Electron and phonon spectra dynamics and features of phase transitions in sodium at P=0-100 GPa

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Abstract. An electron and phonon spectra dynamics, features of structural phase transitions, and melting of sodium under the pressure ranging from 0 to 100 GPa are investigated. The electron and the phonon spectra of crystal sodium are calculated ab initio within the density functional theory by means of the software package LmtART-7 (see [1-3] and references herein), allowing the fully potential method of linear muffin-tin orbitals (FP-LMTO method). Earlier, this method was used in papers [4-6] for the calculation of a metals band structure within an atomic-spheres approximation (LMTO-ASA method). Using the Lindemann measure and the calculated phonon spectra, the theoretical values of melting points corresponding to the experimental data are obtained. Features of the electron and the phonon spectra dynamics in the melting curve maximum vicinity and within the structural transition range are discussed for cI2 \rightarrow cF4.

1. Introduction

Modern methods of research of a structure of substances with high pressures [7, 8], allow us to reveal not simple behavior of simple metals (e.g. see reviews [9-12] and references therein). Firstly, a low-symmetric and incommensurate host-guest of crystal structures arose from structural phase transitions. Secondly, it is the abnormal character of melting curves T_m(P), showing an existence of the maxima and the minima, and also – the sites in the curve with dT_m/dP < 0 [13, 14]. Thirdly, it is the superconductivity [15, 16] and the transitions of metal-to-semiconductor [17] and semiconductor-to-metal [18] in Li, and the transition of metal-insulator in Na [19].

In experiments [13, 14] the anomalous behavior of the melting curve T_m(P) of sodium was revealed: the maximum of T_m = 1000 K with P=30 GPa and its subsequent falling to room temperatures at P = 118 ± 120 GPa (see curves 1 and 2 designated in Fig. 1a by star symbols at Fig. 1). The negative melting slope of sodium is within the pressure range, in which the stable solid structures are known to be a body-centered cubic (b.c.c. or cI2 in Pearson notation [20]) and to be a more compact face-centered cubic (f.c.c. or cF4 in Pearson notation [20]) above 65 GPa [21]. Under higher pressure of P = 115 GPa, after transition from cF4 to a lower symmetric cubic structure with a 16-atom cell (cI16) [13, 21], the melting temperature is T_m = 300 K, which is lower than that at a normal pressure 371 K. See also Fig. 1a, where the sodium structure in the melting curve minimum vicinity, according to the crystallographic researches of the authors of [14], is shown in a boxed insert.
It can be seen, that the transition range from crystal structures cI16 and oP8 at $P = 118$ GPa and $T = 296.6$ K to the liquid with the diffuse nature of X-ray radiation scattering equals to $\Delta T = 9.4$ K temperature interval. Herein, within the range of $296.6 \leq T \leq 301.4$ K, the sodium structure represents a mixture of crystal structures - a tetragonal tI50 and a rhombic oC120 containing 50 and 120 atoms in unit cells, respectively, and within the range $301.4 \leq T \leq 306$ K – a monoclinic structure mP512 containing 512 atoms in the cell. Therefore, one may assume that the transition range, bounded from the bottom by the melting curve passing through (306 K, 115 GPa), (296.6 K, 118 GPa), (306 K, 119.4 GPa) points, and from the top by a liquid melt, represents rather a polycrystal amorphous body (see [24]), than a mono - or a polycrystalline body. Along the line $T_c = 306$ K, both a density and a volume of the liquid are non-uniform. Thus, the derivatives $\partial V_{cm} / \partial P|_{T=const}, \partial V_{sm} / \partial P|_{T=const}$ are negative and cross each other at $P = 118$ GPa, where $V_{cm} = V_{sm}$.

Figure 1. Left (a): Points (1, 2 - stars) - Na melting temperature experimental values according to [13]; curve 3 - our approximation of [13] data within the range $0 \leq P \leq 64.5$ GPa; curve 4 - melting temperature calculated values, obtained in previous paper [22] where genuine two-phase equation of state was used; points (5, diamonds) - melting temperature calculated values, obtained in current paper (onward introduced); triangles (6) represent crystalline sodium relative atomic volume and its structure variations at pressure rise [13, 14, 23]. On a boxed insert part of the melting curve minimum is shown with transition range structures being indicated according to [14]. Horizontal dash line (7) corresponds to $T_m$ within transition range cI2 → cF4, where $V_m \approx V_{lm}$; line (8) corresponds to $T_m$ of Na having cI16 structure (see boxed insert); line (9) corresponds to the temperature, below which sodium stays in crystalline state with structure, marked on figure with vertical dashed lines; (10) - range, corresponding to the melting curve minimum, where Na liquates from being solid. Right (b): First (1) and second (2) approximation (curve 3 on Fig. 1a) derivatives.

