Molecular Dynamics Simulation of the Pressure Effect on Melting Temperature of HE Molecular Crystal

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Using molecular dynamic (MD) simulation method we have developed the technique for determination of melting temperature dependence on pressure for molecular crystals of some high explosives (HE). The dependencies of melting temperature on pressure were determined for molecular crystals of RDX, HMX and PETN.

We used the approach that was proposed in Ref. [1] to carry out MD simulation of HE molecular crystal melting. Interatomic interaction was calculated using force field developed in Ref. [2]. The computer code LAMMPS [3] was used to perform MD simulation. The melting point of HE molecular crystals at various pressures was determined as a point of discontinuity of the total potential energy dependency on temperature. Fig. 1 shows one of the results of MD simulation of melting process of RDX crystal (hexahydro-1,3,5-trinitro-1,3,5-s-triasine).

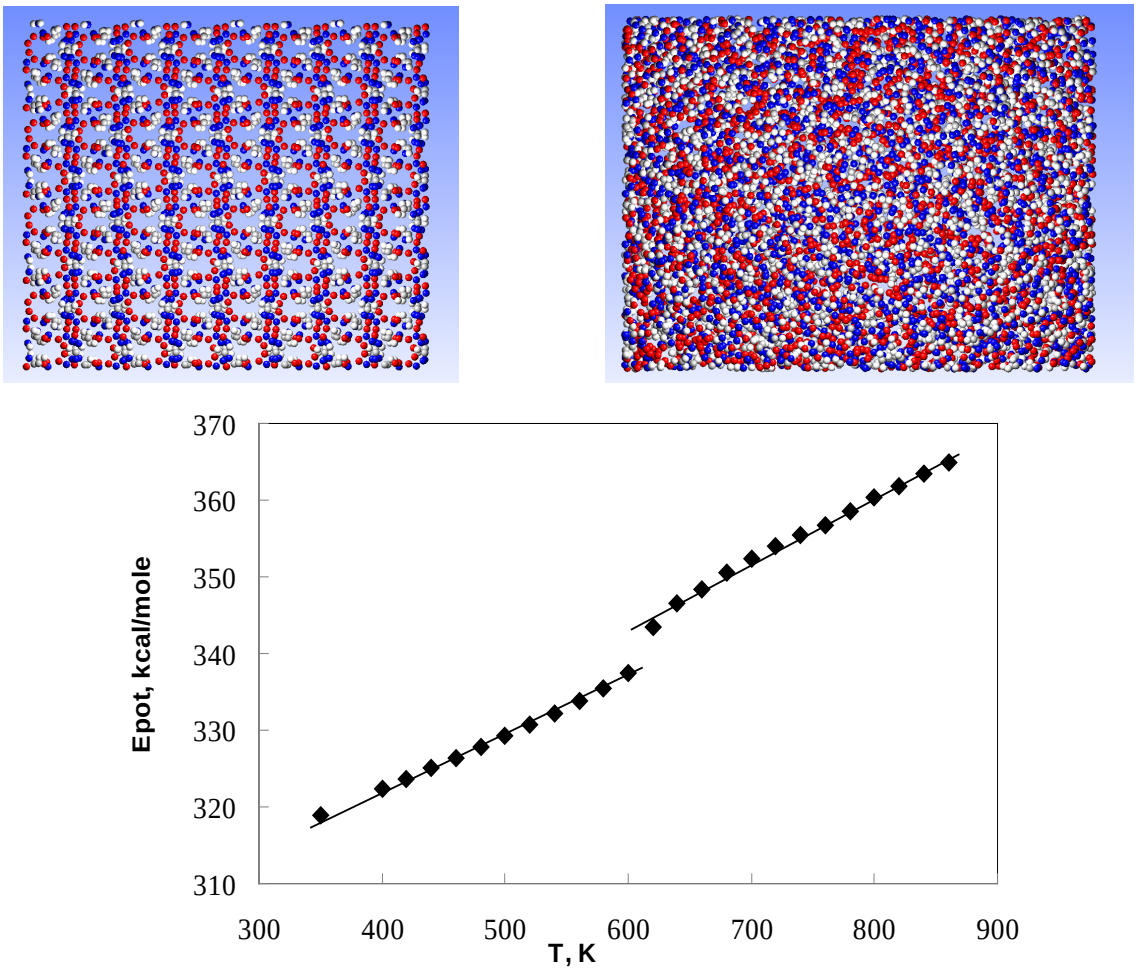

Figure 1. The dependence of potential energy of RDX crystal on temperature

Figure 1 shows the dependence of potential energy of RDX crystal on temperature and a state of RDX crystal lattice (coordinates of atoms) before melting and after crystal melting. Latent heat of melting was estimated using change of specific volume and potential energy of molecule in a melting point.

Figure 2 shows the dependence of RDX crystal melting temperature increment on pressure that was obtained by MD simulation method.

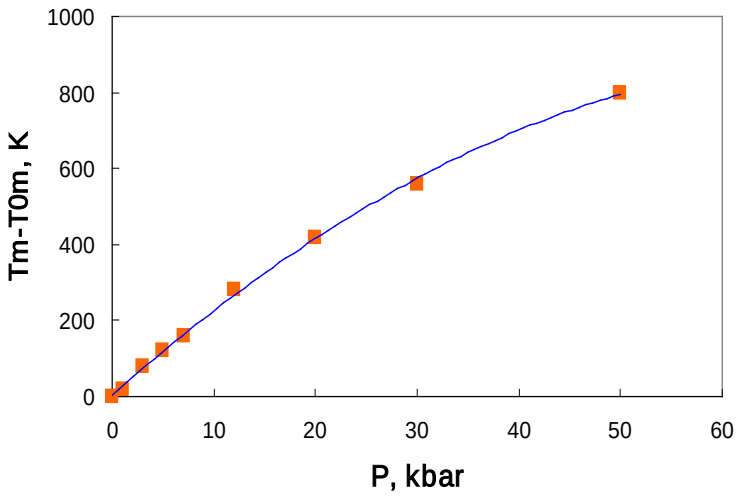

Figure 2.The dependence of melting temperature increment of RDX crystal on pressure

The dependence of melting temperature of RDX crystal on pressure has been calculated also using the Lindemann theory [4]. The comparative analysis of the obtained data has shown that the MD simulation results and the results obtained using the Lindemann theory agree well.

The dependence of Hugoniot temperature on shock pressure has been calculated for molecular crystals RDX, HMX, and PETN also. The comparative analysis of Hugoniot temperatures and melting temperatures showed that melting temperature always essentially greater than Hugoniot temperature at the same pressure.

Thus, from the obtained results it is possible to make conclusion that the aggregate state of the considered HE molecular crystals behind of a shock wave front does not transfer in a liquid phase up to detonation pressure.

Acknowledgment

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References

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