ATOMISTIC SIMULATION OF THE MECHANICAL BEHAVIORS OF CU/SIC NANOCOMPOSITES

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1 Introduction

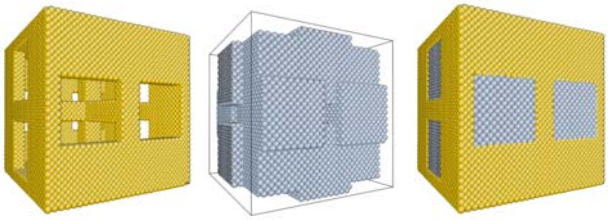
The nanocomposites containing nanosized microstructure have extensively motivated researchers to investigate the mechanical properties of such composites. Metal/ceramics nanocomposites, which are composed of low-melting-point metal and high-melting-point ceramics, can provide desirable mechanical properties including high specific stiffness, high plastic flow strength, creep resistance, good oxidation and corrosion resistance [1-3], and have potential application in thermal protection system (TPS), especially for the usage in thermal shock environment [4,5]. When co-continuous metal/ceramic composites are created in which both the metallic and the ceramic components are of nanoscale size [6], by controlling the nanostructure scale of ceramics nanoporous network, it is possible to significantly enhance the mechanical properties of metal/ceramics nanocomposites. The nature of the high interface/volume ratio and synergy of the combined physical properties may lead to a novel functional materials.

In this paper, we designed Cu/SiC to an interpenetrating phase nanocomposites (IPNC), based on the concept of the co-continuous nanocomposites. Atomistic simulations were employed to investigate the mechanical behaviors of Cu/SiC nanocomposites at different temperatures. The effects of volume fraction of SiC and interfacial strength on the mechanical properties of nanocomposites were characterized. The results of simulations show that temperature and volume fraction (VF) have important influence on the effective properties of nanocomposites, and the interfacial strength vary can change the deformation mechanism of nanocomposites under uniaxial loading. Our findings are helpful for the optimization design of the metal/ceramics nanocomposites with interpenetrating phases.

2 Model and Method

2.1 Model of Cu/SiC nanocomposites

The micro-structures of the co-continuous metal/ceramic nanocomposites are too complicate to directly simulate [6]. Here, based on the experimental observation [6] and the concept of INPC [5], the cubic cell model [7] was used to simulate the micro-structure of the nanocomposites (Fig.1), which is rather simple for molecular dynamics (MD) simulation. With this micromodel of the Cu/SiC nanocomposites, the effects of the parameters of structure and interface on the mechanical properties can be discussed, such as volume fraction, interfacial strength. In this paper, the volume fraction of SiC varies from about 30% to 60 %.



(a) (b) (c)

Fig. 1. (a) Model for nanoporous Cu. (b) Model for nanoporous SiC. (c) The representative unit cell of Cu/SiC nanocomposites, with Cu in yellow and SiC in gray.

2.2 Simulation Method

All the MD simulations presented in this work were performed using the large-scale atomic molecular massively parallel simulator (LAMMPS) [8].

Reliable force fields are very important for obtaining accurate simulation results. Currently, there are many types of force fields available, which have been parameterized to describe a variety of systems. In this paper, the interactions between the Si and C atoms were simulated using Tersoff potential [9], and the embedded atoms method (EAM) [10] potential was assigned to all the Cu atoms. However, no particular force fields exist to describe Si-Cu and C-Cu interactions. So a compromise is taken to choose force fields that, despite not being the most precise on, allows for extracting the physics of the problem in a qualitative manner. The interactions between the SiC and Cu atoms were represented by Lennard-Jones (LJ) (12-6) potentials. For LJ potential, the energy between two atoms is expressed as:

$$U_{ij} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \quad (1)$$

Where U_{ij} is a pair potential energy between the atom *i* and *j*. ε_{ij} and σ_{ij} are the coefficients of well-depth energy and the equilibrium distance, respectively. For different types of atoms, the parameters can be obtained by the mixing rules:

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \quad (2)$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \quad (3)$$

