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ANALYSIS OF TEMPERATURE CHANGES OF STRUCTURE OF FUSIONS TO THE RUBIDIUM WITHIN THE FRAMEWORK OF CLUSTER MODEL

АНАЛІЗ ТЕМПЕРАТУРНИХ ЗМІН СТРУКТУРИ РОЗПЛАВІВ РУБІДІЮ У РАМКАХ КЛАСТЕРНОЇ МОДЕЛІ

A computer program modeled the cluster structure of molten simple metals with a body-centered cubic (BCC) lattice, determining structural parameters of molten rubidium — cluster shape, average interatomic distance, optimal cluster size, and inter-cluster distance — by comparing simulated data with neutron and X-ray diffraction results. Guided by the Wulff principle and high-density atomic planes, the bipyramid cluster (volume-to-surface-area ratio of 0.17) is most stable near the melting point and up to 160°C, correlating with a linear decrease in cluster size. Above 240°C, where viscosity and density change anomalously, the tripyramid cluster (ratio of 0.14) dominates, showing increased surface area and energy, indicating a structural transition from bipyramid to tripyramid.

***Keywords**: coordinationnumbers, short-rangeorder, translationdirection, body-centeredcubic (BCC) crystallattice, surfaceenergy, averageinteratomicdistance, optimalclustersize.*

Розроблена комп'ютерна програма моделювання кластерної структури розплавів простих металів з кристалічною решіткою об'ємноцентрованою кубічною (ОЦК). Шляхом співставлення з експериментальними даними нейтронно-рентгенодифракційного аналізу проведено визначення особливостей структурних параметрів у розплавах рубідію: форми кластерів, середньої міжатомної відстані, оптимального розміру кластера, середньої відстані між кластерами. Вибір форми кластеру визначався у відповідності з принципами Кюрі-Вульфа про мінімум поверхневої енергії кристалу, що знаходиться у рівновазі зі своєю рідиною та принципу Браве, згідно з яким кристал обмежується атомними площинами з максимальною густиною атомів. В ОЦК гратці таким відповідають кластери у формі: біпіраміди, призми, трипіраміди. Перший із названих кластерів відповідає найбільшим відношенням об'єму до площі поверхні, тобто є найбільш ймовірним при температурах близьких до точки плавлення.

У температурних інтервалах, де спостерігаються аномальні зміни макроскопічних фізичних параметрів — в'язкості і густини (~240^{0}C) відбуваються і відповідні зміни параметрів *кластерів. Наведені залежності оптимальних розмірів кластера від температури в інтервалі 40°С — 160°С скоріш за все відповідають формі біпіраміди для якої відношення об'єму до площі поверхні дорівнює 0,17 і є найбільшим, тобто найбільш вірогідним. Про це додатково свідчить і лінійне зменшення розміру кластера зі зростанням температури в цьому інтервалі.*

Для більш високих температур 240°С, 360°С приведені значення для біпіраміди не відповідають дійсності, оскільки не корелюють зі змінами середньої міжатомної відстані від температури та середньої відстані між кластерами від температури в цьому інтервалі, як і для призми (відношення об'єму до площі дорівнює 0,15).

Суттєва кореляція у даному інтервалі температур має місце лише для трипіраміди, для якої відношення об'єму до площі дорівнює 0,14 є найменшим, а сукупна поверхнева енергія кластерів — найбільша. Таким чином приведені результати свідчать про наявність фазового переходу ІІ роду при температурі близько 240°С, що обумовлене зміною форми кластерів від біпіраміди до три піраміди. Цей процес супроводжується збільшенням сукупної площі поверхні кластерів і відповідно їх поверхневої енергії.

***Ключові слова**: координаційні числа, ближній порядок, напрямок трансляції, об'ємноцентрована кубічна кристалічна гратка (ОЦК), поверхнева енергія, середня міжатомна відстань, оптимальний розмір кластеру.*

Problem's Formulation

The objective of this work is to develop a computer program for modeling the cluster structure of melts of simple metals with a body-centered cubic (BCC) lattice in their solid state, such as rubidium, to enable comparison with experimental data from neutron and X-ray diffraction analysis and to determine the shape and key structural parameters of clusters, including average interatomic distance, optimal cluster size, and average distance between clusters.

