Mechanical behaviors of nanocrystalline Cu/SiC composites: an atomistic investigation

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Abstract

Large-scale molecular dynamic (MD) simulations are employed to investigate the mechanical properties of the nanocrystalline Cu/SiC composites. The MD results indicate that the mechanical behaviors are insensitive to the strain rate when the strain rate is below $1.0 \times 10^9 \text{ s}^{-1}$. The Young's modulus and the yield stress of the nanocomposites increase nonlinearly with the volume fraction (VF) of SiC. Furthermore, the Young's modulus obtained by MD simulations fit the theoretical results well. In addition, a critical volume fraction (CVF) of the SiC reinforcement, 0.34 is obtained. Below the CVF, the nanocrystalline composites show metal-like mechanical behaviors. The majority of the dislocations nucleate at the Cu/Cu and Cu/SiC interfaces and then propagate into the Cu matrix. The flow stress almost keeps constant with the increase of strain. When the VF of reinforcement is above CVF, the reinforcement SiC dominates the mechanical behaviors of the nanocomposites. The strain hardening becomes more obvious with the rise of VF of SiC. Cracks prefer to nucleate and propagate along the SiC/SiC and Cu/SiC interfaces due to their strong brittleness. Our results show that adding the reinforcement to obtain high strength and

1 decent plasticity of metal matrix composites (MMC) also works at the nanoscale. A
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3 sharp increase of strength is found for the SiC/Cu nanocomposites when the SiC VF is
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5 around 0.34 due to the switch of the deformation and failure mechanisms. Based on
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7 these investigations, we can design the nanocomposite with quite high strength and
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9 relatively good plasticity.
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53 **Keywords:** molecular dynamics; Cu/SiC nanocomposites; strain rate; dislocations
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1. Introduction

Metal matrix nanocomposites (MMNs), which are reinforced by ceramic components (SiC, Al₂O₃, etc.), have an extensive use in high technology applications [1] due to their high specific stiffness, high plastic flow strength, creep resistance, good oxidation and corrosion resistance [2-4]. To maximize the performance and reliability of such materials, a fine-tuning of the nanostructure is required. Thus, it is necessary to have a fundamental understanding of the deformation and mechanisms of MMNs. It is possible to significantly improve the mechanical and physical properties of MMNs by controlling the nanostructure of materials when the size of both matrix and reinforcement reduce to nanoscale [5]. High ratio of interface and combination of two different phases may lead to a superior material.

Experiments on Al-Cu-Mg/SiC_p-T8 composites showed that both the strength and elastic modulus increase with the volume fraction (VF) of the reinforcement [6]. Fracture of the reinforcements, void growth and coalescence in metal matrix and interfacial decohesion are the main failure modes observed in experiments [7-10]. With development of nanotechnology, nanoscale metal matrix composites (MMCs) can be obtained, which show more surprising physical and mechanical properties. The introduction of the reinforcement leads to the hardness increase of the Cu/Al₂O₃ nanocomposites remarkably [5]. However, it is still significantly difficult and expensive to implement nanoscale experiments due to heterogeneous nature of interfaces in nanocomposites and small time scales of the relevant processes involved

[1].

Molecular dynamic (MD) simulations can provide detail structural information and mechanical behaviors of nanocomposites at atomic scale and may be efficient in the design of nanocomposites Zhou *et al.* systematically studied the effect of loading angle[11], orientation angle[12] and interfacial strength[13] on the deformation process of nanocomposites. Dangare *et al.* [1] observed the strengthening behaviors and the tension-compression strength asymmetry of Al/Si nanocomposites with using MD simulations. It was observed that the strength of the nanocomposites increase linearly with increase of the VF of Si in the Al-rich region. The mechanisms of deformation and failure of Al/Si nanocomposites was investigated by Donald *et al.* [14, 15] with a quasi 2D model and they proved that the deformations of the Al/Si nanocomposites are associated with the sliding/shearing of grain boundaries. Furthermore, it was found that the introduction of a second phase leads to the initiation and propagation of a crack along the interfaces in the Al/Ni nanocomposites [16]. In addition, Yang *et al.* [17] and Feng *et al.* [18-20] found the VF of SiC, interfacial properties and thermo effects play important roles in the plastic deformation of the co-continuous Cu/SiC nanocomposites. Although some studies on nanocomposites had been performed by experiments [3, 5, 21] and simulations [1, 17, 22, 23], the effect of the reinforcement on the deformation and failure mechanism is not clear yet.

