Computer simulation of obtaining thin films of silicon carbide

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The Tersoff potential, which establishes Si-Si, C-C and Si-C bonds, is the main stabilizing factor when considering the autonomous behavior of the resulting SiC films. The deposition of Si and C atoms is carried out at a high temperature (1000 K). At the same time, the substrate in the model is motionless; is actually at zero temperature. We can assume that the film is obtained under cooling conditions. Therefore, when testing the model, the cooling process should be taken into account, including when studying the structure of the deposited SiC film. Since there are no analogues of this work, in which the electrolytic deposition of a SiC film on a substrate is studied by the method of molecular dynamics, we will test the model by obtaining bulky amorphous phases of silicon carbide. We obtain these amorphous phases from the 3C-SiC and 4H-SiC crystalline phases of this compound. The criterion for the adequacy of the model used here will be the obtaining of similar partial radial distribution functions for one of these bulk phases with the corresponding functions obtained by other authors using an identical interaction potential and similar external conditions.
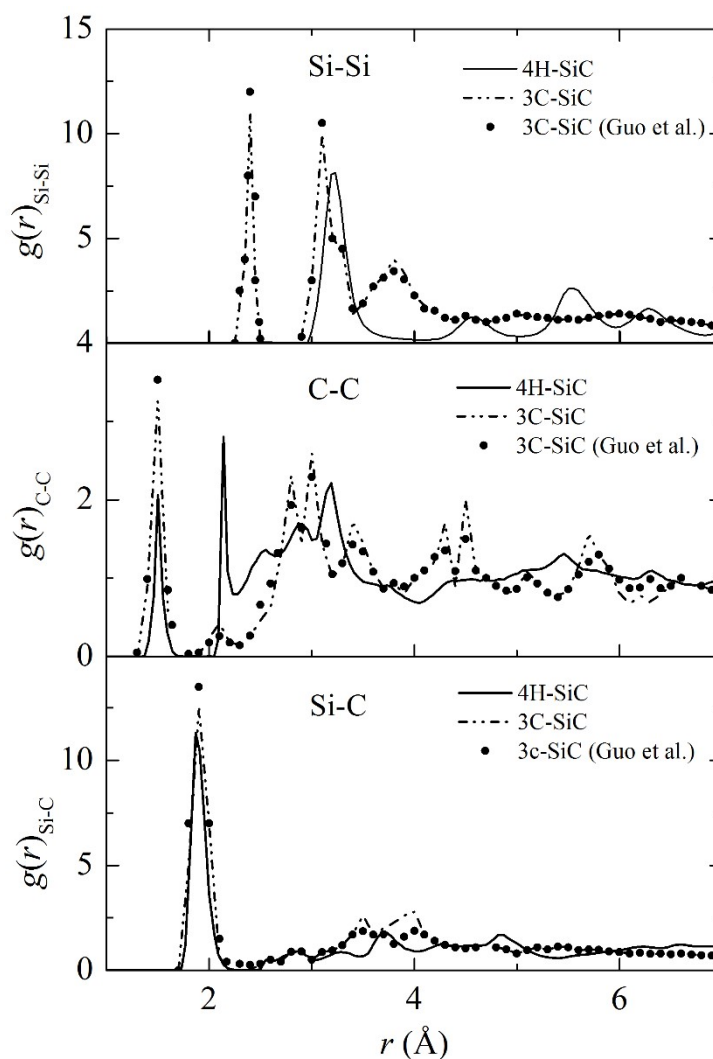
Fig. 1. Partial (Si-Si, C-C and Si-C) radial distribution functions calculated for 4H-SiC and 3C-SiC modified silicon carbide phases at T = 200 K.

Despite the fact that more than 250 polytopes have been discovered among silicon carbide crystals, only a limited number of them lend themselves to controlled synthesis. Periodic boundary conditions (PBC) acted in the system. These stable phases include the zinc blende (3C-) structure and the wurtzite structure (4H-) of SiC. The difference between these structures lies in the stacking of diatomic layers: 3C has three such layers (ABC), and 4H has four layers (ABAC). The 3C-SiC and 4H-SiC phases have similar melting points (3103 K) [1].

In [2], in the molecular dynamics model of 64000 Si and C atoms interacting through the Tersoff potential, the solidification of the molten 3C-SiC phase in contact with its own crystal was studied. The melt was obtained at a temperature of 3500 K and then equilibrated for 1 ns with the 3C-SiC crystalline phase. The lowest temperature to which the system was cooled was 200 K. In this case, the cooling rate was 10^{11} K/s. The authors of [2] believe that due to the lack of time for the rearrangement of atoms at such a cooling rate, amorphization rather than crystallization is observed. In other words, in this computer experiment, they obtained at a predominantly amorphous 3C-SiC phase. It is the result of the study in [2] that we used for comparison with the 3C-SiC and 4H-SiC systems obtained by us during heating and cooling.

Systems of 6000 atoms interacting with the Tersoff potential and representing the 3C-SiC and 4H-SiC phases of silicon carbide were heated from 300 K to 3500 K and then cooled to 200 K at the same rate of 10^{11} K/s. Then the phases were kept at the reached temperature (200 K) for 1 ns. The systems were expanded due to PBC. The structure of the 3C-SiC and 4H-SiC phases obtained at T = 200 K was analyzed by constructing partial radial distribution functions. These functions for the two considered SiC phases are compared in Figs. 1. Note that all partial (Si-Si, C-C and Si-C) functions $g(r)$ obtained for the 3C-SiC system are in good agreement with the corresponding functions found in [2]. At the same time, the partial functions $g(r)$ for the 3C-SiC and 4H-SiC phases noticeably differ from each other. For example, in the case of the Si subsystem, the g(r) function of the 3C-SiC phase contains a pronounced peak at 1.9 Å, which is absent in the $g(r)$ of the 4H-SiC phase. At the same time, in the case of the C subsystem, a pronounced peak at 2.14 Å appears for $g(r)$ of the 4H-SiC phase, which almost does not appear for the analogous function of the 3C-SiC phase. The best agreement is achieved for $g(r)_{SiC}$ of these two phases.

Thus, the closeness of the partial radial distribution functions of this work and work [2] for the predominantly amorphous C3-SiC phase of silicon carbide obtained under similar cooling conditions characterizes the present model as adequate.

References

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