The program is designed to achieve the following:

- Cluster shape: determination of the geometric shape of clusters (e.g., bipyramids, prisms, or tripyramids) that aligns with the Wulff principle, which states that a crystal in equilibrium with its liquid phase minimizes surface free energy, and the tendency of crystals to be bounded by atomic planes with high atomic density (low Miller indices).
- Average interatomic distance: calculation of the average distance between atoms within a cluster, a critical parameter for understanding the local structure of the melt.
- Optimal cluster size: identification of the cluster size that provides the most stable configuration based on energetic characteristics, such as the volume-to-surface-area ratio.
- Average distance between clusters: analysis of the distances between individual clusters in the melt, which influences macroscopic properties such as viscosity and density.

The program enables modeling of cluster behavior in the melt at various temperatures, particularly in ranges where anomalies in physical properties are observed (e.g., around 240°C for rubidium). The modeling is validated by comparison with experimental neutron and X-ray diffraction data, ensuring the accuracy of theoretical predictions. The results help identify features of structural phase transitions (e.g., a change in cluster shape from bipyramid to tripyramid with increasing temperature) and their correlation with changes in macroscopic parameters, such as surface energy and density.

Analysis of recent research and publications

Studies [6, 7] demonstrate that changes in the short-range coordination structure in melts of alkali metals, such as rubidium (Rb) and cesium (Cs), with varying temperature occur abruptly at specific temperatures or within narrow temperature ranges, rather than monotonically. These changes correlate with anomalous phenomena observed in the temperature dependencies of viscosity and density. For rubidium melts, such anomalies are observed in the temperature range of 250°C—300°C, potentially indicating a second-order phase transition associated with a change in the shape of clusters within the melt structure. These findings underscore the importance of interpreting neutron and X-ray diffraction data using a cluster model of the structure of simple liquids, which accounts for the local organization of atoms in clusters and their evolution with temperature.

Neutron and X-ray diffraction studies of simple liquids and melts have been the focus of numerous investigations. Studies [1, 2] are notable examples of research into the structure of liquid metals using diffraction methods. For the structural analysis of melts of simple metals within the framework of the cluster model, this work builds on the results of studies [3, 4, 5, 6,7]. These studies provide the theoretical and experimental foundation for modeling the cluster structure, including the determination of cluster shapes, interatomic distances, and other structural parameters that vary with temperature.

Formulation of the study purpose

The objective of this work is to develop a computer program for modeling the cluster structure of melts of simple metals with a body-centered cubic (BCC) lattice, enabling comparison with experimental data from neutron and X-ray diffraction analysis to determine cluster shapes and key structural parameters, including average interatomic distance, optimal cluster size, and average distance between clusters.

Presenting main material

Interpretation of diffraction studies based on the cluster model of liquid structure requires implementing a set of computational tasks, ranging from selecting cluster shapes to establishing relationships between model parameters and diffraction analysis data. These calculations are presented in this work for clusters derived from the body-centered cubic (BCC) lattice structure.

The choice of cluster shape was guided by the Wulff principle, which states that a crystal in equilibrium with its liquid phase minimizes surface free energy, and the tendency of crystals to be bounded by atomic planes with the highest atomic density (low Miller indices). In a BCC lattice, these planes correspond to the {110} family, including planes such as (110), $(\bar{1}10)$, (101), $(10\bar{1})$, (011), $(0\overline{11})$, $(\overline{11}0)$, $(\bar{1}01)$, $(\overline{101})$, $(0\overline{11})$, $(\bar{0}11)$, and $(\overline{011})$. Clusters constructed from these planes can take the form of bipyramids, prisms, or tripyramids.