The well depth ε and equilibrium distance σ are estimated as 0.165565 eV and 3.05 Å for Cu-Cu [11], 0.019996 eV and 3.225 Å for Cu-C [11], 0.01744 eV and 3.826 Å for Si-Si [12]. So we can obtain the ε and σ as 0.05374 eV and 3.438 Å for Cu-Si interaction, respectively, according to the mixing rules. Actually, the mechanical strength of the interface between Cu and SiC is affected by the chemical reactions at the interface [13]. Special coatings can change the properties of the interfaces [14]. So we take the well depth ε as varying parameters (Tab. 1) to investigate the effects of interfacial strength on the effective mechanical properties. The effects of size parameters σ are beyond the scope of this paper, therefore the size parameters are set to be constant in all the simulations.

Table 1. The well-depth energy ε for interaction between SiC and Cu (eV).

	Interface 1	Interface 2	Interface 3	Interface 4
C-Cu	0.010	0.013	0.016	0.020
Si-Cu	0.020	0.030	0.040	0.050

Simulations were implemented in the NPT ensemble. Periodic boundary condition was imposed in all directions for all simulations in this work. The simulations were performed at temperatures in the range of 300-1200 K. The equations of motion were integrated using the Verlet leapfrog method with a time step of 0.001 ps. The models were applied an uniaxial tensile loading after a 50-ps equilibration. The average stresses in the atomistic systems were calculated using the virial theorem [15] in a microscopic equilibrium configuration after each loading step [16].

3 Results and discussions

Here, the results of MD simulations are given to understand the qualitative mechanism of the mechanical properties of Cu/SiC nanocomposite. By comparing the true stress-strain relationship of Cu/SiC nanocomposites at 300 K (Fig. 2), with the interface 2 ($\varepsilon_{c-cu} = 0.013$ eV, $\varepsilon_{Si-cu} = 0.030$ eV), the SiC volume fraction of 54.36% shows the highest yield strength with the highest initial elastic modulus, which indicates an appropriate volume ration can be chosen to get a nanocomposites with better mechanical properties. When the volume fraction of SiC drops to 38.92%, the nanocomposites show more obvious nonlinear mechanical properties.

Fig. 3 shows the effects of the interfacial parameters on the mechanical properties. According to the stress-strain curves with different well-depth energy of the SiC/Cu interaction, the properties of interface do not affect the elastic moduli of nanocomposites, but the deformation mechanism above the strain of about 3.0%. It indicates that the nanocomposites with weaker interface show stronger nonlinear

mechanical behaviors. Wegner et al. showed the enhanced properties of Ni/SiC IPC may result more from the contiguity of the phase than from the interpenetrating microstructure [17], which also shows the importance of the interface properties. By the snapshots of the tensile deformation of Cu/Sic nanocomposites in Fig. 4, the initial debonding of the Cu/SiC interface was observed at strain of about 3.9%, which degrades the mechanical properties of the nanocompoistes. With the increase of the tensile strain, the debonding of the interfaces grows continuously and leads to redistribution of the stress in the materials nano-networks.

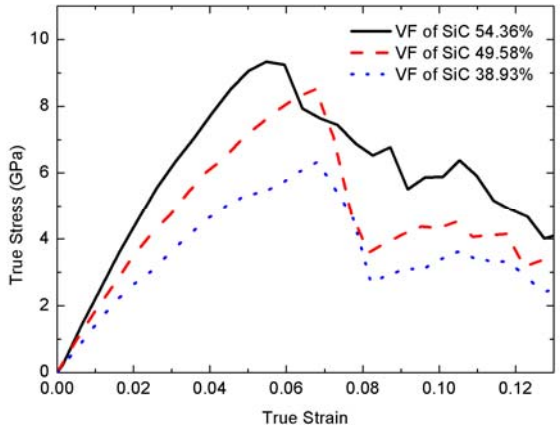


Fig. 2. The true stress-strain relationship of the Cu/SiC nanocomposites with different SiC volume fractions.

