Molecular Dynamics Simulation of Elastic and Temperature Waves Propagation in Graphene Crystal

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The procedures to determine propagation velocities of elastic and temperature waves in a graphene plate have been developed using the molecular dynamics (MD) simulation method. The propagation velocities of the elastic rarefaction (sound) and temperature waves have been determined in the 10-1000 K temperature range in the «Zigzag» and «Armchair» directions of a graphene plate.

Four control and measurement volumes have been selected in graphene plate to determine propagation velocity of elastic and temperature waves (Fig.1). A small tensile deformation has been specified through imparting an initial pulse for all atoms of V1 volume in the negative X direction. Correspondingly, a weak rarefaction wave begins to propagate at the sound velocity in the positive X direction over the graphene plate. The arrival time of rarefaction wave in the V2, V3 and V4 volumes was used to calculate its propagation velocity. Likewise, to determine the temperature perturbation propagation velocity, in V1 volume the constant temperature T_1 has been specified and the arrival time of temperature perturbation has been measured in volumes V2, V3 and V4. The Brenner potential was used for the calculation of interatomic interaction between carbon atoms [1]. The MD simulation was performed using the LAMMPS code [2].

A propagation velocity of elastic rarefaction wave of $C_0 = 21.3\ km/s$ was obtained for the «Armchair» direction. In the temperature range of graphene plate 10-1000 K the propagation velocity of elastic rarefaction wave does not change substantially. A propagation velocity of elastic rarefaction wave in the «Zigzag» direction of $C_0 = 21.9\ km/s$ was also obtained. Over the same temperature range it was found that this value did not change substantially either.

The temperature perturbation velocity has been calculated at two initial graphene plate temperatures 0 and 300 K. The atoms' temperature in the boundary volume V1 in both calculation versions was taken identical and was equal to $T_1 = 1000\ K$. The temperature perturbation propagation velocities calculated using the proposed method have the following values: at the plate temperature 0 K – 20.4 km/s, at the plate temperature 300 K - ~7 km/s.

Using MD simulation method the graphene plate temperature of destruction was explored (Fig.2). Results of MD simulation have shown that the graphene plate is destroyed at the temperature ~ 6500 K.

Based on the MD simulation methodology, techniques for calculating graphene plate thermal conductivity were developed also. The computational curves were derived for the dependence of thermal conductivity of a single-layer graphene plate on the plate length in the heat flux propagation direction, as well as at different mono-vacancy concentrations and plate temperatures.

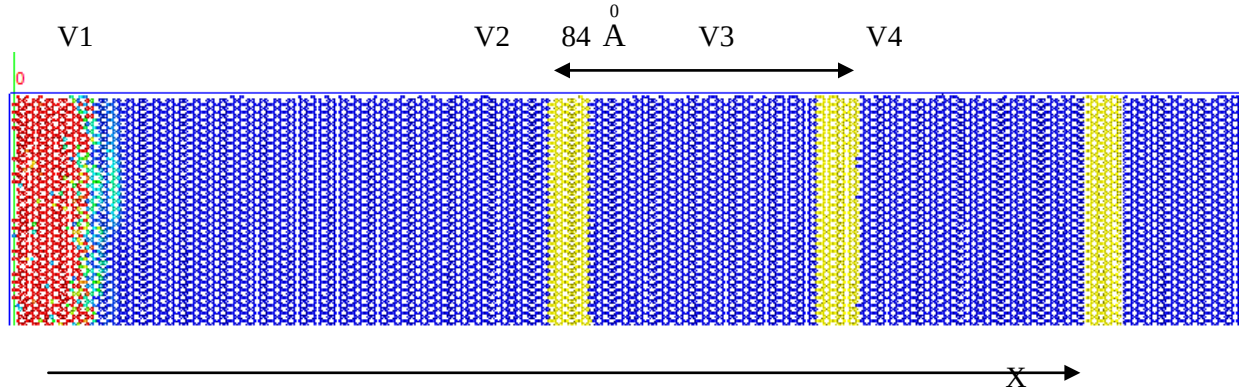

Figure 1. The MD calculation cell to determine propagation velocity of elastic and temperature waves in graphene plate .

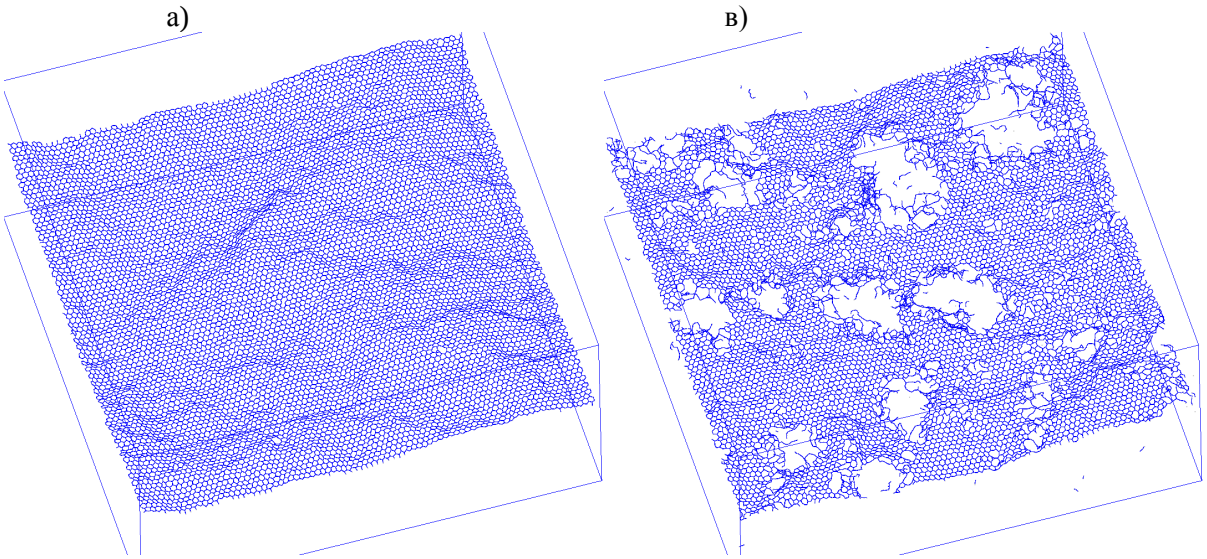

Figure2. The state of graphene plate at the temperature: а - 5900 K and в - 6700 K.

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References

[1] D.W. Brenner, O.A.Shenderova, J.A. Harrison, S.J. Stuart, and S.B. Sinnot, J. Phys.: Condens. Matter 14, 783 (2002).
[2] http://lammps.sandia.gov.