Investigate the fast melting process of 2D SiC model by molecular dynamics

Vo Van On¹*, Nguyen Thị Thúy Nhi¹, Nguyen Thanh Hung¹

¹Group of Computational Physics and Simulation of Advanced Materials – Institute of Applied Technology – Thu Dau Mot University

*E-mail: onvv@tdmu.edu.vn

Abstract. This paper presents the results of the study of fast melting process of 2-dimensional SiC by MD simulation with a sample of 400 atoms which consists of 200 Si atoms and 200 C atoms. The model is melted from 300K to 8000K at a rate of 10¹³ K/s. Investigation of energy dependence on temperature shows a jump of the average total energy of SiC model at temperature T = 5090K. Investigation of material microstructure by a radial distribution function, ring distribution, bonding angle distribution, even distribution number distribution showed that the phase transition temperature was about 5090K.

1. Introduction

There are many engineering applications known for three-dimensional Silicon Carbide (SiC) materials, while bi-dimensional SiC materials still have little research interest. In 2010 scientists began to get interested in the material after discovering graphene, a new two-dimensional form of carbon, from Nobel prize-winning Russian physicians Andrej Geim and Konstantin Sergeiievich Novoselov. Due to its unusual behaviors and promising applications in various technical fields, two-dimensional silicon carbide (2D SiC) has piqued the interest and been intensively studied in recent years [1-6]. Under atmospheric conditions, DFT calculations predict that 2D SiC has a honeycomb structure identical to graphene [1–4]. It is referred to as Hexa-SiC. Hexa-SiC monolayers have a direct bandgap of 2.56 eV and binding energies of up to 2.0 eV [6]. Furthermore, 2D Hexa-SiC has a significant in-plane rigidity and local magnetic moment in the presence of silicon-vacancy [7, 8]. Furthermore, SiC nanotubes or SiC nanoribbons have been extensively investigated for atomic and electronic structure and other properties[9-12]. The armchair's SiC nanoribbons are nonmagnetic semiconductors, while the zigzags are magnetic metals, according to DFT calculations [11]. Ab initio study of electronic and optical actions in 2D Hexa-SiC mono or multilayers [13]. The thickness and geometric structures of these nanosheets have a significant impact on their behavior. The bandgap of 2D Hexa-SiC, which is about 2.5 eV, can be tuned, and this material has promising applications in optoelectronic devices [13]. Other important 2D Hexa-SiC applications predicted by theoretical research are included in [14, 15, 16]. V.V. Hoang et al. used molecular dynamics (MD) simulations to investigate the formation and atomic structure of two-dimensional (2D) tetra-SiC (containing fully quadrilateral) [17]. The team of
Tue Minh L. Ng et al. used the Vashishta interaction potential to simulate the melting of 2D structural SiC and obtained a phase transition temperature of about 4050K [18]. V.V. On et al. used MD simulation with Vashishta interaction potential to investigate the rapid melting of SiC [19]. There have been no previous studies on the rapid melting of SiC using the Tersoff potential. In this paper, we use MD simulation with Tersoff interaction potential to investigate the quick melting process of SiC. The following is how the paper is organized: Part 2 contains the outcomes of the measurements and simulations; part 3 contains the conclusion.

2. Calculations and simulation results

There are 400 atoms in the original model, including 200 Si atoms and 200 C atoms. The periodic boundary conditions of a 2-dimensional SiC lattice heated in NVT mode. The Tersoff potential was used to characterize Si–Si, C–C, and Si–C interactions, and it is a three-body potential feature that can provide a more accurate explanation of covalently bonded materials like silicon and carbon [20],

\[ E = \frac{1}{2} \sum_{i \neq j} f_c(r_{ij}) \left[ A_{ij} \exp(-\lambda_{ij}r_{ij}) - B_{ij} \exp(-\mu_{ij}r_{ij}) \right] \]  

(1)

Here \( b_{ij} \) is described by

\[ b_{ij} = \chi_{ij} \left( 1 + \xi_{ij}^{n_i} \right)^{-1/2n_i} \]  

(2)

The parameters \( \xi_{ij}^{n_i} \) are given by

\[ f_c(r_{ij}) = \begin{cases} 1, & r_{ij} \leq R_{ij}, \\ 0.5 + 0.5 \cos \left( \frac{\pi}{S_{ij} - R_{ij}} \right), & R_{ij} < r_{ij} \leq S_{ij}, \\ 0, & r_{ij} > S_{ij}, \end{cases} \]  

(3)

Here \( A_{ij} \) and \( B_{ij} \) are continuous parameters of Morse potential; parameters such as \( f_c(r) \) have values and the derivative continuously for all \( r \) and go from 1 to 0. Here \( R_{ij} \) is only selected; it consists of the first grain layers of SiC. Standard compound rules are used such that the parameters \( \lambda_{ij} \) and \( \mu_{ij} \) are the arithmetic mean and \( A_{ij} \), \( B_{ij} \), \( R_{ij} \) and \( S_{ij} \) are the geometric mean of the individual i and j component values, respectively [21].

