

RMS Dynamic Displacements of Atoms and Their Complexes from the Equilibrium Position in Crystals

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The thermal characteristics of a group of ionic crystals of cubic crystal system, CaB_6 type hexaborides, and UB_{12} metal dodecaborides were investigated using high-temperature X-ray diffraction using a KROS camera with a thermal nozzle. On the basis of the X-ray characteristic temperature values, full root mean square (RMS) dynamic displacements of hypothetical atoms or their complexes with average and consolidated masses are calculated. The temperature increase of the oscillation amplitudes and the temperature decrease of the X-ray characteristic temperature are explained. The reasons for the slight difference of the X-ray characteristic temperature values with the literary data are described. It is established that the reduced masses of hypothetical atoms are smaller than their average masses. The growth rate of the RMS dynamic displacements of atoms with increasing temperature for ionic crystals is shown graphically, and for hexaborides and dodecaborides of metals – analytically, in the range from room temperature to 700–973 K. The change in RMS dynamic displacements with the change in masses is observed in ionic crystals and is not observed in metal borides. This is explained by the structure of the interatomic bond change. The values of the general measure of the anharmonicity of thermal oscillations are given for hexaborides and dodecaborides. It is shown that in the group of hexaborides there is a regular decrease of the crystal lattice parameter with the increase of the atomic number of metals, which is explained by lanthanide compression. This is due to the strength of the boron frame, which is a consequence of the increase in the atomic radius. It is explained that the increase in the anharmonicity of thermal oscillations of atoms with increasing temperature leads to a linear decrease in the effective X-ray characteristic temperature. Studies have shown that the RMS dynamic displacements are described by a weak quadratic polynomial with positive velocity, which correlates with the temperature dependence of the general measure of anharmonicity of vibrational motion.

Keywords: Oscillation anharmonicity, Oscillation amplitudes, RMS dynamic displacements.

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1. INTRODUCTION

In the field of nanoelectronic physics, the determination of the full RMS dynamic displacements $\overline{u_r^2}$ of atoms or their complexes of equilibrium position is of great theoretical and practical importance. First of all, it concerns the mobility values of these particles in crystals with different atoms. In addition, the values of $\overline{u_r^2}$ carry the information of the temperature limit for the destruction of the crystal. The determination of the amplitudes of thermal oscillations by the X-ray method in crystals with the same atoms does not pose any particular problems. Problems arise in the experimental determination of RMS dynamic displacements of atoms of substances, which are composed of different sorts of atoms, since one must know the temperature dependence of the X-ray characteristic of Debye temperature $\Theta_D(T)$. It, in turn, is related to the average or balanced mass of hypothetical atoms or their complexes. These difficulties were pointed out in [1].

2. DESCRIPTION OF THE OBJECT AND RESEARCH METHODS

The materials selected for the investigation were ionic crystals of the type NaCl, CsCl, hexaborides and

dodecaborides of metals like CaB_6 and UB_{12} . These crystals have face-centered cubic (FCC) (NaCl , UB_{12}) and volume-centered cubic (VCC) (CsCl , CaB_6) lattices.

These substances have wide practical use. This especially concerns hexaborides and dodecaborides of metals due to their heat resistance, refractory properties, abrasion resistance and thermoelectric properties (thermoelectric power, thermoemission, work function, electrical conductivity).

A characteristic feature of the FCC lattice is the presence of faces with all even or odd indices (hkl), which makes it possible to experimentally determine the amplitudes of thermal vibrations of different atoms.

By the structure MeB_6 (metal boron six) (VCC lattice) and MeB_{12} (metal boron twelve) (FCC lattice) can be considered as three-dimensional (possibly tetrahedral) frameworks of boron atoms, in the voids between which there are metal atoms. Octahedral frames of boron atoms in hexaborides are characterized by high rigidity and strong bonding, since the metal atoms are located in the voids between them and do not cause large changes in distances.

Hexaborides and dodecaborides of metals are very refractory: their melting point is within 2400–2923 K.

According to the literature data and accordingly to quantum mechanical calculations, the boron atom can

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form s -, p -, and d -communication functions. It can be assumed that the s - and p -functions, forming hybrid orbits, are realized in bonds between the boron atoms themselves, whereas the d -function, together with the rest of the p -functions, provides metal-boron bonds. This leads to the formation of a common conductivity band composed of overlapping levels of metal and boron. For hexaborides of the rare earth metals, a characteristic feature is the metallic nature of their properties with the exception of SmB_6 . Along with the same characteristics, hexaborides have different, which is manifested in different values $\Theta_R(T)$.

