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Letter

Dislocation-based strengthening mechanisms in metal-matrix nanocomposites: a molecular dynamics study of the influence of reinforcement shape in the Al-Si system

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ABSTRACT

We use molecular dynamics simulations to study the interaction of dislocations with reinforcements of various shape during nanoindentation of Al/Si metal-matrix nanocomposites. Three different geometries of the Si reinforcement are considered: a spherical particle, a cylindrical fiber, and a plate. We show that plate reinforcements may absorb dislocations and emit them back into the matrix with altered glide direction, both strengthening and toughening the composite, in agreement to experiment. This mechanism does not work for spherical reinforcements, since the curved interface does not allow for dislocation emission; the case of fibers is intermediate. It is concluded that the shape of the reinforcement plays a dominant role in dislocation-based strengthening mechanisms in metal-matrix nanocomposites.

1. Introduction

Metal-matrix composites (MMCs) constitute a popular class of materials with promising advantages over unreinforced metals and other composites such as polymer-matrix composites. In their recent monograph [1], Chawla and Chawla list an impressive series of improved properties of MMCs, ranging from mechanical properties over high-temperature capabilities to cyclic-fatigue characteristics. In the context of the present work, the higher strength and stiffness of MMCs as compared to the unreinforced metal are particularly important.

In an MMC, the reinforcements are distributed in the form of particles [2], fibers [3], or plates [4] in the metallic matrix [1]. However, due to the incorporation of particulates and fibrous reinforcements, MMCs usually exhibit a lower ductility and toughness, and thus have a lower damage tolerance, than monolithic metals and alloys [5–7]; this feature constitutes an obvious drawback in practical application. Thus, a strategy to tailor the structure of MMCs that might endow such materials with both high strength and good ductility is in great demand.

Recently, a new type of nanoscale-laminate MMCs, developed by controlling the two-dimensional distribution of the particulate [8,9] and fibrous [10–12] reinforcements, has become a prevailing model for developing a new generation of high-strength MMCs with considerable ductility, due to their remarkable abilities of energy absorption and dislocation storage. Similarly, graphene as plate reinforcement shows excellent mechanical properties including increased stiffness, tensile strength, total elongation under stress and toughness [13–17]. Also it was demonstrated that the deformation behavior of graphene/Al composites is characterized by a significant strain hardening at low strain values [16]. It is therefore interesting to investigate in how far the shape of the reinforcement influences this behavior.

Experimental studies attribute strengthening mechanisms to stress transfer [18] and Orowan looping [19], and the toughening mechanism mainly to crack evolution [20,21]. However, these mechanisms only become dominant at large deformations at the interfaces in MMCs. Thus, it is significant to identify the dominant mechanism in the early stages of deformation in MMCs.

Nanoindentation is a routine technique for testing the mechanical behavior of materials [22,23]. It provides in particular information on the material hardness, and hence on the plastic deformations that can occur in it. While many aspects of the plastic behavior of elemental and homogeneous materials are understood, the response of composite materials to nanoindentation has been investigated less frequently and few experimental [24–27] or modeling [28–31] studies have been published up to now. These studies investigate three aspects: fracture caused by indentation into

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particle reinforcements [24,25,31], mechanical properties including Young's modulus as well as the hardness of the particle and the metal matrix [26,27,30], and debonding and failure of the interface [28,29]. However, none of them investigates the interaction of dislocations with the reinforcement-matrix interface, as we do here.

Molecular dynamics (MD) simulations are often used to study the atomistic processes occurring during nanoindentation in materials [32]. When applied to single crystals, MD gives results in good agreement with experiment [32,33]. In addition, due to the versatility of computer simulation, the influence of materials properties on the indentation can readily be investigated [34,35].

Nanomachining and in particular nanoindentation studies are performed increasingly often using molecular dynamics (MD) simulations [32]. These need only the interatomic interaction potentials as input into the simulation; thus the results obtained are essentially as good as the potentials used. The reliability of such potentials has been investigated in many cases, in particular for fcc [36], bcc [37,38], and hcp [39] metals, but also in Si [40,41] and for Al/Si composites [42].

In this paper, we investigate the plastic deformation behavior for the specific case of an Al/Si nanocomposite under indentation. By choosing three exemplary geometries for the Si reinforcement – a plate, a spherical particle, and a cylindrical fiber – we can shed light on the mechanisms that make the mechanical performance of plate MMCs different from the other reinforcement geometries.

2. Method

We study indentation of an MMC based on fcc Al as matrix and cubic diamond Si as the reinforcement material. The simulation box has a depth of 44.5 nm and a lateral extension of 57.1 nm. The Al matrix is single-crystalline; its free surface has a (100) orientation. As shown in Fig. 1(a)–(c), three different shapes of the Si reinforcement are studied:

1. a spherical particle of radius $R = 16$ nm;
2. a cylindrical fiber of radius $R = 16$ nm;
3. a plate of thickness $d = 5.4$ nm beneath the Al matrix overlayer of 11.5 nm thickness. Note that this plate makes our geometry identical to a nano-layered Al-Si system.