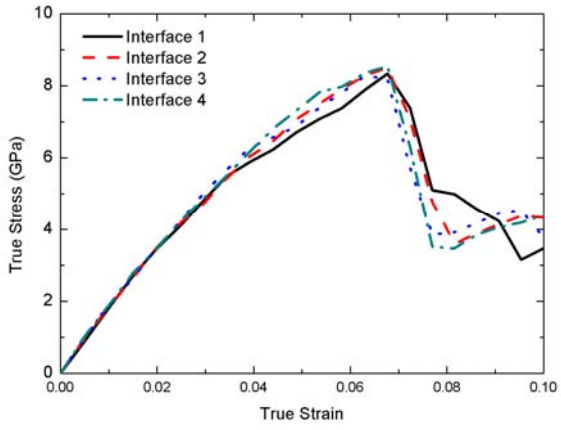


Fig. 3. The true stress-strain relationship of the Cu/SiC nanocomposites with different interfacial parameters.

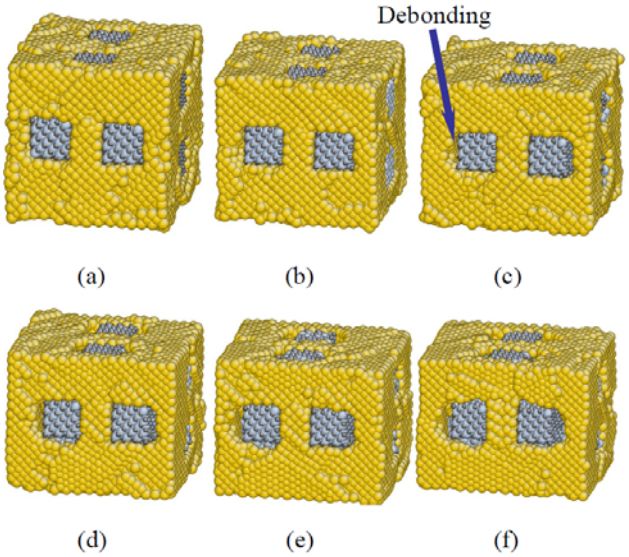


Fig. 4 The deformation process of the Cu/SiC nanocomposites with interface 4 ($\varepsilon_{c-cu} = 0.020$ eV, $\varepsilon_{Si-cu} = 0.050$ eV). The interface debonding can be firstly observed at the strain 3.9% of (c), and the continuous growth is shown in (d)-(f).

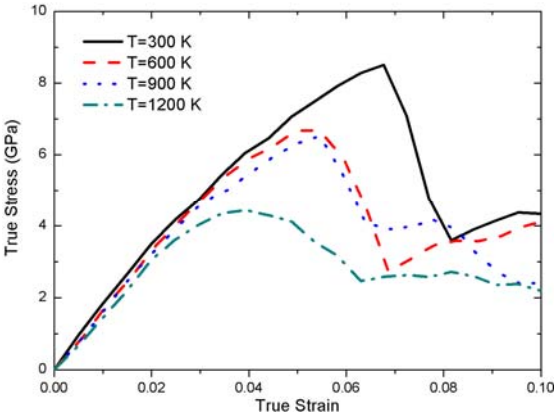


Fig. 5. The temperature effects on the mechanical behaviors of the Cu/SiC nanocomposites.

In order to obtain the temperature effects on the mechanical properties of Cu/SiC nanocomposites, the uniaxial loading processes were simulated in temperature range from 300 K to 1200 K with the parameters of interface 2. As shown in Fig. 5, the nanocomposites yield with the highest stress and maximum failure strain at 300 K. The yield stress drops to about one-half of that in room temperature. With the increase of temperature, the Cu phase shows obviously softening, which decrease the moduli and yield stress of the nanocomposites. The

stress-strain curve of 300 K has a sharp cline at the yield point, but not the 1200 K one, which means a brittle-to-ductile transition.

4. Conclusions

The volume fractions of the two phases in Cu/SiC nanocomposites play important roles in the mechanical properties, which make the nanocomposites designable to certain purpose. The strengths of the interfaces show effects on the plastic deformation of the nanocomposites. Some special coatings are expected to obtain appropriate properties of interfaces. With the temperature increase, the nanocomposites show a brittle-to-ductile transition.

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