In simple NaCl or CsCl structures, oscillations of hypothetical or real atoms are considered, and in complex CaB_6 or UB_{12} (dodecaborides) structures, oscillations of both metal atoms and boron frames and reduced hypothetical atoms are considered.

To determine the RMS dynamic displacements $\overline{u_r^2}$ of atoms and frames, the method of high-temperature X-ray diffraction in the range from room temperature to 773 K for ionic crystals is selected from equilibrium positions and up to 973 K for metal borides by determining the Debye-Waller factor indices $2M$, which is expressed by the known ratio for cubic structures:

$$2M = \frac{3h^2T \sum b_i^2}{mk\theta^2 a^2} \left[\Phi\left(\frac{\theta}{T}\right) + \frac{1}{4} \frac{\theta}{T} \right], \quad (1)$$

or

$$2M = \frac{4}{3} \pi^2 \overline{u_0^2} \frac{h^2 + k^2 + l^2}{a^2} = \frac{4}{3} \pi^2 \overline{u_0^2} \frac{\sum b_i^2}{a^2}, \quad (2)$$

where $\left[\Phi\left(\frac{\theta}{T}\right) + \frac{1}{4} \frac{\theta}{T} \right] = \psi\left(\frac{\theta}{T}\right)$ is the Debye function, h is the Planck's constant, k is the Boltzmann constant, Θ is the effective X-ray characteristic temperature, T is the thermodynamic temperature on the Kelvin scale, a is the crystal lattice parameter, $\sum b_i^2 = h^2 + k^2 + l^2$ is the sum of squares of crystallographic indices (hkl), m is the mass of an atom or complex of boron atoms, $\overline{u_r^2}$ is the total mean square of the dynamic displacement of an atom or complex of boron atoms.

Assimilating (1) and (2) we have:

$$\overline{u_r^2} = \frac{9}{4} \frac{h^2 T \psi(x)}{\pi^2 m k \theta^2}, \quad (3)$$

where $x = \Theta/T$.

At $x = \Theta/T < 2\pi$ function $\psi(x)$ can be expressed as

$$\psi(x) = 1 + \alpha \frac{\theta^2}{T^2} \approx 1 + 0,0267 \frac{\theta^2}{T^2} \quad (4)$$

with a relative error of not more than 0.1 % at room temperature and not more than 0.03 % at high research temperatures. The proportionality factor α is 0.0267 according to the tabular values of function ψ .

It can be seen from (3) that to find $\overline{u_r^2}$ it is necessary to have the values of the reduced or average hypothetical masses of atoms m and Θ . We took m the averages m_{av} and the consolidated m_{con} masses of hypothetical atoms and their complexes, both in definition $\Theta_R(T)$

and in definition $\overline{u_r^2}(T)$. The choice of mass values m depends on the values $\overline{u_r^2}$ and Θ .

There are various methods for determining the characteristic temperature Θ , in particular heat capacity, elastic, X-ray. Among the X-ray methods we have chosen the method of high-temperature X-ray diffraction on a flat film with the help of the "KROS"-type camera with allowance for corrections on temperature diffuse scattering (TDS) of X-rays, the method of determination Θ_R and dependence $\Theta_R(T)$.

We used this method to investigate the substances of cubic crystal system of simple and complex structures. Having analyzed the results, we have come to the conclusion that when determining Θ_R and $\overline{u_r^2}$ we need to use the masses of atoms or their complexes.

Separate determination of $\overline{u_r^2}$ of different atoms by the method described by us in [1] gives illogical values due to the low intensity of the interference lines with odd indices (hkl). Therefore, for the separate determination of $\overline{u_r^2}$ of cations and anions or complexes, we calculated using the conventional formula (3), taking the values Θ_R common to different atoms and their groups for a given substance.

The initial data were the values of the logarithm of the relative intensity $\ln(I/I_0)$ of the interference maximum (hkl) at room temperature T_0 and at $T (T \geq T_0)$, similarly to the logarithm of the relative products of the intensity factors $\ln(B/B_0)$, except Debye's e^{-2M} , the correction β and β_0 on the TDS, crystal lattice parameters a and a_0 , the summed masses of hypothetical atoms or their carcasses.