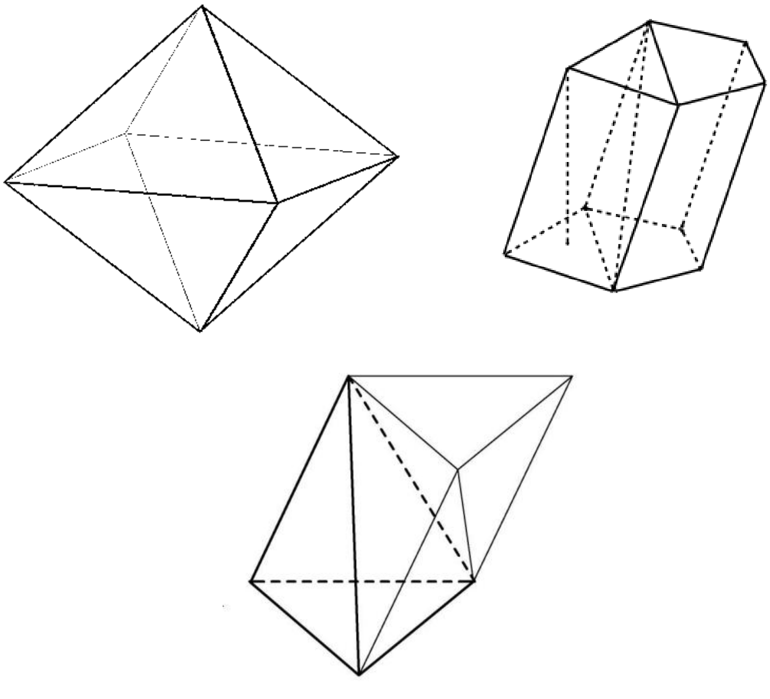

Fig. 1. Examples of bipyramids, prisms, tripyramids

The first of the adopted cluster shapes corresponds to the highest volume-to-surface-area ratio, making it the most probable at temperatures near the melting point.

When interpreting the radial distribution function (RDF) within the framework of the cluster model, methods must be defined for calculating coordination numbers within a cluster, followed by their averaging across the cluster and comparison (or fitting) with experimental RDF data. Unlike an ideal infinite crystal, where the coordination number for the k-th coordination sphere is fixed, in a cluster, the coordination number of an atom depends on its position. Therefore, it is necessary to calculate the average coordination number for each coordination sphere within a cluster. This can be achieved as follows:

$$Z_k = \sum_i N_{ki} Z_{ki} / N(\upsilon), \tag{1}$$

where N_{ki} is the number of atoms with coordination number Z_{ki} in the k-th coordination sphere, and $N(\upsilon)$ is the number of atoms in a cluster with υ atoms along its edge.

Ingeneral case the number of atoms in a cluster is expressed by cubed ependence on υ:

$$N(\upsilon) = \alpha\upsilon^3 + \beta\upsilon^2 + \gamma\upsilon + c, \tag{2}$$

where α, β, γ, c is determined for each of forms of clusters. Numbers:

$$Q_k(\upsilon) = \sum Z_{ki} N_{ki}(\upsilon), \tag{3}$$

Also can be presented by analogical dependence

$$Q_k(\upsilon) = Z_{k\infty}(\alpha_k\upsilon^3 + \beta_k\upsilon^2 + \gamma_k\upsilon + \delta_k). \tag{4}$$

In the first case, parameters are determined relatively simply. However, to obtain α_k, $\beta_k, \gamma_k, \delta_k$, it is necessary to calculate the value of $Q_k(\upsilon)$ for different numbers of atoms along the edge of the cluster, $N(\upsilon)$, for all coordination spheres used in the calculations. To this end, a computational algorithm was developed to determine these parameters, enabling the solution of the problem for all considered cluster shapes.

As known, when analyzing diffraction from a finite object, it is appropriate to incorporate the form factor V(x_p) into the structure factor, as described in [5].

$$a(S) = \sum_{-\infty}^{+\infty} V(x_p) \exp(iSx_p), \tag{5}$$

where x_p isradius which connects some a central atom is arbitrarily chosen from Pb y an atom, S is a factor of dispersions. Function of form

$$V(x_p) = \frac{1}{N} \sum_{-\infty}^{+\infty} \sigma(x_m)\sigma(x_{m\pm p}), \tag{6}$$

$\sigma(x_{m\pm p})$ — Evald functions; $\sigma(x_{m+p}) = \begin{Bmatrix} 1, & x_{mp} \epsilon V \\ 0, x_{mp} \Subset V & \end{Bmatrix}$, where V is a volume of some limited area.

The continuous functions of form were found $V(x_p)$ for all forms of clusters of structure of CVC.

For bipyramid:

1. In direction of normal to the verge

$V_1(x) = 1 - \frac{3x}{2L} + \frac{3x^2}{8L^2} + \frac{1x^3}{8L^3}$ (four directions of translation),

where= $\frac{a}{\sqrt{2}}$, a — large diagonal of bipyramid.