It should be mentioned, that since a cesium melting curve anomalous behavior has been experimentally discovered in 60's of the 20th century [25, 26] (see also reviews [27, 28] and the references therein), numerous attempts of its theoretical explanation have been performed: e.g. see [29-34]. In papers [29-31] the solid-liquid transition is considered as an order-disorder transition within a Lennard-Jones and Devonshire model of liquids [35, 36] under Bragg-Williams approximation which is technically applicable to alloys (solutions) only. Despite the faint applicability of Lennard-Jones and Devonshire theory and Bragg-Williams approximation for simple monoatomic liquids, such as melts of alkali metals (see some reasonable criticism of the theory in Ya.I. Frenkel's book [37]), in the noted papers, a qualitative confirmation of a chance of a maximum emergence resulting from a long-range order deviation in solids has been obtained. For the cause of maximum formation on melting curve papers [32-34] calls repulsive potential and its softness to attention and also point at possible dependence of the vicinity. I. e. the repulsive potential probable relation to the near-order local structure of a solid metal and its melt. The paper [38] should also be noted, since it
reports that the substance model used in [29-34] cannot provide any clear statement for the melting curve abnormal behavior. The authors of [38] rather convincingly showed the possibility of a model fluid, with only one type of a local structure, to have a wide features range of melting, structural transitions in solids under condition of interparticle repulsion extreme softening, leading to the nearest neighbors division reduction. In other words, the extreme softening of the interparticle repulsion promotes the fluid clustering (a polycluster amorphous body in terms of A.S. Bakai [24]). For the extra proof, let’s consider a liquid phenomenological model suggested in our papers [22, 39]. According to the model, a liquid consists of the clusters having a quasicrystal short-range ordering and an intercluster space occupied with a monoatomic gas (the monoatomic clusters). A sodium melting curve (see curve 4 on Fig. 1a) and a curve of the pressure relative change in the course of melting (see curve 2 on Fig.2a) were obtained within a two-phase approximation. A comparison with experimental data shows, that up to 15 GPa, a good coincidence between theoretical and experimental melting curves is observed. The melting temperature growth deceleration and the volume jumped reduction acceleration is observed under increasing pressure. However, this fact is not sufficient for gaining a zero-value volume jump at $P = 28.3$ GPa. See for example curve 3 in Fig. 3a (marked with stars), we obtained the extrapolation to zero for the experimental data represented in [28] (the curve 1 marked with triangles in Fig. 2a). In our estimation, it was concerned both the actual two-level model and the identical number of atoms in clusters, thus not allowing to obtain a denser, in comparison with a solid body, packing of atoms in its melt, which was observed on the sites of the melting curve with a negative slope.

**Figure 2.** Left (a): Relative volume variation of Na while melting within the range I-1 according to experimental date from [28] - triangles (1), our calculations from [22] - diamonds (2) and our extrapolation to zero of data provided by [28] - stars (3). Right (b): Relative volume of solid and liquid sodium qualitative behavior versus pressure according to the experimental data and our interpolation (see Fig. 2 (a)).

At present time, in order to describe the melting curves behavior, the so called ab initio methods are used, in which forces acting on atoms enforcing them to gain their instantaneous arrangement (well-ordered or not) are computed within quantum dynamical methods [40-47]. For example, the ab initio molecular dynamics simulation of Na solid and liquid phases has been carried out in papers [40, 41] reporting about the coherence between a structure and a density and determining the reasons of the melting curve negative inclination. In papers [42, 43, 45], the explanation of sodium melting is suggested via ab initio calculations of the phonon spectrum and the mean square deviation of atoms, where only the matter solid phase properties are used. The cited papers show the rebuilding of sodium with an essential role of the phonon spectrum in a melting curve abnormal character within a single-phase approximation, using the well-known Lindemann measure as the melting criterion. In our opinion, little attention is payed to the analysis of the lattice atomic zero fluctuations contribution, to the features of a melting curve behavior, because under pressure, the lattice atomic zero fluctuation
energy increases. Thus, close to zero temperatures, the equilibrium locations of atoms may not coincide with the ideal lattice nodes. In favor of this assumption, it is possible to deduce the c16 equilibrium crystal structure, which can be a superposition of eight c12 cells, however atoms of the latter would not reside in nodes of it.