To achieve equilibrium, the model was relaxed at 300 K in \( 10^5 \) simulation steps; then, in NVT mode, the SiC model was heated from 300 to 8000 K at a speed of \( 10^{13} \) K/s, with \( 770000 \) simulation steps. The MD simulations are done with LAMMPS software [22], and the ring statistics are calculated with ISAACS software [30]. The Guttman rule [23] is used in the measurement of the rings. The atomic configurations are visualized in 2D using the VESTA program [24]. The following sections describe the findings of microstructure analysis and data processing.

2.1. Investigate the correlation between the average total energy per atom and the temperature

Figure 1 shows the total energy dependency on temperature when melting SiC model using molecular dynamic simulation at a rate of \( 10^{13} \) K/s,
Figure 1. The temperature dependence of total energy when melting a two-dimensional SiC model.

At a rate of $10^{13}$ K / s, the original SiC model was melted. The tangent leaves the energy line at $T = 5090$ K, which is the temperature of SiC phase transition in the model, as shown in Figure 1. Due to the high heating rate and the difference in interaction potential for investigation, this study's phase transition temperature varies from the previous study [18].

2.2. Radial distribution function

The radial distribution function (RDF) during SiC melting is shown in Figure 2 at various temperatures.

Figure 2. Temperature dependence of radial distribution functions.

Figure 2 illustrates the model's structural changes during the melting process. The radial distribution function has a sharp first peak at 300K, and then second and third peaks appear, indicating that SiC’s close and far orderly structure is very stable. As a result, the SiC model is solid-state. The elevation of
the distribution peaks decreases as the temperature rises, while its width increases. The elevation of the first peak decreases as the phase transition temperature $T=5090K$ approaches, while the heights of the second and third peaks steadily decrease. This demonstrates that the ordered structure in the close and far distances is unstable. The SiC model has started to decompose. The peaks almost vanish at 6120K, and the radial distribution curves are relatively smooth. SiC’s close and far order system was precarious. At this temperature, the SiC model totally melted.

2.3. Ring distribution function

Figure 3 illustrates the ring distribution at temperatures of 300K, 5090K, and 6120K.

Ring size 3 reaches a ratio of 100 percent at a temperature of 300 K. The bonds between the atoms in the model started to break at the phase transition temperature $T = 5090 K$, with a sharp increase in the ring size 3, reaching a ratio of 51 percent. In comparison to before the phase transition, ring sizes 3 and
4 increased and ring sizes 6 decreased, and there were more rings (such as rings size 7, 8, 10) showing more and more defects in the model structure. The ring size 3 dominates at a temperature of 6120K. When the model is heated to a higher temperature, the remaining rings appear to decrease sharply, demonstrating that the structure's variance is more evident.

2.4. Mean ring distribution

Figure 4 illustrates the influence of temperature on the average ring distribution.

![Figure 4. Temperature dependence of mean ring size](image)

The mean ring size fluctuated around ring size 3 before the phase transition. The average ring number continues to increase from 2340K to 5080K, but it is not stable. At a phase transition temperature, the ring size abruptly increases to nearly 4.8, suggesting that the SiC structure is changing. The average number size increases and decreases continuously from 3.6 to 5.25 after the phase transition temperature. It can be shown that when the model is heated to higher temperatures, the mean ring size appears to vary quickly.

2.5. The angle distribution function

Figure 5 illustrates the bonding angle distribution at different temperatures of 300K, 5090K, and 6120K.
Figure 5. Bond angle distributions at 300 K (a), at 5090 K (b), and at 6120 K (c).

At 300K, the Si-C-Si bond angle is mainly distributed at 119°, with a ratio of 26%. The Si-C-Si angle distributes from 102° to 142° at T = 5090K and peaks at 122° with a ratio of 6.8%. The Si-C-Si bond angle varies from 20° to 180° when the temperature is gradually increased up to 6120K. The SiC in the model has turned into a liquid at this temperature.

2.6. The distribution function of mean angle

Figure 6 shows the temperature dependence of the mean bond-angle distribution.
Figure 6. The temperature dependence of the mean angle distribution

The mean angle almost reached $119^0$ before the phase transition temperature, indicating that the structure has not changed. There is a jump in mean angle at the phase transition temperature $T = 5090K$, and the structure starts to modify. The mean angle distribution continued to decrease after phase transition, reaching $104^0$ at $6120K$.

2.7. Coordination number distribution function

Figure 7 illustrates the distribution of coordination number at 300K, 5090K, and 6120K temperatures.
Figure 7. Coordination number distribution at 300 K (a), at 5090 K (b), and at 6120 K (c).

All of the SiC atoms in the model have a coordinate number of 3 at 300K, reaching in a ratio of 100%. The 3, 4, 5 coordinate numbers do not change much at T = 5090K, but the coordinate number of 6 increases dramatically from 0.4 percent to 2.3 percent, demonstrating that the structure of SiC in the model begins to change. When the model was heated to 6120K, coordinate numbers 1 and 8 appeared, with the coordinate number 4 dominating with a ratio of 34%. The SiC melted at this temperature.