In this paper, MD simulations are implemented to investigate the effects of VF of the reinforcement on the mechanical behaviors of Cu/SiC nanocomposites. The strain

rate effects and VF of SiC on the mechanical behaviors of the Cu/SiC nanocomposites are studied firstly. The deformation and failure mechanisms in the Cu/SiC nanocomposites with varying VF of SiC are analyzed based on the observations of atomistic structure evolution in the Cu/SiC nanocomposites. A comprehensive understanding of the deformation and failure mechanisms of Cu/SiC nanocomposites is achieved.

2. Computational details

The initial nanocrystalline Cu/SiC nanocomposites model with an average grain size of 8 nm and containing 26 grains are created with using the Voronoi construction method proposed by Derlet and Van Swygenhoven [24]. The orientations and distributions of grains are chosen randomly depending on the desired composition of the nanocomposites. With this method, the quasi isotropic homogeneous Cu/SiC nanocomposites can be obtained.

Fig.1 illustrates the geometry details of the representative unit cell model of the Cu/SiC nanocomposites. The size of the model is $23.5 \text{ nm} \times 23.5 \text{ nm} \times 23.5 \text{ nm}$, which is much larger than any cut-off distance in three dimensions. The interactions of atoms with their periodic images can be ignored. Furthermore, the center-symmetry parameter (CSP) and the coordination number (CN) are used to identify the deformations in the FCC and diamond cubic lattice.

For MD simulations, reliable force field is very important to obtain the reasonable results. In this paper, the Tersoff potential [25] is used to describe the

interactions between silicon and carbon atoms, which is proved to describe the mechanical properties of SiC nanocrystalline very well [17, 26].

The Tersoff potential is a three-body potential, which computes total energy SiC atoms of the system as [25]

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

where the subscript R and A represent the repulsive and attractive components of the potential, respectively. b_{ij} is the strength of each bond depending on the local environment, and it decreases with the number of the neighbors. f_c is a smooth cutoff function, f_R and f_A are the repulsive and attractive pair potentials, respectively.

The interactions between Cu atoms are simulated with using an empirical embedded-atoms method (EAM) potential [27]. In the EAM method, the total energy of the Cu atoms can be represented as [27]

$$E_{Cu} = \sum_{ij} V(r_{ij}) + \sum_i F(\bar{\rho}_i) \quad (2)$$

$$\bar{\rho}_i = \sum_{j \neq i} \rho(r_{ij}) \quad (3)$$

where $V(r_{ij})$ is the pair potential as a function of atomic separation distance r_{ij} between atoms i and j , and F is the embedding energy as a function of the electron density $\bar{\rho}_i$ given in Eq. (3), which is induced at site i by all other atoms in the system, $\rho(r_{ij})$ is the atomic density function.

Ideally, the potential used to represent the interface should include two-body and three body interactions. Recently, the extended Tersoff potential [28], Charge

optimized many-body (COMB) potential [29] and Tersoff potential [30] have been developed to describe the interactions between Si and Cu atoms. Herein, the Tersoff potential is used to depict the interactions between Si and Cu atoms due to its time-saving and small computational efforts [30]. However, there is no existing three-body potential to represent the interactions between C and Cu atoms, hence a Morse potential is adopted for the C-Cu interaction [31]. The Morse potential is expressed as [31]

$$V = D_0[e^{-2a_0(r-r_0)} - 2e^{-a_0(r-r_0)}] \quad (4)$$

where r is the distance between the atoms, r_0 is the equilibrium bond distance, D_0 is the well depth of the potential, and a_0 is the width of the potential. r_0 , D_0 and a_0 are 0.22 nm, 0.1eV and 0.17 nm^{-1} , respectively. In Ref. [31], researchers firstly used the Morse potential to describe the interactions in Cu-Cu and C-C. The parameters are then fitted by approximating the Morse potential expression to the well-known potentials, e. g., the embedded-atoms method (EAM) potential and the Stillinger-Webber (SW) potential. Then, the parameters in the Morse potential used to depict the Cu-C can be obtained based on the mixing rule. From our results, it is easy to find the interfacial Cu atoms will have higher energy than the interfacial SiC atoms (Fig. 9 and Fig. 10 in our latter results). Thus, the Cu atoms will not wet SiC.