The analysis is also necessary because the anomalous behavior of melting curves under increasing pressure may occur not only with alkali metals, but also with other metals, including noble and transitional, but under significantly greater pressure values. For instance in [48], the structural transition in Au from a cubic centered (fcc) to a hexagonal-close-packed (hcp) structure at \( P = 240 \) GPa has been found experimentally; the same transition for Al at \( P = 217 \pm 10 \) GPa has been observed in [49]. The theoretical paper [50] suggested possibility of existence for Al of an incommensurate host-guest (h-g) structure Al16-I4/mcm at \( P = 3.2 \pm 8.8 \) TPa being similar to the incommensurate host-guest structure of phase IVa of barium.

The objective of the current paper is a careful analysis of the electron and phonon spectra dynamics and the lattice atomic zero fluctuation contribution to the c12\( \rightarrow \)cF4 structural transition features and the melting curve behavior for sodium within the pressures range from 0 to 100 GPa.

2. Calculation method

We used the LMTART-7 software package [2, 3] for the ab initio phonon and electron spectra determination, as well as of the total interaction energy between the electrons and the sodium nuclei. The dynamics of a lattice was computed using a linear response method within a well-known density functional theory (see details of the method in the reviews [51-53]) by LMTART-7. The exchange-correlation potential (Vosko-Wilk-Nussair) [54] was considered in a generalized gradient approximation [55]. We used a pseudo-potential method in the plane wave expansion (PLW). The PLW expansion is a full potential approximation which uses non-overlapping muffin-tin spheres, where the potential is represented via the spherical harmonics, the expansion, and the interstitial region where the potential is expanded in plane waves. The full potential regime provides the best accuracy by an increasing computational time [2, 3]. The number of plane waves 14146 was used, the plane-wave energy cutoff was 138.1 Ry (up to 250 Ry). The integration on Brillouin zone was carried out on grid 32*32*32 special (Monkhorst-Pack) k-points.

The phonon spectra were calculated by means of the interatomic power constants, on the basis of 35 basic q-vectors, in the irreducible Brillouin zone (a grid 8*8*8). The calculated via LMTART-7 c12 Na phonon states densities for various pressure values correspond to normalization requirements within the accuracy, which is substantially lower than one percent. The highest deviation, 1.6%, is obtained for \( P = 0.263 \) GPa.

To obtain Na melting temperature, similar to [42, 43, 45], we use a well-known Lindemann measure

\[
\sqrt{\langle u^2(T_m) \rangle} \approx L_{NN}
\]

where \( \langle u^2(T_m) \rangle \) - is an atom displacement standard deviation at a melting temperature \( T_m \); \( L, d_{NN} \) - is a Lindemann measure and a mean nearest-neighbor distance, correspondingly.

The atomic displacement standard deviation depends on a normalized phonon states density \( g_\omega(\omega) \)

using the relation [56]:

\[
\langle u^2(T) \rangle = \frac{\hbar}{2M} \int \frac{g_{ph}(\omega)}{\omega} \coth \frac{\hbar \omega}{2T} d\omega
\]

Normalization requirement \( g_\omega(\omega) \) is:

\[
\int_{-\infty}^{\infty} g_\omega(\omega) d\omega = 1,
\]
where $g_{ph}^t(\omega_{\text{ex}}) = g_{ph}^c(\omega_{\text{ex}}) = 0$. It should be noted that $\omega_{\text{ex}}$ values, obtained using the LMTART-7 software package, might become negative (results of negative frequencies minimal values emergencies will be further analyzed). Herein, according to our calculations, the normalization requirement (3) is fulfilled with high accuracy.

