Universal Structural and Dynamic Features in Metals Near Their Melting Points

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Abstract. The results of a comparative analysis of experimental data for the equilibrium properties and characteristics of liquid alkaline earth (magnesium, calcium, strontium), alkaline (lithium, sodium, potassium) and transition metal groups: elements of the subgroups of nickel (Ni, Pd, Pt) and copper (Cu, Ag, Au) near their melting points are presented. Reduced spatial \( r/r_m = r_k m / \pi \) and time \( t/t_m = t_k m / \sqrt{\beta} \) scales, in which \( r_m \) is the first peak position of the static structure factor \( S(k) \) and \( \beta = 1/k_B T \) is the inverse temperature, are introduced as the basis for the law of corresponding states. Based on these scale transformations and x-ray diffraction analysis, it was found that the groups of liquid alkaline, alkaline earth, and transition metals are described by universal \( r \)- and \( k \)-dependencies. It has been established that the dispersion law of longitudinal polarization \( \omega_c(k) \), given in accordance with these scale relations, for elements of groups of liquid alkaline, alkaline earth and transition metals has a single universal character. An analysis of the properties of three groups (alkaline, alkaline earth and transition) liquid metals using scale transformations shows that the law of the corresponding states is valid for these substances.

1. Introduction

The problem of a universal description of the structural and dynamic properties of various groups of liquids is relevant for modern condensed matter physics [1]. On the one hand, this would avoid the difficulties associated with the extraction of experimental information. The fact is that almost until recently, the properties of microscopic collective and single-particle dynamics were experimentally studied mainly by the method of scattering of slow neutrons. In this case, various difficulties arose, firstly, with the separation of collective and single-particle contributions, and, secondly, with the presence of significant experimental errors in some \((k,\omega)\)-regions, sometimes leading to the impossibility of extracting reliable experimental information. On the other hand, the possibility of describing in a unified way the properties of various groups of liquids would make it possible to create a universal microscopic theory of the liquid state.

In this paper, based on an analysis of experimental data [2-6] and the principle of the corresponding states [1], we consider the possibility of a unified description of the structural features and microscopic dynamics of various groups of metals (alkaline, alkaline earth and transition metals).

2. The law of corresponding states for liquid metal melts

In accordance with the principle of corresponding states, the equilibrium properties of various groups of liquids can be described in a certain universal way [3]. Here, the main problem is only in
choosing a certain set of scaling transformations, for example, for such parameters and characteristics of the systems under study as temperature, density, spatial and frequency characteristics [4-6]. To compare the structural and dynamic properties of various groups of metals (alkaline, alkaline earth and transition metals) near their melting point \((T/T_m \approx 1)\), we use scale transformations proposed by us in Ref. [3]. Let us choose as the unit of the spatial scale the value \(r_m = 2\pi k_m\), which corresponds to the average interatomic distance in the system; here \(k_m\) is the first peak position of the static structure factor \(S(k)\). As a unit of the time scale, let us consider the value \(t_m = t/k_m\), where \(m\) is the mass of the particle, and \(\beta = 1/k_BT\) is the inverse temperature. Note that the value \(t_m\) is nothing but the mean free path of a particle on the length scale \(l = 2\pi k_m\). Therefore, the value \(\omega_m = 2\pi/t_m\) will represent the frequency scale. We have calculated the characteristics presented above for the systems under study near their melting points on the basis of experimental data on neutron diffraction and X-ray diffraction analysis [2-6]. The calculated values of parameters and characteristics for the studied systems are presented in table 1.