2.8. Interatomic distance distributions

Figure 8 shows interatomic distance distributions at 300K, 5090K, and 6120K temperatures.
Figure 8. The interatomic distance distribution at 300 K (a), at 5090 K (b), and at 6120 K (c).

At a temperature of 300K, the distance distribution reaches a high of 1.78 and a rate of 18%. There is a high of 1.77 with a rate of 4.6 percent at the phase transition temperature of 5090K, and this distribution varies from 1.54 to 2.09. The broken SiC structure no longer exists in its original state when heated to 6120K, and it transforms into a liquid state. The distance distribution with the temperature of 300K has the maximum distribution peak at 1.78 Å, a rate of 18%. At the 5090K phase transition temperature, the maximum distribution peak at 1.77 Å, rate of 4.6%, and this distribution range from 1.54 Å to 2.09 Å. When heated to 6120K, the broken SiC structure is no longer in the original state and changes to a liquid state.

2.9. Visualization of the atomic configuration

Figure 9 shows the visual configuration of the SiC model at temperatures 300K and 8000K by VESTA software.

Figure 9. The visualization configuration of the SiC model at 300K (a), and at 8000K (b).

3. Conclusion

The molecular dynamics simulation of the quick melting of the SiC model at a rate of 1013 K/s is discussed in this paper. When heated with the Tersoff interaction potential of about 5090K, the survey results obtained the 2D SiC phase transition temperature. The ring, angle, and distance distribution all support the model's phase transition temperature of 5092 K. At 8000K, the SiC structure obliterated everything.
References

[1] A. Wander, F. Schedin, P. Steadman, A. Norris, R. McGrath, T. S. Turner, G. Thornton, N. M. Harrison 2001 Phys. Rev. Lett. 86: 17: 3811;
[2] Miyamoto, Yoshiyuki, Byung Deok Yu. 2002 Appl. Phys. Lett. 80.4: 586-588;
[3] Claeyssens, Frederik, C. L., Allan, N. L., Sun, Y., Ashfold, M. N., & Harding, J. H. 2005 Journal of Materials Chemistry 15.1: 139-148;
[4] Freeman, C. L., Claeyssens, F., Allan, N. L., & Harding, J. H. 2006 Physical review letters 96.6: 066102;
[5] Tusche, C., H. L. Meyerheim, J. Kirschner. 2007 Physical review letters 99.2: 026102;
[6] Hsueh, H. C., G. Y. Guo, Steven G. Louie. 2011 Physical Review B 84.8: 085404;
[7] Sahin, H., Cahangirov, S., Topsakal, M., Bekaroglu, E., Akturk, E., Senger, R. T., & Ciraci, S. 2009 Physical Review B 80.15: 155453;
[8] Eliseeva, N. S., Kuzubov, A. A., Ovchinnikov, S. G., Serzhantova, M. V., Tomilin, F. N., & Fedorov, A. S. 2012 Jemp Letters, 95.11: 555-559;
[9] Menon, M., Richter, E., Mavrandonakis, A., Froudakis, G., & Andriotis, A. N. 2004 Physica Review B 69.11: 115322;
[10] Baumeier, Bjorn, Peter Kruger, Johannes Pollmann 2007 Physical Review B 76.8: 085407;
[11] Sun, L., Li, Y., Li, Z., Li, Q., Zhou, Z., Chen, Z., Hou, J. G. 2008 The Journal of chemical physics 129.17: 174114;
[12] Bekaroglu, E., Topsakal, M., Cahangirov, S., & Ciraci, S. 2010 Physical Review B 81.7: 075433;
[13] Lin, X., Lin, S., Xu, Y., Hakro, A. A., Hasan, T., Zhang, B., Chen, H. 2013 Journal of Materials Chemistry C 1.11: 2131-2135;
[14] B.S. Song, S. Yamada, T. Asano, S. Noda 2011 Optics Express 19.12 11084-11089;
[15] Arnold, C., Marquier, F., Garin, M., Pardo, F., Collin, S., Bardou, N., Grefet, J. J. 2012 Physical Review B 86.3: 035316;
[16] N. Wang, Y. Tian, J. Zhao, P. Jin 2016 Journal of Molecular Graphics and Modelling 66 196;
[17] Van Hoang, V., Giang, N. H., Dong, T. Q., & Hanh, T. T. T. 2019 Computational Materials Science 162: 236-244;
[18] Tue Minh Le Nguyen, Vo Van Hoang and Hang T.T. Nguyen 2020 Eur. Phys. J. D 74 108;
[19] V. V. On et al 2020 Materials Science and Engineering (IOP): ICRIET 2020 (accepted);
[20] Xichun Luo, Saurav Goel, Robert L. Reuben 2012 Journal of the European Ceramic Society 32 3423–3434;
[21] D. Powell, M. A. Migliorato, and A. G. Cullis 2007 Phys. Rev. B 75 115202;
[22] S. Plimpton 1995 J. Comput. Phys. 117.1: 1-19;
[23] S. Le Roux, V. Petkov 2010 J. Appl. Crystallogr. 43.1: 181-185;
[24] K. Momma and F. Izumi 2008 J. Appl. Crystallogr. 41.3: 653–658;