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Affect of the graphene layers on the melting temperature of silicon by molecular dynamics simulations

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ABSTRACT

In the paper, molecular dynamics simulations have been used to detect the melting temperature of silicon. The two models have been considered as the graphene/silicon/graphene (GSG) sandwich and the only silicon system. Atoms in the models interact with each other via a 3-body Tersoff potential with a modified part based on a Coulomb potential and the Ziegler–Biersack–Littmark universal screening function. We find that C–Si interaction prevents the melting of the two silicon surfaces adjoining the graphene layers. The melting temperature of the silicon part in the GSG sandwich (T_m = 2450 K) is 1.6 times higher than that of the only silicon system ($T_{m,pure}$ = 1540 K). Difference of these melting temperatures has original from interaction of C–Si pairs, which causes decreasing of the energy of the silicon part in the GSG sandwich during heating process leading to an increase of the melting temperature of this silicon part.

1. Introduction

State of silicon determines its many properties. It is well known that crystalline silicon has a diamond-like structure and is an indirect band-gap semiconductor at low temperature and/or pressure. In liquid phase at high temperature, silicon is metallic in spite of its small population of covalent bonds [1]. These two phases of silicon show separation of system volume [2], density [3] and coordination number [4] with each other. Liquid phase exhibits higher density and volume than solid one, while liquid has the smaller volume of system than solid. Phase transition of the melting has caused structural changes of silicon creating its distinguished properties between solid and liquid phases. Therefore, detecting this phase transition has become an important problem due to scientific meanings and technological viewpoints. Phase pressure–temperature diagram typical for different states of silicon has been established in previous studies [5,6]. Many studies also obtain the melting temperature of amorphous or crystalline silicon systems by experimental observations [7,8] or by using various potential forms in simulation methods [9–13]. However, very few studies have carried out calculations for the melting of silicon on substrates or bordered by other material layers, while silicon adjoining with other material can be seen in many devices [14,15]. The deployment of graphene on top of a silicon waveguide has been used to make the high-speed electro-optical modulators [16,17]. Recently, porous silicon coated with graphene can be used as the stable and high performance electrochemical supercapacitors [18]. Most current silicon-on-insulator devices focus on the sandwich structure [19]. In the present work, we investigate phase transition of the melting of the crystalline silicon in the GSG sandwiches. We choose these sandwich forms because of thermodynamic stability of graphene and its application. In addition, we should also know how the graphene layer affects the melting of silicon. In order to have objective results, we run other simulation (the same as the simulation conditions of the GSG sandwich) with considering only the silicon part in the GSG sandwich, meaning that interaction of C–C and C–Si pairs is excluded. The results of the simulations are compared with each other.

2. Models and simulation methods

The model is the GSG sandwich containing the crystalline silicon part of 3200 atoms and each graphene layer of 1144 atoms (Fig. 1). The distance between the graphene layers and the adjoining silicon surfaces is Δd = 1.36 Å, which is approximate the nearest distance between two silicon atoms along the Z direction. The graphene layers are localized parallel with the (100), (010) and (001) planes of the silicon crystal seen in Fig. 1a, b and c, respectively, .i.e. Names of these models are briefed as the GSG100, GSG010 and GSG001 sandwiches (three numbers subsequent GSG indicating type of the plane). Atoms in the GSG sandwiches interact with each other via the Tersoff/ZBL potential. This

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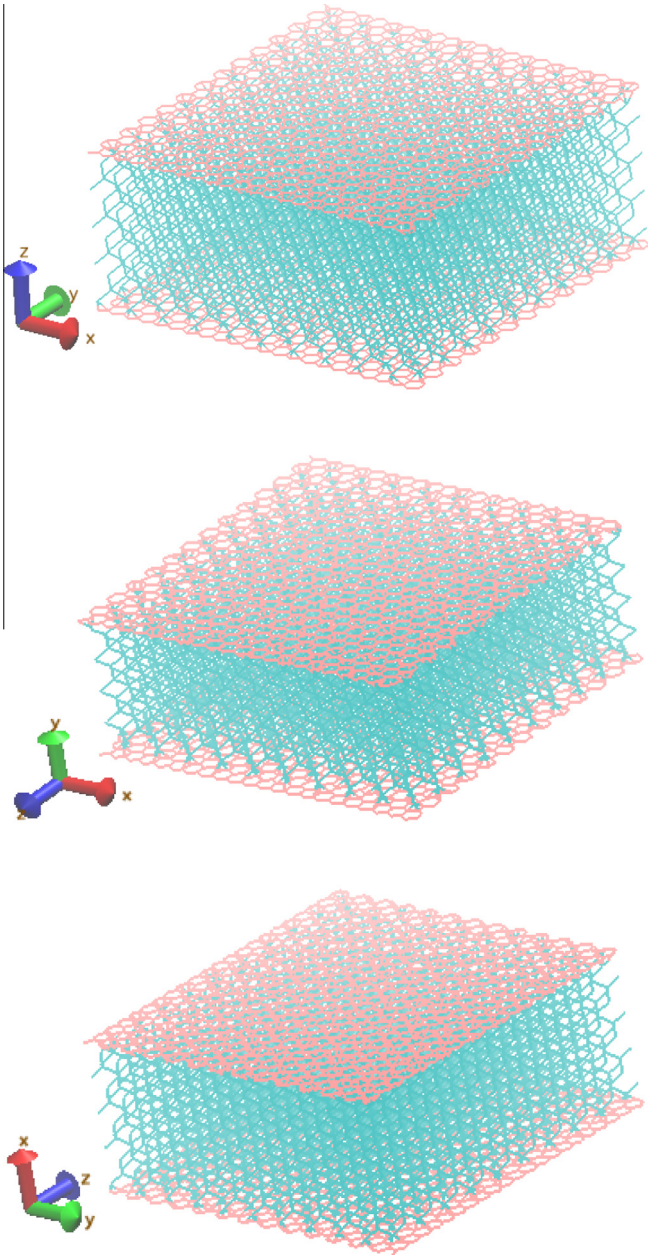