From the analysis of high melting temperatures of metal borides, it follows that the values Θ_R for them must be high and $\overline{u_r^2}$ small. This is possible with the assumption of oscillations of the frames of boron atoms as a whole. Therefore, $\overline{u_r^2}$ masses of metal, the masses of boron frames, and their summed masses of hypothetical lattice atoms were taken into account in the calculations. The technology of sample preparation was similar to that in [2, 3].

The calculations of $\overline{u_r^2}$ are based on the values of the temperature dependences $\alpha(t)$ and $\Theta_R(T)$, which we published in our previous works.

3. DESCRIPTION AND ANALYSIS OF RESULTS

The results of the investigation of the temperature dependence of the total RMS dynamic displacements of atoms on the equilibrium position for the selected ion crystals are presented in Fig. 1-Fig. 4, and for the borides and dodecaborides are given selectively in Table 1 and Table 2.

The researches have shown that the full RMS dynamic displacements $\overline{u_{r,red}^2}(t)$ of hypothetical atoms with reduced masses are larger than the hypothetical ones with average masses. The difference between $\overline{u_{r,red}^2}(t)$ and $\overline{u_{r,av}^2}$ is larger in crystals with a larger difference in the mass of the constituent atoms, such as in KJ , ThB_6 or UB_{12} .

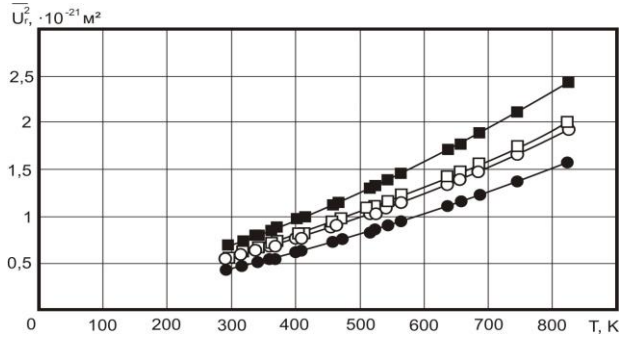


Fig. 1 – Temperature dependence $\overline{u_r^2}(T)$ of hypothetical and real ions in NaCl crystals: \blacksquare – $\overline{u_r^2}$ Na, \bullet – $\overline{u_r^2}$ Cl, \square – $\overline{u_{r,red}^2}$, \circ – $\overline{u_{r,red}^2}$, $\overline{u_{r,red}^2}(T) = 9.417 \cdot 10^{-23} + 1.191 \cdot 10^{-24}t + 1.386 \cdot 10^{-27}t^2$; $\overline{u_{r,av}^2}(T) = 8.989 \cdot 10^{-23} + 1.137 \cdot 10^{-24}t + 1.323 \cdot 10^{-27}t^2$

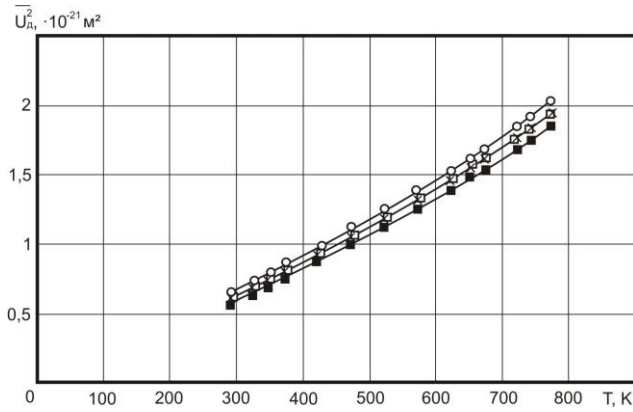


Fig. 2 – Temperature dependence $\overline{u_r^2}(T)$ of hypothetical and real ions in KCl crystals: \circ – $\overline{u_r^2}$ Cl, \blacksquare – $\overline{u_r^2}$ K, \square – $\overline{u_{r,red}^2}$, \times – $\overline{u_{r,red}^2}$, $\overline{u_{r,red}^2}(T) = 7.057 \cdot 10^{-23} + 1.510 \cdot 10^{-24}t + 1.189 \cdot 10^{-27}t^2$; $\overline{u_{r,av}^2}(T) = 7.039 \cdot 10^{-23} + 1.506 \cdot 10^{-24}t + 1.186 \cdot 10^{-27}t^2$

