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DISSERTATION INFORMATION

Thesis title:	Investigation of the structure and thermodynamic properties of the two-dimensional germanene material using simulation method
Major:	Engineering Physics
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Abstract

Recently, two-dimensional (2D) materials have been received a lot of attention of the scientific community, especially 2D materials with a band gap such as germanene. However, up to now, publications related to the phase transitions of germanene are still limited. Factors affecting the formation process of this material have not been investigated in detail, and even the phase transition temperature of germanene has not yet been found, the type of phase transition has not yet been determined. Besides, the microstructure, defect types, or the existance of amorphous germanene have not been thoroughly investigated. In this study, the phase transition phase transitions of the 2D germanene are investigated in detail using Molecular dynamics simulation.

First, the formation process of the crystalline 2D material germanene was investigated in detail by cooling from liquid state. Based on the change in thermodynamics and structural properties, the crystallization temperature of 2D germanene is determined about 1340 K, the phase transition exhibits the first type transition. And germanene with a honeycomb structure is found. However, the final hexagonal germanene is not perfect because it contains a few defects such as Stone-Wales and vacancies. This resulting 2D germanene is called polycrystalline 2D germanene.

Besides, the melting process of monocrystalline and polycrystalline 2D germanene is investigated in detail. The melting temperatures of monocrystalline and polycrystalline 2D germanene are different:

1670 K for single crystalline germenene and 1540 K for polycrystalline one. Although the phase transition temperature are different, the phase transition type is the same, both are the first order phase transition. The main defects in the melting process of 2D germanene are Stone-Wales defects.

In addition, the influence of cooling rate on the formation of 2D germanene is investigated in detail. The resulting configuration can be crystalline or amorphous depending on the cooling rate. The results show that the glass phase transition temperature is 1210 K corresponding to the cooling rate of 10^{13} Ks^{-1} . In addition, structure of 2D amorphous germanene obtained at 300 K is analyzed in detail.

Finally, the influence of configuration size on the formation of 2D germanene is investigated. The results show that the configuration size affects the phase transition temperature and some structural properties.

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