Fig. 1. The GSG sandwich models. From the bottom to the top: the GSG100 sandwich, the GSG010 sandwich and the GSG001 sandwich.

potential includes a 3-body Tersoff potential [20] with a modified part based on a Coulomb potential and the Ziegler–Biersack–Littmark universal screening function [11] having the following form:

$$U = \frac{1}{2}\sum_i \sum_{j\neq i}\left\{[1 - f_F(r_{ij})]U_{ij}^{ZBL} + f_F(r_{ij})U_{ij}^{Tersoff}\right\},$$

$$f_F(r_{ij}) = \frac{1}{1+\exp[-A_F(r_{ij}-r_C)]},$$

$$U_{ij}^{ZBL} = \frac{1}{4\pi\varepsilon_0}\frac{Z_1 Z_2 e^2}{r_{ij}}\phi(r_{ij}/a),$$

$$a = \frac{0.8854 a_0}{Z_1^{0.23} + Z_2^{0.23}},$$

$$\phi(x) = 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x},$$

$$U_{ij}^{Tersoff} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})],$$

$$f_C(r) = \begin{cases} 1 & : \quad r < R - D \\ \frac{1}{2} - \frac{1}{2}\sin\left(\frac{\pi}{2}\frac{r-R}{D}\right) & : \quad R - D < r < R + D \\ 0 & : \quad r > R + D \end{cases}$$

$$f_R(r) = A\exp(-\lambda_1 r),$$

$$f_A(r) = -B\exp(-\lambda_2 r),$$

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-\frac{1}{2n}},$$

$$\zeta_{ij} = \sum_{k\neq i,j} f_C(r_{ik}) g(\theta_{ijk}) \exp[\lambda_3^m (r_{ij} - r_{ik})^m],$$

$$g(\theta) = \gamma_{ijk}\left\{1 + \frac{c^2}{d^2} - \frac{c^2}{\left[d^2 + (\cos\theta - \cos\theta_0)^2\right]}\right\},$$

where r_{ij} is the distance between the atoms i and j, θ_{ijk} is the angle between the vectors $\vec{r}_{ij}$ and $\vec{r}_{ik}$, Z_1 and Z_2 are the numbers of protons in the nuclei of interacting atoms, e is the electron charge, ε_0 is the permittivity of vacuum, a_0 is the Bohr radius, and the value of the other parameters, A_F, r_C, R, D, A, λ_1, B, λ_2, β, n, λ_3, m, c, d and θ_0, can be seen in Ref. [21] or the SiC.tersoff.zbl file of the software package Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).

We use the LAMMPS package to run molecular dynamics simulations. The empty space of $3\Delta d$ is initially added at the two graphene layers of the GSG100, GSG010 and GSG001 sandwiches to create the free surfaces of the systems. The simulations are employed in *NVT* conditions and under periodic boundaries along all the Cartesian dimensions. We use the Verlet algorithm with the simulation time step of $\Delta t = 1$ fs. The models have been equilibrated for 100 ps at $T_0 = 300$ K before heating up. Their temperature is linearly increased via time as $T = T_0 + \gamma_h t$, here $\gamma_h = 4.4 \times 10^{11}$ K/s is the heating rate and t is the heating time.

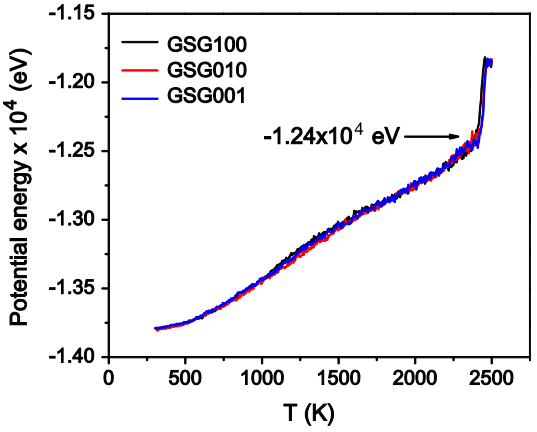

Fig. 2. Temperature dependence of the potential energy of the silicon part in the GSG sandwiches.