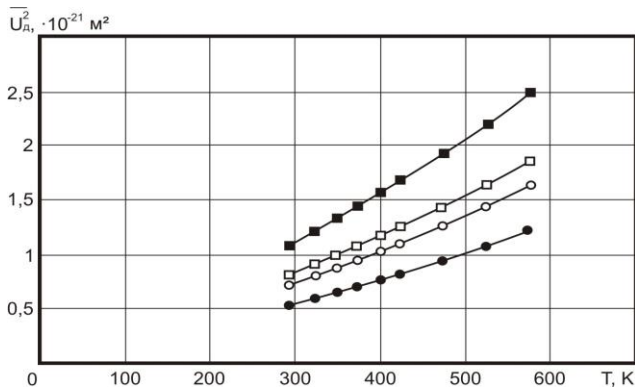


Fig. 3 – Temperature dependence $\overline{u_r^2}(T)$ of hypothetical and real ions in KBr crystals: \blacksquare – $\overline{u_r^2}$ K, \bullet – $\overline{u_r^2}$ Br, \square – $\overline{u_{r,red}^2}$, \circ – $\overline{u_{r,red}^2}$, $\overline{u_{r,red}^2}(T) = 6.058 \cdot 10^{-23} + 1.998 \cdot 10^{-24}t + 1.940 \cdot 10^{-27}t^2$; $\overline{u_{r,av}^2}(T) = 5.345 \cdot 10^{-23} + 1.763 \cdot 10^{-24}t + 1.712 \cdot 10^{-27}t^2$

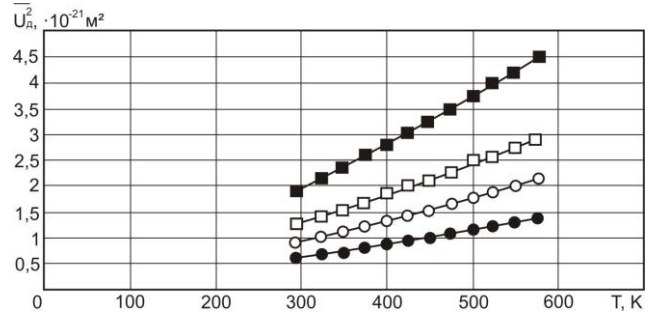


Fig. 4 – Temperature dependence $\overline{u_r^2}(T)$ of hypothetical and real ions in crystals of KI: \blacksquare – $\overline{u_r^2}$ K, \bullet – $\overline{u_r^2}$ I, \square – $\overline{u_{r,red}^2}$, \circ – $\overline{u_{r,red}^2}$, $\overline{u_{r,red}^2}(T) = -8.615 \cdot 10^{-23} + 3.950 \cdot 10^{-24}t + 2.244 \cdot 10^{-27}t^2$; $\overline{u_{r,av}^2}(T) = -6.205 \cdot 10^{-23} + 2.845 \cdot 10^{-24}t + 1.616 \cdot 10^{-27}t^2$

Table 1 – The temperature dependence of the RMS dynamic displacements of atoms on the equilibrium position for borides and dodecaborides

