1 Introduction

Metal matrix nanocomposites (MMNC) reinforced by ceramic components have broad application prospects in aerospace industries because of their excellent mechanical and physical properties such as, high specific stiffness, high plastic flow strength, creep resistance, good oxidation and corrosion resistance [1, 2]. Apart from their high strength, stiffness and wear resistance [3], MMNC has the ability to mitigate damage by spatial optimization of their properties. The most popular reinforcement of such composites is SiC or alumina particles, while the cooper, aluminum and titanium are usually the matrix materials. Ceramics are known for their brittleness, but the combination of ceramics into the ductile metal phase leads to improved mechanical properties like hardness and fracture toughness, especially when metal/ceramic composites are created in which both components are of nanoscale size [3], which is possible to significantly improve the mechanical properties of the materials. Understanding of the deformation and failure mechanisms of these nanocomposites materials can be of benefit to their design and optimization. These mechanisms are complex for the metal/ceramic nanocomposites, which are related to the distribution of the particle reinforcements, grain size and interfacial properties, etc [4-6].

Ceramic particle reinforced metal matrix composites (MMCs) have been studied extensively by using experiments and finite element method (FEM), with the mechanical properties obtained as functions of the microstructure and the volume fraction of reinforcement [7]. Chawla et al. [8] observed the tensile behavior of an Al-Cu-Mg(2080)/SiCp-T8 composites with varying volume fraction \( V_f \) of the reinforcement (at a constant particle size of 5 um) and varying particle size (at a constant volume fraction of 20%) and suggested the elastic modulus and tensile strength both increase with the \( V_f \) of the reinforcement. In addition, the ductility of the material decreases with the increase of particle size. The similar results also were obtained by Mummery et al. [9] and Manoharan et al. [10]. The elastic modulus for different fractions of the fractured particles for Al-3.5Cu matrix reinforced with SiC particles was studied by Shen et al. [11] and Finot et al. [12] with experiments. Furthermore, they used FEM to predict the elastic modulus of these composites, in which the particles were fully intact or all fractured. As expected, their experimental results, which were bounded in the predictions by FEM, implied that even when all the particles in the composites are fractured, the brittle particles contribute to stiffening and strengthening. Nevertheless, treating the cracked particle as a crack in the matrix (or a void for that matter) is not a reasonable assumption. Llorca et al. [13] studied the short-fiber reinforce composites show a distinct Bauschinger effect upon reversed loading under cyclic loading conditions. Fracture of the ceramic reinforcement, void nucleation, growth and coalescence of voids with in metallic matrix, and/or decohesion and crack growth along the interface were the main damage styles in MMCs observed by Llorca et al. [13, 14], Needleman et al. [15] and Laws et al. [16]. Thus, the optimized design of these materials requires a fundamental understanding of the links between the length scales and properties of these composites, which is hope to enable a combination of high strength and good ductility to
improve the failure resistance under various loading conditions in extreme environments (high strain rates, high temperature etc.). It is well realized that the reduction of grain size of the MMCs to nanoscale can improve the strength of the materials [6]. Thus, it can be expected that a nanocrystalline metallic matrix reinforced by nanoscale ceramic particles would result in a MMNC with high strength, toughness and ductility. The hypothesis can be tested using experiments alone, however, are quite difficult and expensive due to the small length scale and small time scale.

The molecular dynamic (MD) simulation method is implemented to investigate the atomic-level structural information and mechanical behaviors of MMNC. This may be helpful in design of composites materials at atomic scales. The strengthening behaviors and the tension-compression strength asymmetry of Al/Si nanocomposite as a function of volume fraction of the reinforcement is observed by Dangare et al. [3, 17] at atomic scales by using MD simulations. Donald et al. [18] investigated the mechanisms of deformation and failure in Al-Si nanocomposites using molecular dynamics, they found the deformations in the Al/Si nanocomposites are associated with grain boundary sliding/shearing at the Al/Si interfaces. A MD study of Ag/Ni composites by Cheng et al. [19] found that introduction of a second phase reduces grain rotation-induced grain growth and leads to the initiation of crack along the Ag/Ni interface, thus decreasing the fracture strain relative to single-phase nanocrystals, which is consistent with general expectations. Cho et al. [20] and Odegard et al. [21] studied that the Young’s modulus of the polymeric nanocomposites is enhanced as the size of nanoparticle decreases by assuming the inclusion modeled in the simulations are spherical nanoparticles.

