Ph.D. DISSERTATION INFORMATION

The Ph.D. Dissertation title: SIMULATION OF MELTING OF THE 2D GLASSY SYSTEMS.

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SUMMARY OF NEW FINDINGS

The success in constructing graphene in 2004, which is a two-dimensional (2D) material, is of great significance in both theory and application, opening a new era for research, fabrication, and development application of 2D systems. The 2D amorphous materials, that combine the benefits of both 2D and amorphous structures, are predicted to be the materials with broad application potential. Up to now, the information about the phase transition of 2D films is mainly observed by the simulation method. The studies show that the melting mechanism of crystalline 2D thin films is affected by the size of the system and the interaction potentials of the atoms in the system. However, information related to the melting of 2D glass is still limited and needs to be investigated.

In this dissertation, the melting of two-dimensional glassy systems, including the monoatomic Lenard – Jones – Gauss and SiC systems, is studied using the molecular dynamics simulation (MD). The temperature dependence of the structural and thermodynamic properties of the systems during heating is analyzed and discussed via the observation of the change in the temperature of potential energy per atom, the radial distribution functions, the coordination number distributions, the ring statistics, the mobility of atoms, and their clustering. The evolution of the model under heating is also analyzed via the tendency to increase mobility and the breaking clusters of atoms upon heating, liquid-like atoms occur/grow.

The dependence on the heating rates and on the size-effect in the melting process of two-dimensional sheets containing Lenard – Jones – Gauss monatomic particles, which interact with each other via Lennard – Jones – Gauss interatomic potential, are investigated. The obtained results indicate that the melting of two-dimensional glassy sheets does not follow any of the previously proposed theories of the melting of two-dimensional crystalline material systems. The melting exhibits a homogeneous nature, i. e. liquid-like atoms appear uniformly throughout the model, and the melting process further leads to the formation of an entire liquid phase. Besides, the obtained results also show that the structural properties of the obtained models are almost not different when using two different heating rates. The melting temperature range is defined from 0.2 to 0.8 (in reduced units). In the melting temperature region, the structural and thermodynamic properties of the systems change sharply with increasing temperature. The glassy transition temperature T_g increases with increasing the size of the systems. This behavior can be observed clearly for small-size models (number of atoms in the models ≤ 3600). When the size of the models is large enough (i.e number of atoms in the models > 3600), the glassy transition temperature T_g is no longer affected.

Glassy SiC nanoribbons (NRs) are studied for modeling, melting, and effect of free edge on the meting. Firstly, modeling of glassy SiC nanoribbons by rapid cooling of the SiC liquid from 8000 K to 300 K is carried out. Two separate molecular dynamics simulations are performed, one using the Tersoff potential and the other using the Vashishta potential. The obtained results show that, compared with the Vashishta potential, the Tersoff potential is more suitable to obtain the glassy SiC on rapid cooling. Unlike the melting of crystalline nanoribbons, which begin to melt from the free edges, the melting of glassy nanoribbons is not affected by the free edges. The melting behavior of the glassy nanoribbons is similar to that of the 2D sheets, liquid-like atoms appear uniformly throughout the model until the whole system completely melts during heating. Transition temperature range and the size-effect on the melting of the glass SiC nanoribbons were found upon heating the obtained nanoribbons.