Rev. Adv. Mater. Sci. 33 (2013) 24-28

MELTING PROCESS OF SiC NANOCERAMIC BY MOLECULAR DYNAMICS

Zhang Ke[1], Ren Juping[1], Tang Yulan[2], Liu Guozhi[1] and Wu Yuhou[1]

[1]College of Traffic & Mechanical Engineering, Shenyang Jian Zhu University, Shenyang 110168, Liaoning, China
[2]Municipal and Environmental Engineering College, Shenyang Jian Zhu University, Shenyang 110168, Liaoning, China

Received: October 17, 2011

Abstract. The sintering and preparation process of nanoceramic materials is simulated by molecular dynamics (MD) simulation. 3D models of molecular dynamics for crystal planes (100) and (110) of SiC nanoceramic crystal is developed. In the models, the Tersoff potential function is used to simulate the inter-atomic force. In order to investigate the microstructure of nanoceramic with crystal planes (100) and (110) after melting, their melting processes are simulated by rapid-heating. Their characteristics are investigated by analyses of energy evolution, pair correlation function and the graph of instantaneous place of the atoms during melting process. Furthermore, melting processes of SiC with crystal plane (100) are also simulated by different heating rate. The results show that density, energy evolution and melting point of SiC nanoceramic crystal with crystal planes (100) and (110) is different, which indicate anisotropy; during the melting process the higher heating rate, the more energy workpiece needs.

1. INTRODUCTION

Nanoceramic has been widely used in a variety of areas due to the properties of high temperature resistance, good thermal conductivity, high hardness, wear-resistant and corrosion [1,2]. SiC is one kind of ceramic materials which has the high temperature mechanical properties, excellent thermal, electronic and semiconductor characteristics, the better high temperature resistance and the lower thermal expansion coefficient. Therefore, SiC is widely used in product and processing of industrial materials [3-5]. Due to the differences of composition and structure between the ceramic material and the traditional ceramic material, the traditional research method is not suitable; now, molecular dynamics simulation method [6] had a great progress to study the nanometer ceramics. H.J. Shen simulated the melting process of SiC nanopole [7], R.S. Averback investigated the sinter and grain growth process of the nanometer ceramics crystal [8], Hideaki Matsubara studied the structure of the nanometer ceramics after melting by the Monte Carlo method and molecular dynamics method [9]. The microcosmic structure of SiC ceramics can be understood better by the simulation of SiC ceramics melting process [10], which is helpful to improve its mechanical properties.

2. THE SIMULATION BASED ON THE MOLECULAR DYNAMICS

2.1. Simulation model

The β-SiC is adopted in the simulation. Molecular dynamics model of SiC (100) and SiC (110) are showed in Fig. 1 and Fig. 2, respectively. In Fig. 1, the workpiece modeled as finite slab consisted of

Corresponding author: Zhang Ke, e-mail: Zhangke@sjzu.edu.cn

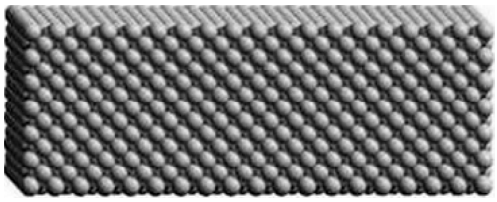

Fig. 1. MD model of SiC(100).

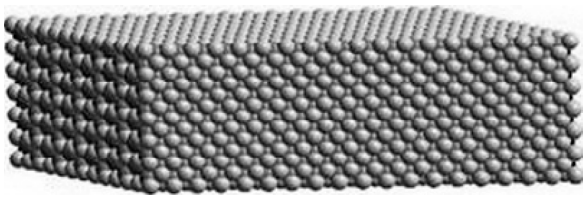

Fig. 2. MD model of SiC(110).

78.48×26.16×26.16 Å^3, containing 11664 atoms, and the workpiece in Fig. 2 consisted of 78.48×36.99×26.16 Å^3, containing 12312 atoms. And, molecular dynamics model of crystal face (100) is cube crystal, and the crystal face (110) is oblique crystal form of β = 145°.

2.2. Simulation method

Molecular dynamics (MD) method is used to study the preparation process of SiC ceramic micro-component. The crystal is simulated in the canonical ensemble (NVT) in this study. Periodic boundary condition is used in the simulation. Before the MD simulation, the system was relaxed 2000 time steps in order to the stability of the system energy. The model have a little changes after relaxation, this is different from the single atomic system. During the simulation, Tersoff potential is used to describe force between the atoms [11] (Tersoff potential function is used to describe the force between SiC crystals [12-14]).

$$E = \sum_i E_i + \frac{1}{2}\sum_{i \neq j} V_{ij}, \quad (1)$$

$$V_{ij} = f_c(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right]. \quad (2)$$

Here, E is the total energy between i and j,
V_{ij} is the potential energy between i and j,
r_{ij} is the distance between i and j,
$f_C(r_{ij})$ is the cut-function between the atoms,
$f_R(r_{ij})$ is the repulsive function,
$f_A(r_{ij})$ is the attractive function,
b_{ij} is low rank function.