This paper focuses on the simulation of the deformation and failure mechanisms of the Cu/SiC nanocomposites, which is expected to achieve a fundamental understanding of the relationship between the length scales and the properties of these composites. The microstructure of the nanocomposite comprises of a random distribution of SiC reinforcement and Cu matrix nanocrystals. The MD simulations are aimed to investigate the process of atom-scale damage evolution in the SiC/Cu nanocomposites. Furthermore, the effects of volume fraction of the reinforcement SiC nanocrystals, the temperature and the grain size on the strengthening behaviors of the composites are also studied. The computational details are discussed in Sec. 2. The process of deformations of the MMNC is presented and discussed in Sec. 3. In addition, the effects of volume fraction of the reinforcement SiC nanocrystals, the temperature and the grain size on the macroscopic strengthening behaviors are analyzed in Sec. 4.

2 Model and Method

2.1 Geometrical Model

The micro-structures of the MMNC are too complicated to be simulated directly. Here, based on the previous works of MMNC [5], the cubic cell model is used in this work. Hence, the cubic computational cell consisting of Voronoi type nanocrystals (as shown in Fig. 1) is adopted in all simulations, which follows the method of Derlet and Swygenhoven [22].

The size of the model is 23.5 nm × 23.5 nm × 23.5 nm, as shown in Fig. 1. The size is much larger than any of cut-off distance in three dimensions, thus the interaction of atoms with their periodic images are vanished. In the model, periodic boundary conditions are implemented in three directions. To study the effect of grain size, MMNC systems are created with an average grain size (AVS) of 6-10 nm. The smallest MMNC have 63 grains.

2.2 Simulation Method

In this study, the MD simulations are implemented in the open source programs large-scale atomic molecular massively parallel simulator
(LAMMPS) [23]. For visualizing the evolution of the atomic structure, the Atomeye [24] and open source ovito [25] are employed. For MD simulation, reliable force fields are very crucial to obtain reasonable results. In the present model, different force fields are employed to reveal the interactions of atoms. Herein, the interactions between Si and C atoms are simulated using Tersoff potential [26]. The empirical embedded-atoms method (EAM) potential developed by Mishin et al. [27] 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

\[ E_{\text{SiC}} = \frac{1}{2} \sum_{i,j} \left[ f_r(r_{ij}) (f_a(r_{ij}) + b_{ij} f_a(r_{ij})) \right] \]  

(1)

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

The total energy of EAM potential [27], revealing the atomic interaction of copper atomic system is expressed as

\[ E_{\text{Cu}} = \sum_i V(r_i) + \sum_i F(\overline{\rho}_i) \]  

(2)

\[ \overline{\rho}_i = \sum_{r_i} \rho(r_i) \]  

(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 \( \rho \), given in Eq. (3), which is induced at site \( i \) by all other atoms in the system, \( \rho(r_i) \) is the atomic density function. All the parameters used here in the Tersoff potential for C and Si atoms and EAM potential for copper are taken from Refs. [26, 27].

However, there is no particular potential exist to describe the Cu-Si and Cu-C interactions. Strictly speaking, the potential used to represent the interface should include two-body and three-body interactions. Two-body interactions are the interactions between Cu-Si and Cu-C while the three-body interactions involve in Cu-Si-C, Cu-C-Si, Cu-Si-Cu and Cu-C-Cu. In this work, we assume the interface of Cu/SiC as a Si-terminate interface. Thus, the potential between Cu and Si atoms should include two and three body interactions. Here, we use the Tersoff potential to represent the interactions between Cu and Si atoms as Zhang et al. [28] used. However, the interaction between Cu and C atoms is quite weaker than that between Cu and Si atoms for the Si-terminate Cu/SiC system, and hence we adopt Morse potential to describe the interactions between Cu and C atoms. The Morse potential is expressed as

\[ V = D_0 \left[ e^{-2\alpha(r-r_0)} - 2e^{-\alpha(r-r_0)} \right] \]  

(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 \( \alpha \) is the width of the potential. The parameters of Morse potential are provided elsewhere [29].