All the simulations are implemented in the NPT ensemble. The equations of motion are integrated with using Verlet leapfrog method with time step of 0.001 ps. Periodic boundary conditions are used in all the three dimensions. The as-created

models are relaxed to achieve zero pressure and then equilibrated at approximate 0 K (10 K in our simulations) for 60 ps. We also increase the temperature of the system to 50 K and then quench down to 10 K, the results show that our conclusion in will not change. The models are deformed in Y direction after the equilibrium, with keeping both dimensions of the mode in X and Z direction constant. The average stresses in the Cu/SiC nanocomposites are calculated with using *virial* theorem [32].

Simulations in our paper are implemented with large-scale atomic molecular massively parallel simulator (LAMMPS) [33]. For visualizing the evolution of the atomistic structure, the open source software Atomeye [34] and Ovito [35] are employed.

3. Results and discussion

3.1. Strain rate effects on mechanical response

In order to study the influence of the strain rate, the Cu/SiC nanocomposites with VF of SiC of 0.259 are loaded with using different strain rates in the range from $1.0 \times 10^8 \text{ s}^{-1}$ to $1.0 \times 10^{10} \text{ s}^{-1}$. Fig. 2 plots the strain rate effects on the stress-strain responses of Cu/SiC nanocomposites under tensile loading. For all strain rates, the stress increases linearly with strain up to about 0.02. When the strain is below this value, the stress-strain curves are almost completely overlapped, which indicates the Young's modulus is essentially independent of the strain rate. Thus the Young's modulus is obtained as about 137 GPa, which is close to the result obtained by previous MD simulations [17]. The peak stress is defined as the yield stress of the nanocomposites [36] and the corresponding strain as the yield strain. The higher strain

rates reduce the dislocations emitting from the Cu/Cu interface or Cu/SiC interfaces (Fig. 3) during the deformation process and thereby render high strength of the nanocomposites [37]. Furthermore, it is more difficult for atoms in the nanocrystalline to overcome the activation energy barrier at the high strain rate due to its short time scale [38-40]. Thus, dislocation slips prefer to occur at the lower load rates. Furthermore, the calculated results show that the yield stress increases with the strain rate nonlinearly (Fig. 4). In addition, plastic flow is observed in these simulations, which shows that the nanocrystalline composites have metal-alike mechanical properties. For the Cu/SiC nanocomposites with low VF of SiC, the mechanical behaviors resemble that of the metal matrix, which is discussed in section 3.3 in details. The stress-strain curves can be divided into two types: below strain rate of $1.0 \times 10^9 \text{ s}^{-1}$, the strain rate dependence of the yield stress is negligible; the yield stress shows strong dependence on the strain rate for the strain rate beyond $1.0 \times 10^9 \text{ s}^{-1}$. Similar phenomenon is found in the tensile simulation of nanowires with using MD methods [41].

3.2. Effects of VF of SiC on mechanical properties

In order to study the effect of VF of reinforcement on the mechanical properties, the Cu/SiC nanocomposites models are created with volume fractions of ~0.0% SiC, 11.5% SiC, ~25.9% SiC, ~33.8% SiC, ~43.7% SiC, ~61.6% SiC, ~78.1% SiC, which are named case I, II, III, IV, V, VI and VII, respectively, as listed in Table 1. Each case has been averaged with 6 simulations. Fig. 5 plots the stress-strain curves of Cu/SiC nanocomposites with various VFs of SiC. The modulus and ultimate strength

are enhanced obviously with the increase of VF of SiC. The plastic behaviors of Cu/SiC nanocomposites can be regarded as the nucleation and reaction of dislocations. Therefore, typical plastic behaviors of metal appear when the matrix Cu is the dominant in the Cu/SiC nanocomposites with relative low VF of SiC (such as case I and II in Fig. 5), such as plastic flow, which are observed nanocrystalline metals commonly [42]. While, when the VF of SiC exceeds 0.34 (such as case VII in Fig. 5), the mechanical behaviors are mainly determined by the SiC reinforcement. The series of stress-strain curves can be divided into two categories as discussed above: For the VF below 0.34, the mechanical behaviors of the nanocomposite are mainly related to the Cu matrix; a strong similarity between the mechanical behaviors of the nanocomposites and the SiC reinforcement is observed with the VF of SiC beyond 0.34. Consequently, 0.34 is characterized as a critical volume fraction (CVF) for the Cu/SiC nanocomposites. It can also be seen clearly that the yield strength increases with the VF of SiC linearly when the VF of SiC belows the CVF, whereas the yield strength increases rapidly with VF of SiC over the CVF. Furthermore, the decrease of Cu/Cu interfaces is another key reason for the brittle behaviors of Cu/SiC nanocomposite with high VF of SiC. It is because that Cu/Cu and Cu/SiC interfaces are the main locations for dislocations nucleation when the grain size is less than 30 nm [43, 44].

