atomistic calculations. It was found that such an interaction leads to a reorientation at the crack tip. As a consequence of the local reorientation, dislocations nucleate on new slip systems leading to crack blunting. Further, they revealed the importance of the cross-slip mechanism on the dislocation multiplication resulting from a change of the stress state near the crack tip. Zhang and Ghosh [16] also presented the MD simulations on characterizing the deformation mechanisms of the Ni single crystal under the mode-I loading including dislocations, twins, and stacking faults near the crack tip. Their results suggested that for the investigated Ni system, dislocation nucleation precedes and thwarts the cleavage crack propagation upon reaching the critical stress during the plastic deformation.

In the present work, molecular statics (MS) and molecular dynamics (MD) methods are employed to investigate the crack–void interaction in α-Fe. The aim of this work is to characterize the failure mechanisms when multiple defects of different natures with different length scales are embedded in a material. The outline of the present study is as follows. The simulated model is described in Section 2. A study of the effect of the crack–void interaction by varying the crack–void distance while keeping the crack length and void radius constant for different crack–void specimens by using the molecular statics and molecular dynamic simulations is presented in Section 3. Conclusions are given in Section 4.

2. Model description

2.1. Modeling crack–void interaction using molecular statics and molecular dynamics

Molecular dynamics (MD) is a numerical tool with which one attempts to simulate the dynamics of atoms while preserving Boltzmann's statistics [17]. When put close to each other, atoms interact by exerting forces on each other. Assuming the force on an atom as the negative gradient of a potential function, one can introduce some elements of physics in a more or less complicated potential function to describe the atom–atom interaction. Associated with a set of boundary conditions, MD is a powerful tool that can be used to reveal and characterize mechanisms. Furthermore, when no kinetic energy is considered (i.e., temperature $T=0$ K), the potential energy of the system can be minimized as a function of the atoms' coordinates using specific algorithms. In that case, the method is defined as molecular statics (MS).

In this study, the crack–void interaction in α-Fe is simulated both via molecular statics and molecular dynamics using LAMMPS [18] in the framework of the embedded atom method (EAM) potential [19–22]. In such a framework, the total energy of the system is expressed as the sum of the effect of the local environment on each individual atom and the pairwise contribution of each pair of atoms, such as

$$E_{tot} = \sum_i F_i(\rho_{h,i}) + \frac{1}{2}\sum_i \sum_{j \neq i} \phi_{ij}(R_{ij}), \quad (1)$$

where F_i is the embedding energy, and $\rho_{h,i}$ is the local electron density around atom "i". ϕ_{ij} is the short-range pair potential and R_{ij} is the distance between atoms "i" and "j". The potential function is correlated to the elastic, structural, and energy properties of α-Fe. In the present work, the Ackland–Mendelev potential [20,21] is employed since it is treated as the most used potential to model α-Fe in past few years [22]. In the work by Terentyev et al. [22], the Ackland–Mendelev potential has been applied for investigating the interaction of a brittle crack with low and high angle grain boundaries in α-Fe at finite temperatures. They indicated that all the principal deformation mechanisms for such problem can be captured by using the Ackland–Mendelev potential, which has qualitatively agreement with the results by using other potentials.

The present simulation setup begins by considering a pre-existing edge crack under tensile loading, as sketched in Fig. 1. The pre-existing crack is along the [100] direction. The crack plane is oriented along the $[0\bar{1}1]$ direction, and the crack edge is parallel to the $[0\bar{1}\,\bar{1}]$ direction. To model the plane strain state, periodic boundary conditions are imposed along the $[0\bar{1}\,\bar{1}]$ direction. The crack length, L, is taken as one-fourth of the simulation cell size in the [100] direction. The crack specimen sketched in Fig. 1 is used as a reference case to compare with the data obtained when the crack–void interaction is taken into account.

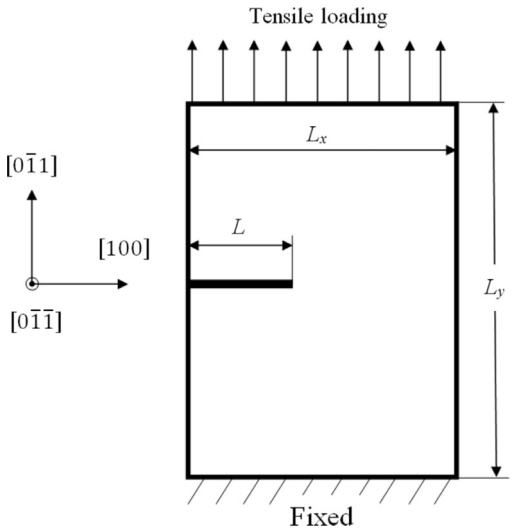

Fig. 1. Crack system in MS–MD simulations. Initial crack, crack plane, and crack edge are oriented along [100], $[0\bar{1}1]$, and $[0\bar{1}\,\bar{1}]$, respectively.