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Crack propagation behaviors at Cu/SiC interface by molecular dynamics simulation

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ABSTRACT

The propagation of the interfacial cracks at Cu/SiC interface under tensile (mode I) loadings and combination of tensile and shear (mixed mode) loadings are studied by molecular dynamics (MD) simulations. For the mode I, the asymmetrical interfacial crack propagation is observed at the interface, and the stress concentration is found both at the crack tip and somewhere of interface due to the lattice mismatch. Six loading methods with different loading angles are considered in this work, the behaviors of the crack propagation are found to be dependent on the loading angles. In addition, the Rice and Thomson (R–T) model is also used to predict the behaviors of interfacial crack growth theoretically. With pure tensile loading, the energies necessary for dislocation nucleation at the two crack tips are found to be different, which leads to asymmetrical crack propagation. For the mixed modes, the behaviors of the crack propagation are predicted by comparing the dislocation nucleation energy and the decohesion energy. The predictions of the R–T model are consistent with the MD results qualitatively. This research is intended to provide a fundamental explanation of the asymmetrical crack propagation at interface from atomscale.

1. Introduction

Ceramics reinforced metal matrix nanocomposites (MMNCs) have gained widespread concern in recent years because of their high strengths, high stiffness, good oxidation and corrosion resistance [1,2]. The most popular reinforcement of such composites is SiC or alumina particles, and the matrix is usually cooper, aluminum or titanium. There are increasing applications for the MMNCs in the aerospace, micro-electro-mechanical systems and the biomedical industries, which have attracted extensive attentions to the mechanical properties of such composites [3]. The interface between the reinforcement and the matrix plays a crucial role in determining the mechanical properties of the MMNCs [4]. Generally, the mechanical properties of MMNCs can be drastically altered by the interface, making it necessary to understand the behaviors of the interfacial crack [5]. Interfaces are the narrow regions separating the well-defined domains and are primarily responsible for a range of key properties including stiffness, strength, and fracture behaviors of entire composites, because interface is very important to the stress transfer between the reinforcement and matrix under various loading conditions [6].

Beltz et al. [7] divided the crack propagation in single phase materials into two categories: the cleave propagation for "intrinsically brittle" materials and the blunting of crack tip for "intrinsically ductile" materials. For "intrinsically ductile" materials, dislocations nucleate and emit at the crack tip along the slip plane, which makes the crack tip blunted [7] with the stress released and the radius of the crack tip enlarged [8]. Compared with single phase materials, the propagation of interfacial crack in MMNCs is different. Obviously, the interfacial cracks in MMNCs are influenced by both the ductile matrix and the brittle reinforcement. For interfacial crack in MMNCs, the part of which in the ductile matrix exhibits blunting at the crack tip, while the part of the interface crack in reinforcement always shows a brittle characteristic [9].

Liechti and Chai [10] investigated the asymmetric shielding in interfacial fracture under in-plane shear conditions and suggested the inelastic behavior and three-dimensional effects at near crack tip should be considered. Asymmetric rupture propagation on an interface that combines a bulk elastic mismatch was observed by Bhat et al. [11]. They concluded that the asymmetry was introduced by damage which depends on whether the tensile or compressive region of the rupture tip stress concentration lies on the damage side of the fault. Wang et al. [12–15] observed interfacial cracks propagate in metal/sapphire composites by the growth of voids or microcracks and then are blunt at the tip and finally merge

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with the main crack. In addition, they found that the loading condition and the crystal orientation of metal determined the growth behaviors of the interfacial cracks.

Considering the difference between the energy necessary for dislocation nucleation G_{disl} and the interfacial decohesion G_{cleave}, Rice and Thomson (R–T) [16] established a criterion to distinguish the ductile and brittle behaviors of a crack in crystal. When $G_{cleave} < G_{disl}$, the crack propagates in a cleave style, and $G_{cleave} > G_{disl}$ for a blunting style (Fig. 1), which indicates dislocation nucleation depends strongly on the atomic scale loading phase angel and the crystallographic configuration at the crack tip [12].