The average stresses in the atomistic systems are calculated as [30]

\[ \sigma_{ij}(t) = -\frac{1}{\Omega_0} \left[ \frac{1}{2} \sum_j F_{ij} F_{ij} + M_i \dot{V}_i \dot{V}_i \right] \]  

(5)

where \( \alpha \) and \( \beta \) are the Cartesian components, \( \Omega_0 \) is the atomic volume, \( F_{ij} \) is the force on atomic \( i \) due to atom \( j \), \( M_i \) is the mass of atom \( i \), and \( \dot{V}_i \) is the velocity of atom \( i \).

The system is relaxed for 50ps by NVT ensemble to obtain an equilibrium state. Then, we use NPT ensemble to make stress of the model be zero in all directions. The time-step of 0.001 ps is adopted for all of the MD simulations in this paper. Furthermore, the temperature is allowed to evolve during the deformation process. The strain rate of the loading in MD simulation is about \( 1 \times 10^6 \text{s}^{-1} \).
3 Results and Discussion

3.1 Stress-strain relationships

In order to understand the mechanism of the mechanical properties of Cu/SiC nanocomposites, the stress-strain curves and corresponding snapshots of structural evolution are recorded. The stress-strain relationship of Cu/SiC nanocomposites at 0.5K, with the SiC volume fraction of 58.0% is obtained and illustrated in Fig. 2. The curve is initially linear up to the yield point, after which the nanocomposites show obviously nonlinear deformation. The Cu/SiC nanocomposites exhibit an evident plastic mechanical behavior due to the existence of Cu matrix. The flow stress is also calculated for uniaxial loading in tension process, which is used to measure the level of plastic of Cu/SiC nanocomposites. Furthermore, the Cu/SiC nanocomposites also show a remarkable brittle mechanical behavior as a result of the influence of SiC reinforcement. In addition, the ultra high maximum stress is a result of high strain rates (1 × 10⁹ s⁻¹).

The deform configurations of the Cu/SiC under uniaxial tension are shown in Fig. 3, which are corresponding to the A-F points in Fig. 2. It can be observed that the grain boundaries (GBs) are the regions with obvious stress concentration (as shown in Fig. 3A). The stress concentration is observed in the grains and interfaces when the stress is larger than the yield stress (Fig. 3B), and the dislocations in the Cu matrix appear as well. Almost all the SiC grains endure the maximum stress and more dislocations appear in the Cu matrix (Fig. 3C). Then, cracks appear in the interfaces due to the existence of interspaces in the interfaces (Fig. 3D), and some region in the Cu/SiC are not bear the loads and the dislocations in Cu matrix is decreasing. The material begins to damage when the crack penetrates the computational cell (Fig. 3E) and break soon. The process shows the cracks appear in the interface, which is due to the stress concentration at the interface, and propagate along the interface result in a partial failure (Fig. 3E) to a entire failure (Fig. 3F) transition.

3.2 Effects of temperature on mechanical properties

In order to obtain the temperature effects on the mechanical properties of Cu/SiC nanocomposites, the simulations are conducted in the temperature range from 300 K to 1100 K, with the tensile stress-strain curves shown in Fig. 4. With the increase of temperature, the Cu phase shows obvious softening, which decrease the modulus and maximum stress of Cu/SiC nanocomposites. The modulus and maximum stress of Cu/SiC nanocomposites at different temperatures are listed in the table 1. The region of the nonlinear before the maximum stress is extending, which imply the plasticity of Cu/SiC nanocomposites is improved as temperature increasing.

The common neighbor analysis (CNA) [31] method is used to identify the local deformations in the FCC and diamond cubic lattice. The relaxed configurations at different temperatures are shown in Fig. 5 with atoms colored according to the CAN values. The arrangement of atoms in the interface becomes more irregular (Fig. 5) and implies the voids in the interface increasing with temperature, which corresponds to the decreasing of yield stress of Cu/SiC nanocomposites. In addition, a mount of dislocations appear in Cu due to the temperature increasing, which weaken the load bearing capability of Cu/SiC nanocomposites. The atoms at the interface posses enough kinetic energy diffuse to the Cu matrix as the temperature increases, thus the stress concentration at the interface vanishes when the temperature arrives or exceeds the melt temperature of Cu matrix.