3. SIMULATION RESULTS AND ANALYSIS

3.1. The melting process of SiC (100) and (110)

The melting processes of SiC (100) and (110) were simulated by the system heated to 3000K. In order to keep the balance of system energy, the relaxation was performed 5000 time steps per 500K. Fig. 3 shows the evolution of temperature and energy. The energy and temperature increase with the time. The mode of internal energy increase is similar to the temperature. Before temperature raised 2000K, temperature and energy curve are relatively rising smoothly, but after 2000K, energy curve changed

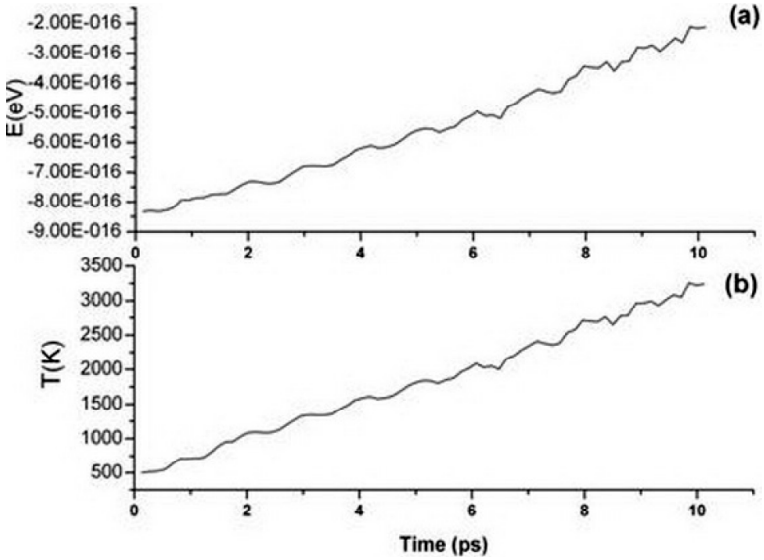

Fig. 3. The evolution of temperature and energy during the melting process of SiC(100).

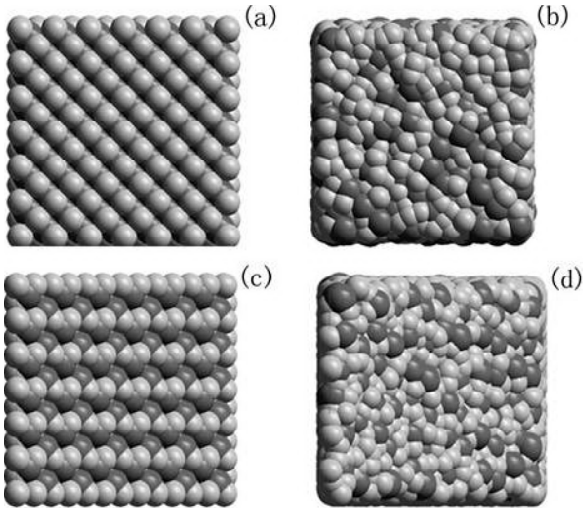

Fig. 4. The instant atomic positions.

irregularly. Fig. 4a shows the instant atomic positions of SiC(100) after the relaxation and Fig. 4b demonstrates the instant atomic positions of SiC(100) after 2000K. Atomic arrangement in Fig. 4b has a great change compared with the system relaxed. Fig. 3 shows that SiC(100) of the melting stage, atomic structure in the model is disorder.

Pair correlation function (PCF) is used to describe the position between atoms in this study. The formula of PCF is defined as (3):

$$g(r,r') = \frac{V^2}{N(N-1)}\left[\sum_{i,j;i\neq j}\delta(r-r_i)\delta(r'-r_j)\right]. \quad (3)$$

Fig. 5 is the PCF curve of SiC(100), the dotted line shows positional relationship between SiC atoms after relaxation, and the solid line represents

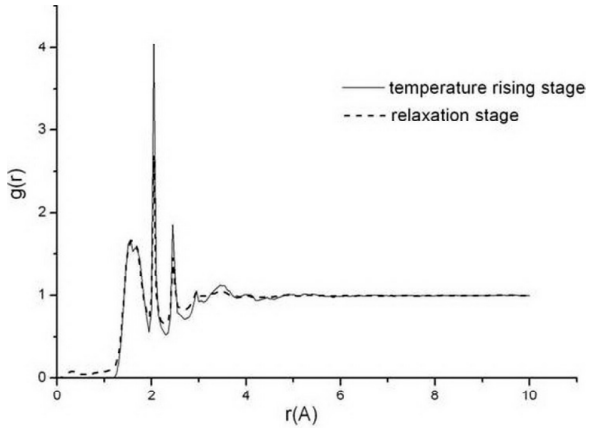

Fig. 5. The PCF curve of SiC(100).

