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Tight-Binding Quantum Chemistry Molecular Dynamics Study on the Semiconductor Temperature Sensor Materials

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【Introduction】

The temperature dependence of bulk resistance characteristics for semiconductor materials allow the manufacture of simple temperature sensors. Solid-phase crystallization silicon was often used as the integrated heater and feedback temperature sensor due to its easy processing and electrical characteristics diversity. In the present work, a novel methodology based on our original tight-binding quantum chemistry theory was introduced and employed to simulate the temperature dependence of the band gap and electrical conductivity for semiconductor of silicon.

【Method】

Firstly, New-Colors, quantum chemistry dynamics program developed in our laboratory was employed to obtain the crystal structures under various temperatures. In the following, the same program was used to calculate the electronic structures for each obtained crystal structure. Finally, based on the obtained electronic structure information, electrical conductivity for a given system is estimated by Monte Carlo simulation [1].

【Results and discussion】

Semiconductor material investigated in our study is silicon in diamond structure. The calculation model contains 64 atoms and belongs to Fd-3m space group. We first simulated silicon crystal model at 300 K using our molecular dynamics program, New-Colors with total time of 8 ps with a time step of 0.1 fs. With this obtained structure, electronic structure was calculated with New-Colors program. It was found that the HOMO energy is located at –7.288 eV, and LUMO energy is located at –6.122 eV, hence calculated energy band gap for silicon crystal at 300 K is 1.126 eV, which agrees with the experimental value of 1.124 eV. And the obtained density of 2.33 g cm^{-3} for silicon at 300 K is also the same with availed experimental data of 2.33 g cm^{-3}. In the following, silicon structures at 250 K, 350 K, 400 K, 450 K and 500 K are also simulated by New-Colors program. We summarized our band gap results combined with the empirical value in literatures [2,3] in Fig. 1. The trend of energy band gap deceased with increased temperature is qualitively well reproduced. The evaluated electrical conductivities of silicon crystal structure at different temperatures are displayed in Fig. 2. One can find that electrical conductivity of Si linearly increased with temperature. The detailed description will be presented at the conference.

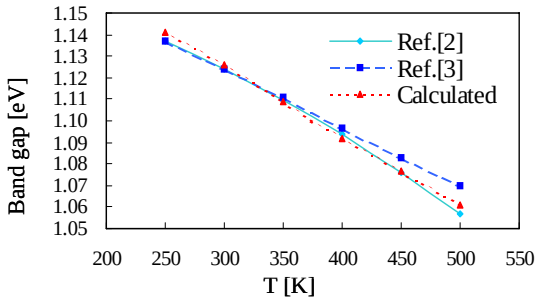

Fig. 1 Temperature dependence of band gap for Si: calculated, data given by [2], data given by [3].

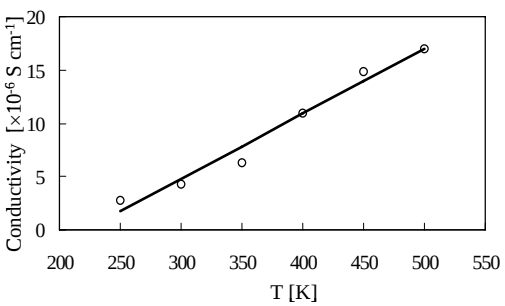

Fig. 2 Calculated temperature dependence of electrical conductivity.

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