Collective motion of atoms in solids

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

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

(1)

which characterizes correlation of particle motion. Here $\mathbf{r}_i(t)$, $\mathbf{r}_k(t)$ are the radius-vectors of particles i and k located at a distance $R \pm \delta$ at the initial time t. Brackets $\langle \ldots \rangle_R$ means averaging over all selected pairs of particles.

We found that the correlations in crystals is much greater than in liquids. The temperature dependence CC(T) demonstrates the hysteretic behavior varying along the isochore. Correlator values are higher in crystal with defects than in pure one. In addition, its values increase during phase transitions and crystal lattice reorganizations. Radial dependence CC(R) exhibits crystal structure in more sensitive way than radial distribution function.

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