Boride	$\overline{u_{r,red}^2}(t)$
CaB ₆	$\overline{u_{r,red}^2}(t) = 6.181 \cdot 10^{-23} + 4.433 \cdot 10^{-25}t + 2.564 \cdot 10^{-28}t^2$
SrB ₆	$\overline{u_{r,red}^2}(t) = 1.093 \cdot 10^{-22} + 2.438 \cdot 10^{-26}t + 5.744 \cdot 10^{-28}t^2$
YB ₆	$\overline{u_{r,red}^2}(t) = 5.932 \cdot 10^{-23} + 4.602 \cdot 10^{-25}t + 2.369 \cdot 10^{-28}t^2$
BaB ₆	$\overline{u_{r,red}^2}(t) = 2.146 \cdot 10^{-22} + 3.325 \cdot 10^{-25}t + 1.555 \cdot 10^{-27}t^2$
LaB ₆	$\overline{u_{r,red}^2}(t) = 6.041 \cdot 10^{-23} + 5.160 \cdot 10^{-25}t + 2.700 \cdot 10^{-28}t^2$
LaB ₆	$\overline{u_{r,red}^2}(t) = 6.041 \cdot 10^{-23} + 5.160 \cdot 10^{-25}t + 2.700 \cdot 10^{-28}t^2$
CeB ₆	$\overline{u_{r,red}^2}(t) = 5.875 \cdot 10^{-23} + 5.127 \cdot 10^{-25}t + 1.722 \cdot 10^{-28}t^2$
PrB ₆	$\overline{u_{r,red}^2}(t) = 6.346 \cdot 10^{-23} + 3.891 \cdot 10^{-25}t + 2.662 \cdot 10^{-28}t^2$
NdB ₆	$\overline{u_{r,red}^2}(t) = 5.693 \cdot 10^{-23} + 3.085 \cdot 10^{-25}t + 1.187 \cdot 10^{-28}t^2$
SmB ₆	$\overline{u_{r,red}^2}(t) = 1.170 \cdot 10^{-22} + 3.354 \cdot 10^{-25}t + 1.267 \cdot 10^{-27}t^2$
EuB ₆	$\overline{u_{r,red}^2}(t) = 5.655 \cdot 10^{-23} + 1.546 \cdot 10^{-25}t + 8.821 \cdot 10^{-29}t^2$
YbB ₆	$\overline{u_{r,red}^2}(t) = 6.064 \cdot 10^{-23} + 5.899 \cdot 10^{-25}t + 1.547 \cdot 10^{-28}t^2$
ThB ₆	$\overline{u_{r,red}^2}(t) = 6.125 \cdot 10^{-23} + 2.731 \cdot 10^{-25}t + 1.893 \cdot 10^{-28}t^2$
TbB ₁₂	$\overline{u_{r,red}^2}(t) = 6.216 \cdot 10^{-23} + 2.421 \cdot 10^{-25}t + 1.384 \cdot 10^{-28}t^2$
DyB ₁₂	$\overline{u_{r,red}^2}(t) = 6.010 \cdot 10^{-23} + 1.314 \cdot 10^{-25}t + 8.231 \cdot 10^{-29}t^2$
HoB ₁₂	$\overline{u_{r,red}^2}(t) = 5.975 \cdot 10^{-23} + 1.680 \cdot 10^{-25}t + 9.922 \cdot 10^{-29}t^2$
ErB ₁₂	$\overline{u_{r,red}^2}(t) = 6.055 \cdot 10^{-23} + 4.336 \cdot 10^{-26}t + 1.381 \cdot 10^{-28}t^2$
TmB ₁₂	$\overline{u_{r,red}^2}(t) = 5.977 \cdot 10^{-23} + 2.200 \cdot 10^{-25}t + 9.890 \cdot 10^{-29}t^2$
UB ₁₂	$\overline{u_{r,red}^2}(t) = 6.191 \cdot 10^{-23} + 1.176 \cdot 10^{-25}t + 1.210 \cdot 10^{-28}t^2$

Note: $\overline{u_{r,red}^2}(t)$ with the reduced mass of the hypothetical atom

Table 2 – A general measure of anharmonicity $(d\ln\Theta/dT)(t)$ for hexaborides and dodecaborides

Hexaborides/ Dodecaborides	$(d\ln\Theta/dT)(t)$
CaB ₆	$(d\ln\Theta/dT)(t) = -1.239 \cdot 10^{-4} - 1.831 \cdot 10^{-8}t$
SrB ₆	$(d\ln\Theta/dT)(t) = -2.521 \cdot 10^{-4} - 9.781 \cdot 10^{-8}t$
YB ₆	$(d\ln\Theta/dT)(t) = -1.145 \cdot 10^{-4} - 1.538 \cdot 10^{-8}t$
BaB ₆	$(d\ln\Theta/dT)(t) = -3.424 \cdot 10^{-4} - 2.426 \cdot 10^{-7}t$
LaB ₆	$(d\ln\Theta/dT)(t) = -1.199 \cdot 10^{-4} - 1.701 \cdot 10^{-8}t$
CeB ₆	$(d\ln\Theta/dT)(t) = -7.277 \cdot 10^{-5} - 5.837 \cdot 10^{-9}t$
PrB ₆	$(d\ln\Theta/dT)(t) = -1.319 \cdot 10^{-4} - 2.103 \cdot 10^{-8}t$
NdB ₆	$(d\ln\Theta/dT)(t) = -6.152 \cdot 10^{-5} - 4.105 \cdot 10^{-9}t$
SmB ₆	$(d\ln\Theta/dT)(t) = -2.953 \cdot 10^{-4} - 1.515 \cdot 10^{-7}t$
EuB ₆	$(d\ln\Theta/dT)(t) = -5.011 \cdot 10^{-5} - 2.681 \cdot 10^{-9}t$
YbB ₆	$(d\ln\Theta/dT)(t) = -5.191 \cdot 10^{-5} - 2.885 \cdot 10^{-9}t$
ThB ₆	$(d\ln\Theta/dT)(t) = -1.126 \cdot 10^{-4} - 1.485 \cdot 10^{-8}t$
TbB ₁₂	$(d\ln\Theta/dT)(t) = -8.105 \cdot 10^{-5} - 7.328 \cdot 10^{-9}t$
DyB ₁₂	$(d\ln\Theta/dT)(t) = -3.833 \cdot 10^{-5} - 1.544 \cdot 10^{-9}t$
HoB ₁₂	$(d\ln\Theta/dT)(t) = -6.034 \cdot 10^{-5} - 3.943 \cdot 10^{-9}t$
ErB ₁₂	$(d\ln\Theta/dT)(t) = -1.632 \cdot 10^{-4} - 3.398 \cdot 10^{-8}t$
TmB ₁₂	$(d\ln\Theta/dT)(t) = -5.140 \cdot 10^{-5} - 2.826 \cdot 10^{-9}t$
LuB ₁₂	$(d\ln\Theta/dT)(t) = -1.218 \cdot 10^{-4} - 1.764 \cdot 10^{-8}t$
UB ₁₂	$(d\ln\Theta/dT)(t) = -9.170 \cdot 10^{-5} - 9.533 \cdot 10^{-9}t$

