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Universality of Microscopic Structural and Dynamic Features in Liquid Alkali Metals near the Melting Point

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The assumption proposed in [U. Balucani et al., Phys. Rev. B **47**, 3011 (1993)] that the space and time dependences of the characteristics of the microscopic structure and dynamics for the group of liquid alkali metals are reduced to a common general form through scaling transformations has been discussed. It has been found that such description is possible when scale units are (i) the effective size of a particle corresponding, in particular, to the experimentally measured position of the main peak in the static structure factor, (ii) the characteristic time scale of the thermal mean free path of the particle, and (iii) the parameters of the "liquid"–"crystal" phase separation (in particular, the melting temperature). This conclusion follows directly from the comparative analysis of experimental data on X-ray diffraction, as well as on the inelastic neutron and X-ray scattering data. This work develops the ideas proposed in [A. V. Mokshin et al., J. Chem. Phys. **121**, 7341 (2004)].

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The statement that microscopically structurally dynamic features of liquids of a certain type (groups of liquefied inert gases Ar, Ne, Kr, Xe; groups of liquid single-component semiconductors with the same coordinate number, e.g., Ge, Si; liquid alkaline earth metals Be, Ca, Mg, Sr; liquid alkali metals; etc.) are universal for this type appears to be not so unambiguous as one could expect. This is most clearly seen in the case of ambiguous treatment of experimental data and results of molecular dynamics simulation for liquid alkali metals, which are typical representatives of the class of simple liquids [1–3].

According to the general concepts of the molecular kinetic theory, it is reasonable to expect that the general character of the interaction between particles in systems of a certain type in identical (equilibrium) thermodynamic phase states should generate a similar structure as well as the single-particle and collective dynamics of a similar character. These concepts underlie the development of theories (usually microscopic) for the description of microscopic dynamics, where one of the key input parameters is the potential of interaction between particles (as was done, e.g., for liquid alkali metals in [4]). It is remarkable that the molecular dynamics simulations [1] for liquid alkali metals (Na, K, Rb, and Cs) near the melting point with the Price–Singwi–Tosi model pseudopotential also indicate that static and dynamic structural correlations for all alkali metals are universally scaled. Earlier attempts at testing the manifestation of such "universality"[1] with theoretical and molecular dynamics considerations were reported in [5–9]. Nevertheless, the most reliable evidence of correctness of these considerations and conclusions could be their confirmation by experimental data. This became possible owing to the development of technique of inelastic X-ray scattering [10]. This technique allows obtaining the corresponding experimental data for liquid lithium [11], sodium [3, 12, 13], and potassium [14, 15] and, thereby, supplementing previous experimental results obtained with the inelastic neutron scattering for liquid potassium [16], rubidium [17], and cesium [18]. It is noteworthy that all these measurements provided the dynamic structure factor $S(k,\omega)$, which contains information on the structure and collective dynamics of particles with the characteristic time $t = 2\pi/\omega$ and spatial $\ell = 2\pi/k$ scales (here, ω and k are the frequency and wavenumber, respectively). Furthermore, an important feature of these experiments is that they were performed for melts at temperatures near the melting point (see Table 1). For this reason, the thermodynamic phase state of systems can be characterized by only the reduced temperature T/T_m, where T_m is the melting temperature of the corresponding system (see Table 1).

Comparing experimental spectra of the dynamic structure factor [2, 3, 19] and features of these spectra

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[1] Corresponding to the so-called "principle of corresponding states" [1].