Meanwhile, the strain-hardening modulus is usually defined as the slope of the curve at large strains (deformation above 3.8% in the present simulations). The least-squares method is used to fit the data in the strain-hardening regime. It is

apparent that the stress-strain curves do not exhibit strain hardening when the Cu matrix is dominant in the Cu/SiC nanocomposites. i.e., the flow stress does not increase with strain after the initial yield (Fig. 6). A large number of dislocations emit from the interfaces then be absorb by other interfaces should be responsible for this phenomenon [42]. Thus, the lack of strain hardening is believed to contribute to the tensile ductility of Cu grains in the Cu/SiC nanocomposites [42]. As for the cases that VF of SiC in the Cu/SiC nanocomposites over CVF, strain hardening is observable distinctly. In these cases, the dislocation density is high inside the grains due to the increase of SiC/SiC interfaces which are thought to be the locations of dislocation absorption. Therefore, the strain hardening becomes more significant with the increase of dislocation pile-ups in the Cu/SiC nanocomposites [42] which is resulted by the rise of VF of SiC in the Cu/SiC nanocomposites (Fig. 6).

In addition, basing on the variation principles of linear elasticity, an effective method have been proposed to estimate the bounds for the effective Young's modulus of the particle reinforced MMCs [45]. The lower and upper bounds for effective Young's modulus of the composites can be calculated as [45]

$$E_{lower} = \frac{9K_{lower}}{1 + 3K_{lower} / \mu_{lower}} \quad (5)$$

where,

$$K_{lower} = K_M + f \left[\frac{1}{K_R - K_M} + \frac{3(1-f)}{3K_M + 4\mu_M} \right]^{-1} \quad (6)$$

$$\mu_{lower} = \mu_M + f \left[\frac{1}{\mu_R - \mu_M} + \frac{6(1-f)(K_M + 2\mu_M)}{5\mu_M(3K_M + 4\mu_M)} \right]^{-1} \quad (7)$$

And the upper bond of the Young's modulus is expressed as [45]:

$$E_{upper} = \frac{9K_{upper}}{1 + 3K_{upper} / \mu_{upper}} \quad (8)$$

where,

$$K_{upper} = K_R + (1-f) \left[\frac{1}{K_M - K_R} + \frac{3f}{3K_R + 4\mu_R} \right]^{-1} \quad (9)$$

$$\mu_{lower} = \mu_R + (1-f) \left[\frac{1}{\mu_M - \mu_R} + \frac{6f(K_R + 2\mu_R)}{5\mu_R(3K_R + 4\mu_R)} \right]^{-1} \quad (10)$$

where μ and K are the shear and bulk modulus, respectively, and f is the volume fraction of SiC in the nanocomposites. The subscripts “upper”, “lower”, “M” and “R” refer to the upper and lower bound estimates, and matrix and reinforcement, respectively. E is the effective Young’s modulus of the Cu/SiC nanocomposites.

In order to compare the MD results with the theoretical predictions, the shear and bulk modulus of single-crystalline Cu and SiC are calculated with using MD simulations, which are 30.26 and 119.7 GPa for Cu, 152.2 and 218.4 GPa for SiC, respectively. The effective Young’s modulus of the Cu/SiC nanocomposites in our simulations are obtained by fitting the initial linear elastic region of the stress-strain curves. Furthermore, as we discussed in section 2, our model can be regarded as a quasi-isotropic homogeneous model. Fig. 7 shows the comparison between the result of MD simulation and the theoretical predictions. For the Cu/SiC nanocomposites with VF below about 0.25, the Young’s moduli calculated with MD are smaller than the lower bound. While for VF above 0.25, the MD results locate between the upper and lower bounds and are approaching to the upper bound with increasing of VF of SiC. It has been proved that the surface effects of SiC can be neglected while the surface effects of Cu matrix must be considered in Cu/SiC nanocomposites [17]. The

phenomenon that surface of Cu is softer than bulk has been approved by MD simulations [46]. Young's moduli of Cu were found to decrease with the later dimension and the size of surface [46], Thus, when Cu matrix is dominant in the Cu/SiC nanocomposites, the fact that modulus obtained by MD simulations are lower than theoretical results is due to the overwhelming of Cu interfaces in the Cu/SiC nanocomposites.

