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The effect of linear imperfection in [001] direction on the thermal properties of silver crystal

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Abstract
The aim of this investigation was to calculate the thermal properties of silver crystal in the presence of linear imperfection. The simulations were performed by molecular dynamics simulation technique in NPT as well as NVT ensemble based on quantum Sutton-Chen many body potential. The thermal properties including cohesive energy, melting temperature, isobaric heat capacity and thermal expansion of imperfect silver crystal were calculated and compared to those of the perfect crystal. Moreover, the quantities such as radial distribution function, order parameter and lindemann index were calculated in order to obtain information on crystal structure and disorder in atoms. All calculations were done both with liner imperfection in [001] direction and without imperfection at different temperature. The simulation results show that cohesive energy, linear thermal expansion coefficient increase and melting temperature, latent heat of fusion decrease with increasing linear imperfection. Also, the results show that linear imperfection has no effect on the heat capacity.

Keywords: molecular dynamics simulation, liner imperfection, Silver crystal, thermal properties

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