The theoretical description of the fracture at interface includes not only nonlinearities in the vicinity of the crack but also bonding breaking between atoms, as well as the formation of extended defects (e.g., dislocations) [17]. Thus, molecular dynamics (MD) method was adopted to study fracture at the atomic scale. Yamakov et al. [18] observed asymmetrical crack propagation along the grain boundary under hydrostatic tensile loading by MD simulations in aluminum crystal. In one direction, the crack propagates in a brittle manner by a cleave style with very little or no dislocation emission, while in the other direction, the propagation is ductile through the mechanism of deformation twinning or dislocation fault. Luque et al. [19] analyzed the crack growth along the symmetrical tilt grain boundary $\Sigma 9\,(1\,1\,0)/[2\,2\,1]$ under mode I loading in twin cooper crystal. They investigated the process of dislocation emission from the crack tip till the material yield, two different critical stress intensity factors (SIFs) for dislocation nucleation have been calculated by matching the displacement fields at the crack tip neighborhood with the continuum elastic fields. The different SIFs of two crack tips [19] and different style of crack propagation in two directions [18] are thought corresponding to the crystallographic orientation of two crystals in these passages. Furthermore, loading conditions can also be crucial for crack propagation, the propagation of a crack along the interface under six difference mixed mode loading conditions was simulated by Zhou et al. [20,21]. They investigated relation between stress and opening displacement under the mixed mode loading conditions and derived various cohesive zone models under different loading conditions. Vatne et al. [22,23] observed a crack in single crystal iron under mode I, II and III and mixed loading mode and calculate the critical stress intensity factors for crack propagation and dislocation emission under different loading conditions. In addition, due to the lattice mismatch between two materials, there exist dislocations in the interface which can alter the style of crack propagation [9]. Wang et al. [24] investigated the structures, energies and Burgers vectors of misfit dislocations in metal (Au, Ag, Al, Pt)/SiC interfaces, and found partial dislocations and full dislocations at the metal/SiC interface. However, the effects of the interfacial dislocations and the loading phase angle on the interfacial crack propagation has not related to the physical mechanisms, so further research at atomistic scale is necessary.

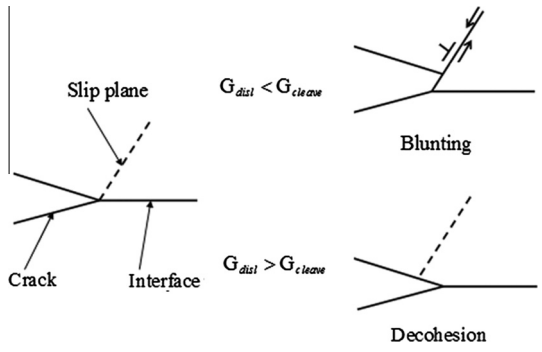

Fig. 1. A sharp crack with inserting a slip plane (left), showing the competition between dislocation emission (upper right) and decohesion of the interface ahead of the crack (lower right) [12].

Understanding of the crack behaviors at the interface is helpful to lay foundation to the knowledge of fracture mechanisms of MMNCs and is benefit to understand complex phenomena like the brittle-to-ductile transition. In this work, MD simulations are used to investigate the effects of lattice mismatch on the interface crack growth. The loading phase angle influence is also analyzed based on the observation of the atomic structure evolution in the simulations. In addition, we use the R–T model to predict the crack growth behaviors. A comprehensive understanding of the behaviors of interfacial crack growth is achieved.

2. Model and method

2.1. Crack model

The micro-structures of MMNCs interface are too complicated to be modeled directly [25]. As observed by the transmission electron microscopy (TEM), the metal in Cu/sapphire nanocomposites can be considered as single crystalline on a length scale of close to 1 μm [26]. Accordingly, the metal of present model is assumed to be single crystalline. Unlike the assumption in the theoretical model, the interface of real material has a physical thickness [27]. In this work, we take the thickness of interface as about 4 nm, which is considered as an optimization size to represent the mechanical behavior of interface by Gall et al. [27].

The size of the model is $80a \times 84a \times 15a$, and a is the lattice constant of SiC, as shown in Fig. 2. The size is much larger than any of cut-off distances in three dimensions, thus the interaction of atoms with their periodic images are vanished. An initial central crack along X-axis is introduced by removing the corresponding atoms at the interface. The length and width of the crack are about 10 nm and 2 nm, respectively. In the model, the periodic boundary conditions are adopted in X and Z directions, with non-periodic boundary condition for Y direction. The cubic axes for FCC Cu and SiC are aligned, with a lattice mismatch of about 16.7%. There are about 7×10^6 atoms in the simulation cell. Two rigid zones with thickness of 0.88 nm are placed in the upper and bottom boundary of the unit cell, and denoted as 1 and 2 regions in Fig. 2a, respectively. They are acted as loading layers in the simulation. Furthermore, the initial dislocation exists in the interface of the model as shown in Fig. 2b, which is initial defect at the interface leaded by lattice mismatch. The slip planes in the copper of the model are $(1\,1\,1)$ and $(\bar{1}\,1\,\bar{1})$ planes as illustrated in Fig. 2c.

2.2. Details of MD simulations

In this study, the MD simulations are implemented in the open source programs large-scale atomic molecular massively parallel simulator (LAMMPS) [28]. For visualizing the evolution of the atomic structure, the Atomeye [29] and open source ovito [30] are adopted. For MD simulation, reliable force fields are very important to obtain reasonable results. In the present model, different force fields are employed to describe the interactions of atoms. Herein, the interactions between Si and C atoms are simulated using Tersoff potential [31]. The empirical embedded-atoms method (EAM) potential developed by Mishin et al. [32] is adopted to describe the interactions between Cu atoms. The Tersoff potential for Si and C atoms is a three body potential. The total energy of the system of SiC atoms is given as [31]

$$E_{SiC} = \frac{1}{2}\sum_i \sum_{i \neq j} \{f_c(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})]\} \quad (1)$$