3.3. Deformation and failure mechanisms

3.3.1. Nanocomposites with VF of SiC below CVF

As discussed in section 3.2, the mechanical behaviors of the nanocomposites are mainly related to the Cu matrix when the VF of SiC is below CVF. Here, the typical case (case II) is taken as a representative to explain the deformation and failure mechanisms of the nanocomposites with comparison with other cases. Fig. 8 shows the snapshots of configurations deformation of the nanocomposites under uniaxial tensile loadings. In the tensile process, the nanocomposites start with elastic deformation from its initial state to a strain of 0.027 (Fig. 5). Then dislocations begin to emit from the Cu/Cu or Cu/SiC interfaces (Fig. 8a), which lead to the plastic deformation of the Cu/SiC nanocomposites. More dislocations appear in the Cu matrix with the increasing loading (Fig. 8a and b). Furthermore, recrystallization is also observed in our simulations, which is indicated by a yellow arrow in Fig. 8. The nucleation of the new grain starts by the emission of partial dislocations from the GBs (Fig. 8a). The complex core structures labeled 1 are formed by these emitting dislocations (Fig. 8b). Finally, the lamellas link up to form the new grain (Fig. 8c).

This phenomenon is also found in other simulations [44] and experiment [47] on the nanocrystalline metal deformation. Fig. 9 and Fig. 10 display the average energy of Cu and SiC atoms in the deformation process. Here, the bulk and interfacial atoms are defined in the initial configuration without deformations, and the coordination numbers of atoms not equal to 12 or 4 are regarded as the interfacial atoms. The average energy of bulk Cu atoms increases with the loading (Fig. 9), which means that there are increasing atoms involved into dislocations. For the interfacial Cu atoms, the average energy of them decreases within the deformation process (Fig. 9). Dislocations emissions release the energy of the interfacial atoms, which is also observed by Su and Tang [48]. However, for the phase of SiC in the nanocomposites act almost as a rigid body on the Cu atoms due to its much higher modulus. Therefore, the average energy of bulk SiC atoms almost remain unchanged (Fig. 8 and Fig. 10). While the average energy of interfacial SiC atoms decreases with the strain (Fig. 10), which can be attributed to the dislocation emission from the Cu/SiC interface. For the Cu/SiC nanocomposites with VF of SiC below CVF, a large number of dislocations appear in the Cu matrix lead to the strong plasticity of Cu/SiC nanocomposites (Fig. 11a₂, b₂ and c₂). At the same time, the reinforcement SiC improves the loading capacity of Cu/SiC nanocomposites remarkably (Fig. 11a₁, b₁, c₁ and Fig. 5). Furthermore, strong stress concentration occurs on the Cu/SiC interfaces due to the lattice mismatch [11], which leads to a significant grain boundary sliding/shearing at the Cu/SiC interfaces [14, 49]. It is proved that the sliding/shearing at the Cu/SiC interfaces and dislocation activity at the GBs dominant the early stages of plastic

1 deformation in the Cu/SiC nanocomposites [14]. Meanwhile, when the VF of SiC
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3 closes to CVF, a small crack is observed in the simulation (Fig. 12a). For the Cu/SiC
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5 system, the bulk modulus of SiC is about 218.4 GPa while the bulk modulus of
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7 copper is only 119.7 GPa [11, 50]. It is well known that the crack will be easier to
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9 activate at the brittle (SiC/SiC) interface (Fig. 12b) since it is easier to have stress
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11 concentration at the brittle interface. While for the SiC/Cu and Cu/Cu interfaces, the
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13 dislocation generated at the interfaces will weaken the stress concentration, and
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15 therefore, it is difficult to activate crack at such interfaces. However, the crack is
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17 blunted quickly when the crack propagates into Cu (Fig. 12c). Thus, the deformation
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19 and failure mechanisms are mainly corresponding to the Cu matrix when the VF of
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21 SiC is below about CVF. For the cases below CVF, dislocations generating at Cu/Cu
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23 and Cu/SiC interfaces and the later sliding/shearing at the Cu/SiC interfaces dominant
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25 the mechanical behavior of the Cu/SiC nanocomposites, which leads such
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27 nanocomposites to show an excellent ductility.