At $T \gg \hbar \omega$, the equation (2) transforms to:

$$\langle u^2(T) \rangle = \frac{T}{M} \int \frac{g_{ph}(\omega)}{\omega^2} \, d\omega$$

(4)

The resultant expressions, we used for $T_\alpha$ calculations in both a quantum case and a classical limit, are written as:

$$\langle L d_{\alpha} \rangle = \frac{h}{2M} \int_{\omega_{\text{ex}}}^{\omega_{\text{in}}} \frac{g_{\omega}(\omega)}{\omega^2} \coth \frac{\hbar \omega}{2T} \, d\omega = 0;$$

(5)

$$T_\alpha = \langle L d_{\alpha} \rangle \frac{M}{T} \left( \int_{\omega_{\text{ex}}}^{\omega_{\text{in}}} \frac{g_{\omega}(\omega)}{\omega^2} \, d\omega \right)^{-1}.$$  

(6)

The replacement of $\omega_{\text{ex}}$ in (5) and (6) by $\omega_{\text{cut}}$ is caused by an infeasibility to obtain the physically sensible data. The curve $T_\alpha(P)$ calculations within full frequency range $[\omega_{\text{ex}}, \omega_{\text{cut}}]$ ($\omega_{\text{ex}}(P), \omega_{\text{cut}}(P)$ behavior will be analyzed later). We should note that our $\omega_{\text{ex}}$ values calculated using the LMTART-7 are close to those obtained in [43] using the Quantum ESPRESSO software package [57].

Calculations of $T_\alpha$ using (5) and (6) were performed in MATHEMATICA 7 software package. For Na taken, the Lindemann constant value was $L=0.14$, which was similar to [43].

3. Results. Discussion

An important characteristic of the FP-LMTO method is a non-touching muffin-tin sphere radius, $R_T$. It separates the electrons belonging to an atom core from the electrons of external orbitals. Fig. 3 shows the pressure dependent relation $R_T/\langle R \rangle$ (\langle R \rangle - an average nearest neighbors distance determining the macroscopic density (i.e. a volume)). It can be seen that for the given lattice type, the value is constant (curve 2), while the relative volume per atom (curve 1) smoothly decreases. Within the region II, where the structural transition cI2→cF4 takes place, it decreases abruptly. Inside this region, at least within the range $P \approx 65-75$ GPa, the simultaneous existence of the phases cI2 and cF4 is observed.

Let's return to Fig.1. We obtained the analytical approximation of the experimental results in the region I (cI2 lattice, the curve 3 on Fig.1a) as follows:

$$T_\alpha = T_{\alpha 0} + A \left( \exp\left( -\alpha_1(P - P_1) \right) - \exp\left( -\alpha_2(P - P_2) \right) \right),$$  

(7)

where $T_{\alpha 0} = 371$ K; $A = 1.70981 \times 10^4$ K, $\alpha_1 = 3.49197 \times 10^2$ GPa$^{-1}$; $\alpha_2 = 3.492 \times 10^{-2}$ GPa$^{-1}$. The first and the second derivatives of the melting curve are shown in Fig.1b. It is obvious that the $T_\alpha$ maximum point does not belong to a simple second-order phase transition, if the existence of the implicit local order parameter is not assumed, suggested like a tensor irreducible part in paper [58]

$$T_{\alpha 0}(x) = \sum_{i=1}^{3} n_i(x)n_i(x)n_i(x)n_i(x),$$

(8)

where the orthogonal unit vectors $\{n_i(x)\}$ ($i = 1, 2, 3$) define the local cubic order direction at a point $x$. The real situation is apparently much more complicated. Firstly, because the order parameter (8) can be applied to a simple cubic lattice only. Secondly, the melting curve and a dashed vertical line at
$P = 28.3$ GPa divide the phase plane into four areas with various local densities and symmetries. Within the region I-1, a metal density below $T_m(P)$ is greater than the melt density above $T_m(P)$. Within the region I-2, the situation is vice versa: above $T_m(P)$, the melt density exceeds the metal density below $T_m(P)$. Unfortunately, the single-phase Lindemann measure along with \textit{ab initio} molecular dynamics methods are not capable of solving the problem uniquely. The calculated values (diamonds, Fig. 1a), we obtained over the relations (5) and (6), are well consistent with the experimental data. However, this agreement is achieved by cutting off the initial frequencies of the phonon states density (see curve 2 on Fig. 4a). Moreover, the behavior of curve $\omega_m(P)$ qualitatively repeats the melting curve behavior, its more flat maximum being shifted to the side of larger pressures. It indicates that the melting curves data are to be accepted cautiously when we use the Lindemann measure or similar molecular dynamics methods. In our opinion, investigating the melting curves abnormal behavior at high pressures, it is necessary to pay more attention to the research of a condensed matter structure and a near order symmetry.