positional relationship between SiC atoms after heating. Compared with two curves, SiC atoms' position have a great change after melting, and SiC(100) shows amorphous structure. Fig. 6 shows the evolution of temperature and energy during the melting process SiC(110). In Fig.6, the melting processes between SiC(100) and SiC(110) are similar, energy evolution changes along with temperature. Fig. 4d shows the instant atomic positions at 1900K, compared with Fig. 3, energy evolution become irregular at about 1900K. Therefore, SiC(110) is melting at about 1900K.

After melting, the density of SiC (100) is 3.62 g/cm^3, and the density of SiC(110) is 3.86 g/cm^3. Compared with the melting process between SiC(100) and SiC(110), the melting state of SiC(100) and SiC(110) is similar, but the melting point is different, and the internal energy of SiC(110) is higher than SiC(100).

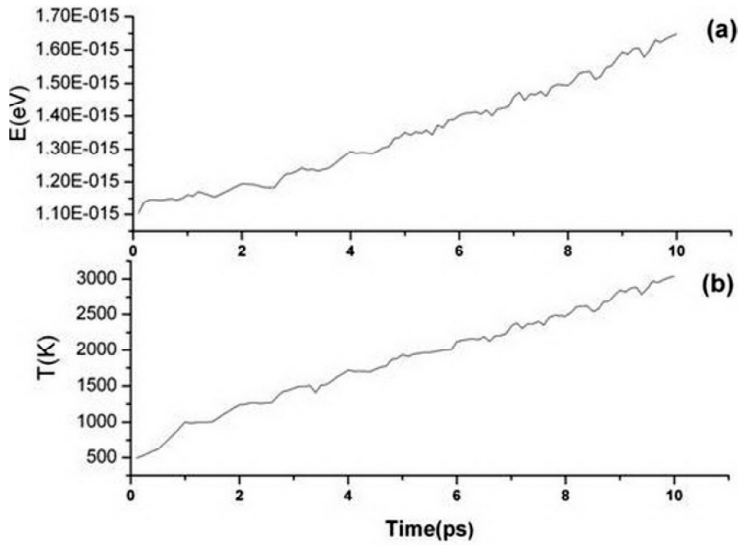

Fig. 6. The evolution of temperature and energy during the melting process SiC(110).

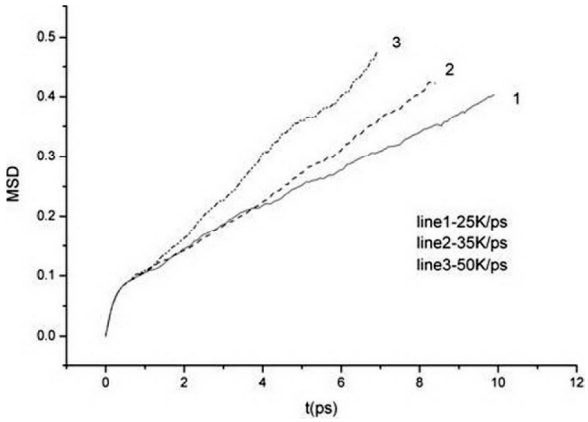

Fig. 7. The MSD curve of C atoms with different heating rates.

3.2. Effect of the heating rate on the melting process of SiC(100)

In order to study the influence of heating rate on the melting behavior of SiC crystal, the SiC(100) melting process is simulated in different heating rate. First, system which contained 4050 atoms is relaxed about 100 ps under the temperature of 300K, in order to keep the system balance. Then the melting process is simulated by the system heated to 2200K under different rate.

Because the ratio of Mean Square Displacement (MSD) to time is equal to diffusion coefficient, the spread of atoms with time can be described by MSD. Fig. 7 shows the MSD curve of carbon atom in different heating rates. In Fig. 7, curves 1 to 3 respectively represents the heating rate 25 K/ps, 35 K/ps, and 50 K/ps. At the beginning, the diffusion of atoms is not influenced by heating rate. With the time increasing, the diffusion speed of C atoms with the heating rate 10 K/ps is higher than others, and atoms are more disorder. Fig. 8 is the MSD curve of Si atoms with different heating rates. The MSD value of Si is slightly lower than that of C, which indicates the diffuse speed of Si atoms is slower than that of C atoms in the same temperature. Fig. 9 shows the curve of SiC internal energy in different heating rates. Curves 1 to 3 still respectively represents the heating rate 25 K/ps, 35 K/ps, and 50 K/ps. At the beginning, the internal energy of nanoceramic is not influenced by heating rate. The internal energy is same and quickly raises under three heating rates. With the temperature increasing, internal energy is influenced by the heating rate obviously. The gradients of the three curves are almost constant. The gradient of Curve 3 is more than others which indicates the system of Curve 3 has the bigger internal energy than others. The internal energy of curve 1 is lowest. So the higher heating rate, the higher melting point.