3.3.2. Nanocomposites with VF of SiC beyond CVF

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42 When the VF of SiC achieves a relative high value (over CVF), the deformation
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44 and failure mechanisms changed surprisingly, which are mainly determined by the
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46 mechanical behaviors of the reinforcements (cases V, VI and VII). The sharp increase
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48 (Fig. 5) of the strength is attributed to the large VF of nanocrystalline SiC grains,
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50 which result in more SiC/SiC grain boundaries, wherein plastic deformation is only
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52 limited to the flow of disordered atoms at SiC/SiC grain boundaries [1]. Furthermore,
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54 it is obvious that Cu/SiC nanocomposites become more brittle with the increasing of
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VF of SiC due to inability of SiC/SiC to nucleate dislocations and the limited flow of atoms at the SiC/SiC grain boundaries. For these cases, the reinforcement SiC dominates the properties of Cu/SiC nanocomposites. With taking all cases into account, the snapshots of case VII are used as an example to identify the deformation and failure process of nanocomposites with VF above CVF. The composites system starts with elastic deformation from its initial state to the yield stress at a strain of 0.02 in the tension loadings. A small percentage of dislocations, which emit from the Cu/Cu or Cu/SiC interfaces, appears in the Cu matrix and leads to the decrease of stress (Fig. 13a). Stress drops abruptly after the first yield point, and cracks arise on the triple junction meanwhile (Fig. 13b). The cracks propagate along the interfaces (Fig. 13) due to high activation energy of interfacial atoms [26]. Furthermore, cracks are easy to penetrate the model due to the existence of abundant SiC/SiC and Cu/SiC interfaces (Fig. 13c), which are thought to be more brittle than the Cu/Cu interfaces generally .

Fig. 14 shows the energy of the interface atoms during the deformation process. For the initial model, many interfacial atoms are in the high energy state due to the lattice mismatch between different grains. In region I, indicating elastic deformation of the Cu/SiC nanocomposite, the interfacial atoms more stable with the energy decrease. In region II, the energy of the interfacial SiC atoms increases with the loads. While for the interfacial Cu atoms, their energy still decreases in the deformation process. It is because that the dislocations emitted from the Cu/Cu and Cu/SiC interfaces release the energy of interfacial Cu atoms. When the strain increases to

about 0.09 (Fig. 14), cracks appear in the SiC/SiC and Cu/SiC interfaces. It means the bonds between atoms at the interface rupture. This phenomenon is expected to lead to the decrease of the total energy of interfacial atoms (region III in Fig. 14). For such nanocomposites, cracks prefer to nucleate at the triple junction [14, 15] and propagate along the Cu/SiC and SiC/SiC interfaces, which are thought to be more brittle than the Cu/Cu interfaces.

4. Conclusion

In this paper, the structure evolution and deformation behaviors of the nanocrystalline Cu/SiC nanocomposites are studied by MD simulations. It is found that the mechanical behaviors of Cu/SiC nanocomposites are insensitive to the strain rate when the strain rate is below $1 \times 10^9 \text{ s}^{-1}$. For the Cu/SiC nanocomposites with VF of SiC below CVF, their mechanical behaviors are mainly determined by the matrix Cu and the stress-strain curves do not exhibit strain hardening. A lot of dislocations emit from the Cu/Cu and Cu/SiC interfaces are observed during the plastic deformation process, which means the nanocomposites have good ductility. When the VF of the SiC beyond CVF, the mechanical behaviors of the nanocomposites are dominated by the reinforcement SiC. Strain hardening becomes more distinct with the increase of VF of SiC. The nanocomposites become more brittle with the increased VF of SiC due to the inability of SiC/SiC to nucleate dislocations and the limited flow of atoms at the SiC/SiC grain boundaries. Furthermore, because of the brittleness of the SiC/SiC and Cu/SiC interfaces, cracks prefer to nucleate and propagate along the

SiC/SiC and Cu/SiC interfaces. The phenomenon leads to the abrupt failure of the Cu/SiC nanocomposites. In addition, the Young's moduli obtained by MD simulations increase with the VF of SiC nonlinearly, which are in good agreement with the theoretical predictions. Our results prove that the enforcement has the similar strengthen effect on metal-matrix nanocomposites, which is well known in the MMCs. We also find the increase of the strength of SiC/Cu nanocomposites is quite different when the VF of SiC is different, e. g., a sharp enhancement is observed when the VF of SiC is larger than 0.34.