The researches have shown that the full RMS dynamic displacements $\overline{u_{r,red}^2}(t)$ of hypothetical atoms with reduced masses are larger than the hypothetical ones with average masses. The difference between $\overline{u_{r,red}^2}(t)$ and $\overline{u_{r,av}^2}(t)$ is larger in crystals with a larger difference in the mass of the constituent atoms, such as in KJ, ThB₆ or UB₁₂.

The dependence $\overline{u_r^2}(T)$ is described by a weak quadratic polynomial with positive velocity, which correlates with the temperature dependence of the general measure of anharmonic vibration motion $(d\ln\Theta_R/dT)(T)$. The pattern of increasing crystal lattice parameter in the NaCl < KCl < KBr < KJ series is revealed, which is related to the increase in the ion radii of the constituent crystals and the decrease in the effective X-ray characteristic temperature in the same series, which is explained by the increase in the anharmonicity of thermal oscillations.

The growth rates of $\overline{u_{r,red}^2}(t)$ and $\overline{u_{r,av}^2}(t)$ in the experimental ion crystals are analytically expressed by the corresponding ratios given in the work [4].

For ionic crystals with a small difference of reduced and average masses (NaCl, KCl), the growth rate $\overline{u_r^2}$ of hypothetical ions is almost the same. In KBr and KJ crystals, with a significant difference of reduced and average masses, the growth rate $\overline{u_{r,red}^2}$ and $\overline{u_{r,av}^2}$ is significant but of the same type. This concerns to CsCl, although the crystal structure is also affected in this case.

In the group of hexaborides, there is a regularity of decrease in the crystal lattice parameter with increasing atomic number of metals, which is explained by lanthanide compression, with the exception of ErB₆ and YbB₆. This is explained by the strength of the boron framework, which is a consequence of the increase in the atomic radius, for example, in Yb, which is in a

two-wave boride state unlike other metals of the cerium subgroup.

Increase in the anharmonicity of thermal vibrations of atoms with increasing temperature leads to a linear decrease in the effective X-ray characteristic temperature. Depending on the method of calculating the magnitude Θ (by elastic, heat, X-ray, and other mixed characteristics, including the use of values of the reduced and average masses of hypothetical atoms and their complexes), the characteristic temperatures are different. So when using the combined masses Θ_R is greater than when using the average masses. The values of Θ_R are closer in magnitude to those Θ obtained by the elastic characteristics.

A clearer pattern is a slight decrease in the lattice parameter a of dodecaborides as the ordinal number grows in the Mendeleev periodic table, however, there is no explicit pattern for Θ_R and for the universal measure of anharmonicity $d\ln\Theta_R/dT$. However, in the case of substances of type MeB₆ and MeB₁₂, the full RMS dynamic displacement values $\overline{u_r^2}$ from equilibrium positions increase with increasing temperature. Universal measures of anharmonicity also increase in size, which is explained by the weakening of interatomic bonds and the temperature decrease $\Theta_R(T)$.

