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Journal of Experimental and Theoretical Physics 2015 vol.121 N5, pages 828-843

Short-range order and dynamics of atoms in liquid gallium

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Abstract

© 2015, Pleiades Publishing, Inc. The features of the microscopic structure, as well as one-particle and collective dynamics of liquid gallium in the temperature range from T = 313 to 1273 K, are studied on the p = 1.0 atm isobar. Detailed analysis of the data on diffraction of neutrons and X-rays, as well as the results of atomic dynamics simulation, lead to some conclusions about the structure. In particular, for preset conditions, gallium is in the equilibrium liquid phase showing no features of any stable local crystalline clusters. The pronounced asymmetry of the principle peak of the static structure factor and the characteristic “shoulder” in its right-hand part appearing at temperatures close to the melting point, which are clearly observed in the diffraction data, are due to the fact that the arrangement of the nearest neighbors of an arbitrary atom in the system is estimated statistically from the range of correlation length values and not by a single value as in the case of simple liquids. Compactly located dimers with a very short bond make a significant contribution to the statistics of nearest neighbors. The temperature dependence of the self-diffusion coefficient calculated from atomic dynamics simulation agrees well with the results obtained from experimental spectra of the incoherent scattering function. Interpolation of the temperature dependence of the self-diffusion coefficient on a logarithmic scale reveals two linear regions with a transition temperature of about 600 K. The spectra of the dynamic structure factor and spectral densities of the local current calculated by simulating the atomic dynamics indicate the existence of acoustic vibrations with longitudinal and transverse polarizations in liquid gallium, which is confirmed by experimental data on inelastic scattering of neutrons and X-rays. It is found that the vibrational density of states is completely reproduced by the generalized Debye model, which makes it possible to decompose the total vibrational motion into individual contributions associated with the formation of acoustic waves with longitudinal and transverse polarizations. Comparison of the heights of the low-frequency component and of the high-frequency peak in the spectral density of vibrational states also indicates a temperature of T ≈ 600 K, at which the diffusion type of one-particle dynamics changes to the vibrational type upon a decrease in temperature. It is demonstrated that the modified Einstein–Stokes relation can be derived using the generalized Debye model.

http://dx.doi.org/10.1134/S1063776115110072