3.3 Effects of Vf on mechanical properties

Fig. 6 plots the stress-strain curves of Cu/SiC nanocomposites with the varying Vf of SiC. In the simulated composite system, SiC acts almost as a rigid body, while large deformation is observed in
Cu matrix due to its flexibility. Thus, the modulus of Cu/SiC nanocomposite increases with the increase of the $V_f$ of SiC. In addition, with the increase of $V_f$ of SiC, the capacity of elastic deformation of the nanocomposites is enhanced. The maximum stress in each stress-strain curve is defined as the ultimate strength of the nanocomposites. The dependence of the ultimate strength of nanocomposites on the $V_f$ is illustrated in the upper left corner of Fig. 6. The ultimate strength increases nonlinearly with the increase of the $V_f$ of SiC. Furthermore, the increasing fraction of SiC results a large fraction of the SiC, which limits the diffusion of the atoms at the interface renders a high strength values for the Cu/SiC nanocomposites.

The plastic behaviors of polycrystalline metals before failure can be regarded as the nucleation and propagation of dislocations in Cu matrix. Plasticity in nanocrystalline metals, however, has contributions from the dislocation-based and grain boundary-based processes. The GB becomes more dominant at grain size less than 30 nm [32], which includes GB sliding/rotation and GB diffusion. The processes of the deformation with different $V_f$ of SiC at 0.5 K are shown in Fig. 7. Here, we give two representative $V_f$ of SiC, 10.8% and 78.3%, which are named case A and case B, respectively. For case A, little dislocation appears in the Cu matrix, the GB-based process is the dominant mechanism in the deformation process, which is responsible to the high plasticity of Cu/SiC nanocomposite. While the dominant mechanism in the Cu/SiC nanocomposite with high $V_f$ of SiC is not only GB-based process, a mount of dislocations appear in the Cu matrix as well (Fig. 7). The high fraction of SiC results a high strength of Cu/SiC nanocomposites, which leads to the high deformation in the Cu matrix. Thus, the dislocations in the Cu matrix are activated. Moreover, we also analyze the Cu/SiC nanocomposites with other $V_f$ of SiC and the similar result is observed.

### 3.4 Effects of grain size on mechanical properties

Previous experimental results of the yield stress of single-phase nanostructured metals or metallic clearly indicates that the yield stress increases with increasing grain size (inverse Hall-Petch effects) [33, 34] when the size of the polycrystals below 20 nm. However, the yield stress of MMNCs (grain size bellows 20 nm) does not show such a relation clearly [35] due to the fraction of the reinforcement and the interface between the reinforcement and the matrix, etc. Here, the size of the polycrystals used in our simulations range 6 to 10 nm. Fig. 9 shows the stress-strain curve of Cu/SiC nanocomposites with different grain size. The yield stress and the volume fraction of reinforcement SiC are list in Table. 2. The AVS of the MMNs, which has the maximum stress, is 10 nm, while the AVS of 8 nm has the minimize yield stress. The increase of the grain size also results in the change of the interface between SiC and Cu and the fraction of SiC reinforcement, etc. Thus the strength of the Cu/SiC nanocomposites has no obvious relation with the grain size in our results. A mount of dislocations appear in the Cu matrix before the stress reach the maximum stress. The AVS of MMNs, 10 nm, is the favorite size which dislocations to be activated. While the AVS of 8nm is more difficult for dislocations to be activated than other AVS (Fig. 10)

### 4 Conclusion

MD simulations are carried out to investigate the deformation behaviors of Cu/SiC nanocomposites under high strain rates. Cracks nucleate at interfaces and penetrate the grains leads to the failure of the Cu/SiC nanocomposites. A mount of dislocations are observed in the Cu matrix during the process of the deformation. In addition, strengthening behaviors of the ceramic (SiC) particle reinforced nanocrystalline metal (Cu) are strongly dependent on the temperature, the $V_f$ of SiC and the grains sized. With the temperature increasing, the ultimate yield stresses of Cu/SiC nanocomposites decrease almost linearly. Furthermore, the dislocations in the Cu matrix and the thickness of the specific interface increase with temperature. The strength of the
Cu/ SiC nanocomposites is observed to increase nonlinearly with the increasing of the $V_f$ of SiC. At the low $V_f$ of SiC, the dominant plastic behavior of the Cu/SiC nanocomposites is the BG-dominated process, while the dislocation-based process is a typical style for the Cu/SiC nanocomposites with high $V_f$ of SiC. The effects of the grains size is also studied in this paper. The inverse Hall-Petch effects, which is obvious in the single-phase nanostructured metals, are not found in the Cu/SiC nanocomposites.