**Table 1: A set of reduced physical parameters for the systems under study.**

|                 | \(T_m(K)\) | \(\rho_m(g/cm^3)\) | \(m(10^{-24}g)\) | \(T/T_m\) | \(k_m(\AA^{-1})\) | \(r_m(\AA)\) | \(t_m(10^{-14}s)\) |
|-----------------|-------------|---------------------|-----------------|----------|-----------------|------------|-----------------|
| **Alkali metals** |             |                     |                 |          |                 |            |                 |
| Li              | 453.70      | 0.534               | 11.50           | 1.021    | 2.503           | 2.51       | 5.29            |
| Na              | 371.00      | 0.971               | 38.20           | 1.019    | 2.001           | 3.14       | 13.32           |
| K               | 336.35      | 0.856               | 64.90           | 1.019    | 1.599           | 3.93       | 23.14           |
| Rb              | 312.64      | 1.532               | 141.9           | 1.002    | 1.500           | 4.19       | 37.79           |
| Cs              | 301.55      | 1.873               | 221.0           | 1.005    | 1.441           | 4.36       | 50.08           |
| **Alkaline earth metals** |         |                     |                 |          |                 |            |                 |
| Mg              | 923.0       | 1.740               | 40.374          | 1.032    | 2.400           | 2.62       | 7.30            |
| Ca              | 1115        | 1.540               | 66.575          | 1.007    | 1.950           | 3.22       | 10.63           |
| Sr              | 1050        | 2.640               | 145.55          | 1.003    | 1.780           | 3.53       | 17.78           |
| **Nickel subgroup elements** |         |                     |                 |          |                 |            |                 |
| Ni              | 1728        | 8.90                | 97.497          | 1.026    | 3.100           | 2.03       | 6.45            |
| Pd              | 1828        | 12.0                | 176.18          | 1.014    | 2.780           | 2.26       | 9.46            |
| Pt              | 2041        | 21.5                | 324.06          | 1.006    | 2.750           | 2.28       | 12.29           |
| **Copper subgroup elements** |       |                     |                 |          |                 |            |                 |
| Cu              | 1358        | 8.96                | 105.56          | 1.048    | 3.00            | 2.09       | 7.73            |
| Ag              | 1235        | 10.5                | 179.18          | 1.031    | 2.60            | 2.42       | 12.28           |
| Au              | 1337        | 19.3                | 327.19          | 1.064    | 2.65            | 2.37       | 15.40           |

Experimental data on neutron diffraction and X-ray diffraction analysis for the static structure factor \(S(k)\) of alkali metallic melts (except for francium), alkaline earth (magnesium, calcium, and strontium), and transition (nickel, palladium, platinum, copper, silver, and gold) metals near their melting points \((T/T_m \approx 1)\) [2] are presented in Fig. 1a. Here, \(S(k)\) is a function of the reduced wave number (in units of \(k/k_m\)). As can be seen from the figure, all experimental data can be described by the universal dependence on reduced wave number. In Fig. 1b shows the pair correlation functions \(g(r)\), given in accordance with the values from Table 1. As can be seen from the figure, the reduced pair correlation functions for the systems under consideration are collapse onto a universal master curve.

Raw experimental and reduced longitudinal dispersion curves for liquid melts of alkali, alkaline earth and transition metals are shown in Figs. 2a and Fig. 2b, respectively. As can be seen from the figure, the dispersion curves in the reduced form for all the systems under study are described by a universal master curve. Thus, the results presented in this work testify to the validity of the law of the corresponding states for various groups of liquid metals. It is gratifying that the equilibrium characteristics for liquid alkali, alkaline earth and transition metals can be described by universal
dependencies. This conclusion provides a basis for understanding the mechanisms of microscopic processes in various groups of liquids from a unified standpoint and is some prerequisite to creation of a unified theory of the liquid state.

**Figure 1.** Structural characteristics [$S(k)$ and $g(r)$] for liquid alkaline, alkaline earth and transition (elements of nickel and copper subgroups) metals in reduced units: $r_m = 2\pi/k_m$, where $k_m$ is the maximum position in $S(k)$ [2].

**Figure 2.** Longitudinal dispersion curves for liquid alkaline, alkaline earth, and transition metal groups in absolute (a) and reduced (b) units (where $\omega_0 = 2\pi k_m\sqrt{k_B T/m}$).
3. Conclusions
An important result of the present work is the possibility of a single description of the structural features and dynamic processes of metals near their melting point (groups of alkaline, alkaline earth and transition metals). Based on experimental data on neutron diffraction, X-ray analysis [2] and scale transformations, it was shown that the structural properties of groups of liquid alkaline, alkaline earth, and transition metals near their melting temperatures are characterized by universal features. Thus, the reduced forms of the pair correlation function \( g(r) \) and the experimental quantity – the static structural factor \( S(k) \) for elements of the group of alkali, alkaline earth, and transition metals are described by uniform \( r \)- and \( k \)- dependencies. It is shown that the longitudinal dispersion curves, given in accordance with scale transformations, for the systems under consideration have a single universal character. The results presented in this work indicate the validity of the law of the corresponding states for various groups of liquid metals.

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