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Figure Captions

Fig. 1. Atomistic model of Cu/SiC nanocomposites. The atoms in the models are colored according to the coordinate number (CN).

Fig. 2. Normal stress along Y-direction as a function of the tensile strain for Cu/SiC nanocomposites at approximate 0 K. The applied strain rates are from $1.0 \times 10^8 \text{ s}^{-1}$ to $1.0 \times 10^{10} \text{ s}^{-1}$.

Fig. 3. The atomic configuration of Cu/SiC nanocomposites at $t = 60 \text{ ps}$. (a) $\dot{\epsilon} = 1 \times 10^{10} \text{ /s}$, (b) $\dot{\epsilon} = 2.5 \times 10^8 \text{ /s}$, (c) $\dot{\epsilon} = 1 \times 10^8 \text{ /s}$. Atoms are colored according to the CNA values: green balls for the FCC atoms, blue balls for the BCC atoms, red balls for the HCP atoms which indicate stacking faults, and gray atoms represent atoms in other states.

Fig. 4. Yield stress of the nanocomposites as a function of strain rate.

Fig. 5. The stress-strain relationship of the Cu/SiC nanocomposites with VF varying from 0 to 0.781 at approximate 0 K.

Fig. 6. Stress-strain curves with the different VFs of SiC at approximate 0 K. Straight lines with arrow represent the least-squares fit of the data in the strain hardening regime, the slopes of which represent the strain-hardening modulus.

Fig. 7. Young's modulus of Cu/SiC nanocomposites is obtained as a function of the VF of SiC, comparing with micromenchanics methods.

Fig. 8. Snapshots of the configurations during the tensile deformation. (a) $t = 30 \text{ ps}$; (b) $t = 70 \text{ ps}$; (c) $t = 210 \text{ ps}$. Atoms are colored with CNA values.

Fig. 9. Average energy of the bulk Cu atoms and the interfacial Cu atoms during the

deformation process.

Fig. 10. Average energy of the bulk SiC atoms and the interfacial SiC atoms during the deformation process.

Fig. 11. Snapshots of the case II under the pure tensile loading. (a) $t = 20$ ps, (b) $t = 46$ ps, (c) $t = 85$ ps. (a₁)-(c₁) are plotted by the atomic tensile stress field. (a₂)-(c₂) are colored with CN.

Fig. 12. Snapshots of the case IV under the pure tensile loading. (a) $t = 16$ ps, (b) $t = 83$ ps, (c) $t = 165$ ps. Atoms are colored as similar to Fig. 1. The red circle highlights the micro crack.

Fig. 13. Snapshots of the deformation of the case VII under uniaxial tensile loading. (a) $t = 23$ ps, (b) $t = 97$ ps, (c) $t = 175$ ps. (a)-(c) are colored as similar to Fig. 1. (1)-(4) are magnified of the red region in (a), represents the crack propagation along the interfaces. Atoms in (1)-(4) are labeled using the energy of the atoms.

Fig. 14. Total energy of the interfacial SiC atoms and the interfacial Cu atoms of case VII during the deformation process.

Table 1. Summary of initial Cu/SiC nanocomposites with varying Cu grains and SiC grains.

Case	Cu grains	SiC grains	Atoms
I	26	0	1225149
II	23	3	1229098
III	21	5	1219945
IV	16	10	1230012
V	13	13	1229701
VI	11	15	1228893
VII	6	20	1231003

Figure1

Figure2

Figure3

Figure4

Figure5

Figure6

Figure7

Figure8

Figure9

Figure10

Figure11

Figure12

Figure13

Figure14

Adding the reinforcement to obtain high strength and decent plasticity of metal matrix composites (MMC) is proving to work at the nanoscale as well. A sharp increase of strength is found for the SiC/Cu nanocomposites when the SiC VF is around 0.34. Detail deformation process is explained using the dislocation evolution. Based on these investigations, we can design the nanocomposite with quite high strength and relatively good plasticity.