Two types of atoms' collective motions in crystals

Negodin V D[1,2,@], Fleita D Iu[1,2,3] and Norman G E[1,2,3]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
[3] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

[@] vdnegodin@gmail.com

The work is devoted to the study of the collective motion of atoms in crystals of Lennards-Jones systems using the method of molecular dynamics. We continue started in [1] analysis of pair correlator

$$\mathrm{CC}(T,R,\tau)=\left\langle \frac{[\mathbf{r}_i(t+\tau)-\mathbf{r}_i(t)]\cdot[\mathbf{r}_k(t+\tau)-\mathbf{r}_k(t)]}{|\mathbf{r}_i(t+\tau)-\mathbf{r}_i(t)|\cdot|\mathbf{r}_k(t+\tau)-\mathbf{r}_k(t)|}\right\rangle_R = \\ =\langle\cos\varphi\rangle_R, \quad (1)$$

which characterizes correlation of atoms motions. Here $\mathbf{r}_i(t)$, $\mathbf{r}_k(t)$ are the radius-vectors of atoms i and k located at a distance from interval $[R-\delta, R+\delta]$ at the initial time t. Brackets $\langle\ldots\rangle_R$ means collecting the CC values statistics over all selected pairs of atoms. We plotted histograms of correlator values and extrapolated them to zero temperature. This allowed us to distinguish two parts of collective motions of atoms in crystals. The first part, the phonon one, is temperature independent and is a cause of high CC values in crystals in comparison with liquid. The second part is related to interaction potential anharmonicity, crystal lattice imperfection, and defects. The second part depends on temperature. The increase of CC values with temperature in crystals is under consideration.

[1] Negodin V, Polyachenko Y, Fleita D, Pisarev V and Norman G 2021 *Journal of Molecular Liquids* **322** 114954