In all three cases the thickness of Al on top of the Si reinforcement amounts to 11.5 nm, and the embedded Si particles are situated such that they touch the bottom of the simulation box. This arrangement helps to create analogous indentation scenarios in which the indenter moves only through the pure Al matrix, but the plasticity generated in the Al interacts with the Si reinforcement. The Si reinforcements are oriented such that their [100] direction is aligned with the Al [100] direction. We introduce a cartesian coordinate system centered in the middle of the top surface aligned with the cubic axes of the Al (and Si) crystals; the z axis points in the direction normal to the surface and the x axis points along the cylinder axis, see Fig. 1.

Since Al and Si have different lattice constants – 4.05 and 5.43 Å, respectively – the assemblage of the Si and Al parts to the composite structure has to be done with care. We follow the recipe of Noreyan et al. [43] and choose the lateral sizes of the interface such that they are commensurate for both the Al and Si lattices. Thus, for instance, the lateral extension of 57.1 nm can be filled by 105 lattice constants of Si and by 141 lattice constants of Al.

Before starting the indentation simulations, the systems are relaxed such that all components of the stress tensor reach values <12 MPa, when averaged over the entire specimen, and the temperature drops below 1 K. In detail, the relaxation is performed in several steps: first an energy-minimization algorithm is applied relaxing the systems with periodic boundary conditions in both lateral directions. After an anneal at 30 K, the systems are quenched again and energy-minimized using conjugate-gradient techniques.

During the indentation simulations, the bottom of the system (width of 1 nm) is fixed in all the substrates in order to prevent any rigid-body motion of the substrate during the indentation process. The next 1-nm layers at the bottom as well as the outermost 1-nm layers at the lateral sides of the substrate are thermostatted to 0.01 K using a velocity-scaling algorithm. The small temperatures are employed in order to ease the detection of dislocations; they are routinely used in MD simulations of indentation [44,45]. For metals it was demonstrated previously that indentation at room temperature and at 0 K lead to closely comparable results [38,44]. In Si, a slightly enhanced tendency for phase transformation was reported at room temperature as compared to 0 K [46]; but this issue is not relevant for the present study.

The interactions between atoms in these three systems are described by the Al-Si potential developed by Saidi et al. [47]. They modified the Stillinger-Weber potential [48] of Si to obtain a more accurate description of the phase transformation behavior, and then combined it with the embedded-atom-model (EAM) description of pure Al developed by Mendelev et al. [49]. The combined potential is of the angular EAM type (AEAM). The performance of the Al part of the potential has been studied previously; it has been found to describe plasticity well [38]. Also plasticity in Si is described satisfactorily by the Stillinger-Weber potential [50–53]. The interspecies term added by the AEAM potential was designed to correctly describe the phase diagram and the heat of mixing as a function of composition [47]; it also describes Al-Si interfaces satisfactorily [42].

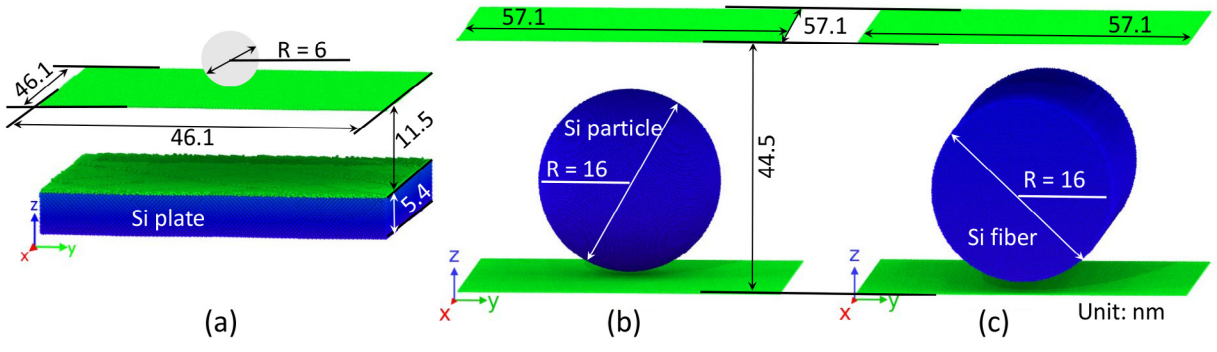

Fig. 1. The three systems studied: (a) plate reinforcement, (b) spherical particle, (c) cylindrical fiber. Green: Al. Blue: Si. Only surface and interface atoms are shown for the Al part. The shape and position of the indenter is indicated in (a). Dimensions of the simulation volume and of the reinforcements are given in units of nm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)