4. CONCLUSION

The SiC(100) and (110) melting process is simulated by molecular dynamics, and the influence of different heating rate on the melting process is investigated. The simulation results are analyzed and the conclusions are that:

(1) Based on the analysis of the melting process of SiC(100) and (110), their melting point and energy are different, which show the anisotropy.
(2) When the temperature of environment is more than the melting point of SiC, its atom array is disorder, and the crystal structure is amorphous; the density of crystal with different crystal orientations is different.
(3) During the melting of process the higher heating rate, the higher melting point.

ACKNOWLEDGEMENTS

This work is supported by National Natural Science Foundation (50975182), the Support Program for

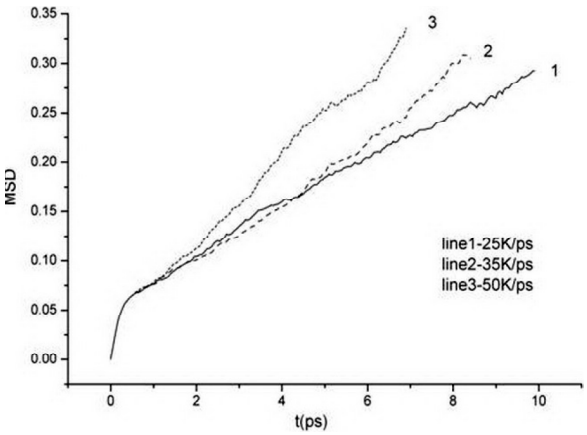

Fig. 8. The MSD curve of Si atoms with different heating rates.

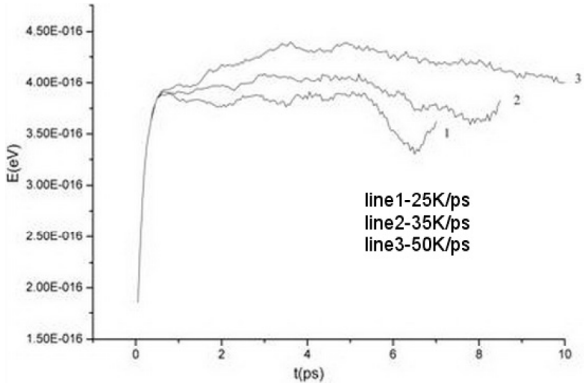

Fig. 9. The curve of internal energy with different heating rates.

Ministry of Education Innovation Team (IRT1160), Natural Science Foundation of Liaoning province (20102186).

REFERENCES

[1] M.E. Levinshteain, S.L.Rumyantsev and M. Shur, P*roperties of Advanced Semiconductor Materials:GaN, AlN, InN, BN, SiC, SiGe* (New York:Wiley, USA, 2001).

[2] A.Pechenik, R.K.Kalia and P.Vashishta, *Computer-Aided Design of High-Temperature Materials* (New York: Oxford University Press, USA, 1999).

[3] Y. G. Gogotsi, S. Welt and D.A. Eesoy // *Nature* **411** (2001) 283.

[4] B. Basavalingu, J.M. Calderin Moreno and K. Byrappa // *Carbon* **39** (2001) 1763.

[5] K. Zhang and Y.H. Wu // *Key Engineering Materials* **315-316** (2006) 364.

[6] Yulan Tang, Yingchun Liang and Dongxu Wang // *Key Engineering Materials* **315-316** (2006) 792.

[7] J. P. Rino and I. Ebbsjö // *Physical Review B* **70** (2004) 045207.

[8] R.S. Averback, H. J. Hofler, H. Hahn and J.C.Logas // *Nanostruct. Master.* **1 (**1992) 173.

[9] H. Matsubara // *Computational Materials Science* **14** (1999) 125.

[10] Ruisong Guo and Sh. Cai, *Engineering structural ceramics* (Tianjin, Tianjin University Press, 2002), In Chinese.

[11] J. Tersoff // *Phys. Rev. B.* **39** (1989) 5566.

[12] Ju-Young Kim and Baik-Woo Lee // *Thin Solid Films* **467** (2004) 94.

[13] Izabela Szlufarska and Rajiv K. Kalis // *Phys. Rev. B.* **71** (2005) 174113.

[14] F. Gao and W. J. Weber // *Nuclear Instruments and Methods in Physics Research B* **207** (2003) 10.