![Graph](image)

**Figure 3.** Relative volume [23] (1) and $R_{\omega}/R_0$ ratio calculated via LmtART-7 [2] dependences versus pressure comparison.

Fig. 4b shows the dependence of the zero fluctuation energy relation to the latent melting heat at normal conditions, obtained within the Debye model of a metal with a boundary frequency $\omega_m(P)$ (curve 1) and

$$\epsilon_0 = \frac{h}{2} \int_{\omega_m}^{\infty} \ln \omega \phi_\omega(\omega) d\omega$$

(curve 2). It is obvious that in the region I, the vacuum fluctuation energy can reach up to 20% of the latent melting heat, thus, encouraging the disorder growth when the pressure rises. The suggested conclusion assigns a necessity of considering a zero fluctuations contribution to both cases of a lattice long range order destruction during melting, and a crystalline structure reconstruction at high pressures. The additional pro argument can be found in paper [59]. It claims that the growth of the pressure promotes the anharmonicity increase of lattice fluctuations, which suppresses a superconductivity and leads to a superconductor-to-semiconductor transition of lithium at $P = 80$ GPa.
(See [18] and references therein).

Figure 4. Values of boundary (1) and cutoff (2) frequencies of phonons (a) and vacuum fluctuations energy to latent melting heat ratio at normal conditions (b). Curve 1 is calculated within Debye model approximation taking into account the boundary frequency value; curve 2 is obtained according to phonon states density computed via LMTART-7 [2].

Figure 5. Electron (a) and phonon (b) states density computed via LMTART-7 [2], and also phonon spectrum (c) for $P = 0.263$ GPa.

Let's consider a dynamics of a phonon spectrum and a density of electron and phonon states near the melting curve maximum and at the beginning of a phase transition $c12\rightarrow cF4$. Fig. 5 shows the electron (a) and the phonon (b) states densities, and the phonon spectrum for $P = 0.263$ GPa (c). The curves numbers in Fig. 5b correspond to the pressure values designed in Fig. 5a. Since all calculations were made for the unit cell containing two atoms, three acoustic branches and three optical branches do exist. Our calculated acoustic spectrum qualitatively coincides with the sodium spectrum given in textbooks, e.g. [60].
Figure 6. Left: Electron and phonon densities of states (a) and a phonon spectra of Na b.c.c. lattice in the vicinity of melting curve maximum: (b, c, d). Right: Density of electron b.c.c. and f.c.c. lattices states and phonon b.c.c. lattices states for sodium in the range of b.c.c.-f.c.c. transition (a), phonon spectrum of sodium b.c.c. lattice in the vicinity of transition b.c.c.-f.c.c. (b, c) and in the range of only f.c.c. lattice existence (see also Fig. 1).
Fig. 6 shows the electron and the phonon densities of states (a) and the phonon spectra (b, c, d), in the vicinity of $T_m$ maximum (left); the electron (for b.c.c. and f.c.c. lattices) and the phonon densities of states for the b.c.c. lattice at $P = 64.494$ GPa (a), the phonon spectra of the b.c.c. lattice for three pressure values: (b) 61.9 GPa, (c) 64.494 GPa, and (d) 92.371 Gpa (right). The features of the phonon spectra, in the vicinity of the melting curve maximum are the existence of a non-zero positive frequency value at $k = 0$ and the small negative transverse acoustic branch frequency at $k/k_{max} \approx 0.2$. It demonstrates the sodium local structure transformation. The existence of larger segments at the acoustic and the optical branches lying in the region of frequencies negative values testifies the instability of these branches and the lattice itself.

4. Conclusion

Thus, in present paper we obtained the energy distribution of the electrons and the phonons as well as the density of states for all experimental points within the range of Na b.c.c. lattice existence. Using the one-phase Lindemann measure and the calculated phonon spectra, the theoretical values of the melting points matching the experimental data has been obtained. An energy of zero fluctuations was defined, and the necessity to account its contribution to the dynamics of the electron and the phonon spectra has been shown. Features of the volume jump behavior during melting under the increasing pressure are discussed.

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