References:


[16] J. R. Brockenbrough, S. Suresh "Constitutive behavior of a microcracking brittle solid in
7


Table 1. The modulus and maximum stress of Cu/SiC nanocomposites at different temperatures, $E$ and $\sigma_{\text{max}}$ are the modulus and maximum stress of Cu/SiC nanocomposites, respectively.

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>$E$ (GPa)</th>
<th>$\sigma_{\text{max}}$ (GPa)</th>
</tr>
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<tbody>
<tr>
<td>300</td>
<td>187.5</td>
<td>8.53</td>
</tr>
<tr>
<td>500</td>
<td>186.2</td>
<td>7.76</td>
</tr>
<tr>
<td>1100</td>
<td>133.4</td>
<td>5.03</td>
</tr>
</tbody>
</table>

Table 2. The maximum stress of Cu/SiC nanocomposites with various grain sizes, AGS and $\sigma_{\text{max}}$ are the average grain size and maximum stress of Cu/SiC nanocomposites, respectively. VF represents the volume fraction of SiC in the Cu/SiC nanocomposites.

<table>
<thead>
<tr>
<th>AGS (nm)</th>
<th>VF (%)</th>
<th>$\sigma_{\text{max}}$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>31.06</td>
<td>10.82</td>
</tr>
<tr>
<td>8</td>
<td>29.94</td>
<td>10.24</td>
</tr>
<tr>
<td>10</td>
<td>30.39</td>
<td>11.31</td>
</tr>
</tbody>
</table>

Fig. 1. Atomistic model of Cu/SiC nanocomposites. Yellow balls for Cu atoms, blue balls for Si atoms and green for C atoms. The other atoms are interfacial atoms.

Fig. 2. The tensile stress-strain relationship of Cu/SiC nanocomposites with the $V_f$ of SiC of 0.580 at 0.5 K.

Fig. 3. The snapshots of damage evolution of Cu/SiC nanocomposites at the marked points A-F in Fig. 2. 1 represents the Cu matrix, the black arrows show the region of dislocations in the Cu matrix. The white circle is the place where a crack nucleates.

Fig. 4. The tensile stress-strain curves of Cu/SiC nanocomposites at different temperatures.
Fig. 5. The relaxed configurations at different temperatures. The structure in the red circle is scaled at the left bottom. The dashed circle indicates the dislocations in Cu matrix. Atoms colored according to the CNA values. The dark blue atoms represent the bulk FCC stacking, the cyan atoms are in the tetrahedral bonding in the diamond cubic lattice, and the atoms in other color represent the atoms at the interface.

Fig. 6. The stress-strain relationship of the Cu/SiC nanocomposites with $V_f$ varying from 0.000 to 0.783 at 0.5 K. The maximum stress of the nanocomposites is shown at the upper left corner.

Fig. 7. The deformation configuration of Cu/SiC nanocomposites with a $V_f$ of SiC of 0.108. Atoms colored according to the coordinate numbers ($Z$). The black circle shows the region of dislocation diffusion. The red circle represents the dislocations in the Cu matrix.

Fig. 8. The deformation configuration of Cu/SiC nanocomposites with a $V_f$ of SiC of 0.783. Atoms are colored according to the coordinate numbers ($Z$). The red circle represents the dislocations in the Cu matrix.

Fig. 9. The stress-strain relationship of the Cu/SiC nanocomposites with grain size varying from 6 nm to 10 nm at 0.5 K. The flow stress of the nanocomposites is shown at the lower.

Fig. 10. The configurations with different grain size. The state A, B and C corresponds to states in Fig. 9. The red arrows represent the dislocations in the Cu matrix. Atoms are colored according to the CNA values.