4. CONCLUSIONS

On the basis of the experimental data for the determination of the crystal lattice parameter and the effective X-ray characteristic temperature $\Theta_R(T)$, the temperature dependence $\overline{u_r^2}(T)$ of the full RMS dynamic displacements on the equilibrium position of atoms and their complexes for a wide class of NaCl, CsCl, CaB₆ and UB₁₂ cubic substances is calculated. It is set up that the values of Θ_R and $\overline{u_r^2}$ depend not only on the temperature, but also on the values of the reduced or average masses (m_{red} , m_{av}) of atoms and their complexes taken in the calculations.

It is established that the magnitude of the reduced masses of hypothetical atoms are smaller than their average masses ($m_{red} < m_{av}$). This, in turn, leads to that $\overline{u_{r,red}^2}(t) > \overline{u_{r,av}^2}(t)$ at all temperatures.

Rapid growth $\alpha(T)$ with temperature for the test substances in the range 293-773 K (ionic crystals) and 293-973K (metal borides) is described by the increasing quadratic polynomial, whereas $\Theta_R(T)$ is described by a linear recession. The temperature rise of all species $\overline{u_r^2}(T)$ is described by a slight quadratic dependence.

The temperature dependences $\alpha(T)$, $\Theta_R(T)$ and $\overline{u_r^2}(T)$ are explained by the anharmonic nature of the thermal vibrations of atoms and their complexes.

By the magnitude, a general measure of the anharmonicity of thermal fluctuations $d\ln\Theta_R/dT$ is smallest in UB₁₂-type compounds, is greater in CaB₆-type compounds, and even greater in ionic crystals. These values differ twice.

According to the literature, a slight difference in values is explained not only by different methods of study and mathematical processing of experimental

data obtained by elastic or heat-capacitive methods of study, but also by the different sensitivity of these data to the shape of the phonon spectrum of the lattice. In other words, the difference between the real shape of the phonon spectrum and the Debye's parabola has a

different effect on the value of the Debye 2 M thermal factor than on the heat capacity or other elastic characteristics. For the most part $\Theta_{el} > \Theta_{av}$, $\Theta_R \approx \Theta_{el}$.

Extensive work on the experiment was performed only on the basis of radiographic data.

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Середньоквадратичні динамічні зміщення атомів та їх комплексів від положення рівноваги в кристалах

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Методом високотемпературного рентгенографування за допомогою камери КРОС з температурною насадкою проведено дослідження теплових характеристик групи іонних кристалів кубічної сингонії, гексаборидів типу CaB_6 та додекаборидів металів типу UB_{12} . На основі значень рентгенівської характеристичної температури розраховані повні середньоквадратичні динамічні зміщення гіпотетичних атомів або їх комплексів з середніми та зведеними масами. Пояснені температурне зростання амплітуд коливань та температурний спад рентгенівської характеристичної температури. Описані причини незначної розбіжності значень рентгенівської характеристичної температури з літературними даними. Встановлено, що зведені маси гіпотетичних атомів менші за їх середні маси. Стрімкість зростання середньоквадратичних динамічних зміщень з підвищенням температури для іонних кристалів показана графічно, а для гексаборидів і додекаборидів металів – аналітично, в діапазоні від кімнатної температури до 700-973 К. Зміна середньоквадратичних динамічних зміщень зі зміною мас спостерігається в іонних кристалах і не спостерігається в боридів металів. Це пояснюється структурою зміни міжатомних зв'язків. Для гексаборидів і додекаборидів наведені значення узагальнюючої міри ангармонізму теплових коливань. Показано, що у групі гексаборидів спостерігається закономірне зменшення параметра кристалічної ґратки зі зростанням атомного номера металів, що пояснюється лантанічним стискуванням. Це обумовлено напруженістю борного каркасу, що є наслідком збільшення атомного радіуса. Наведено пояснення, що збільшення ангармонічності теплових коливань атомів з підвищенням температури призводить до лінійного спаду ефективної рентгенівської характеристичної температури. Дослідженнями показано, що середньоквадратичні динамічні зміщення описуються слабким квадратичним поліномом з додатною стрімкістю, що корелює з температурною залежністю узагальнюючої міри ангармонізму коливного руху.

Ключові слова: Ангармонізм коливань, Амплітуди коливань, Середньоквадратичні динамічні зміщення.