2. In direction of diagonals

$V_2(x) = \left(1 - \frac{x}{2L}\right)^3$(two directions of translation),

where $L = a\sqrt{2}$.

For both cases of $0 \le x \le L$

An important task is the application of Fourier transforms to characterize the types of diffraction peaks.

$$i(S) = \frac{1}{d} \int_{-L}^{L} V(x)\, e^{iS_0x} dx. \tag{7}$$

The characteristic cluster size L is taken into account for normals to the family of reflecting planes. Additionally, the multiplicity of different translations is considered.

In the first case of translation.

$i_1(S) = \frac{3L}{2d\alpha^4}[(1 - \cos\alpha) + 2\alpha^2\left(1 - \frac{1}{4}\cos\alpha\right) - 2\alpha\sin\alpha]$.

In second case of translation

$i_2(S) = \frac{3L}{2d\alpha^4}[2\alpha^2 - (1 - \cos 2\alpha)]$.

General intensity —

$i(S) = \frac{L}{2d\alpha^4}[6\alpha^2 - \alpha^2\cos\alpha - 2sin^2\alpha - 4\alpha\sin\alpha - 2\cos\alpha + 2]$.

For tripyramid:

1. In direction of normal to the verge

$V_1(x) = (1 - \frac{x}{L})^3$(two directions of translation),

2. In direction of diagonals

$V_2(x) = \left(1 - \frac{x}{L}\right)^3$(two directions of translation),

For the first case of 0 ≤ x ≤ L/2, for the second 0 ≤ x ≤L.

In first case of translation

$i_1(S) = \frac{3L}{2d\alpha^4}[(1 - \cos\alpha) + 2\alpha^2\left(1 - \frac{1}{4}\cos\alpha\right) - 2\alpha\sin\alpha]$

In second case of translation

$i_2(S) = \frac{3L}{4d\alpha^4}[2\alpha^2 - (1 - \cos 2\alpha)]$.

General intensity —

$i(S) = \frac{L}{2d\alpha^4}[6\alpha^2 - \alpha^2\cos\alpha - sin^2\alpha - 4\alpha\sin\alpha + cos^2\alpha + 1]$.

For a prism, there are three independent translational directions perpendicular to its faces. These directions are also perpendicular to the faces of a bipyramid that forms part of the prism’s complement. By knowing the form factors for the bipyramid and tripyramid (two of which compose the prism), a discrete form can be derived:

$$V(x) = \frac{V_{bp} \cdot V_{bp}(x) + 2 \cdot V_{thp} \cdot V_{thp}}{V_{bp} + 2 \cdot V_{thp}},$$

where $V(x) = \frac{V_{eq}}{V}$

$$V_1(x) = \frac{2}{3}\left(1 - \frac{3}{2}\cdot\frac{x}{L} + \frac{3}{8}\cdot\frac{x^2}{L^2} + \frac{1}{8}\cdot\frac{x^3}{L^3}\right) + \frac{1}{3}(1 - \frac{x}{L})^3.$$

1. In direction of "short" diagonals

$V_2(x) = (1 - \frac{x}{L^1})^3$ (two directions of translation),

where $L^1 = 2L$.

2. In direction of "long" diagonal

$V_3(x) = (1 - \frac{x}{L^1})^2$ (one direction of translation),

where $L^1 = 2L$.

In first case of translation

$i_1(S) = \frac{L}{d\alpha^4}[\alpha^2\left(4 - \frac{1}{2}\cos\alpha\right) - 3(1 - \cos\alpha) - 2\alpha\sin\alpha]$.

In the second —

$i_2(S) = \frac{3L}{2d\alpha^4}[2\alpha^2 - (1 - \cos 2\alpha)]$.

In the third —

$i_3(S) = \frac{L}{d\alpha^4}[2\alpha^2 - \alpha\sin(2\alpha)]$.

General intensity —

$$i(S) = \frac{1}{2}i_1 + \frac{1}{3}i_2 + \frac{1}{6}i_3$$

$$i(S) = \frac{L}{d\alpha^4}[\frac{10}{3}\alpha^2 + \frac{1}{4}(6 - \alpha^2) \cdot \cos\alpha - \frac{1}{2}(1 - \cos(2\alpha) - (1 + \alpha \cdot \sin(\alpha)) - \frac{1}{6}(3 + \alpha \cdot \sin(2\alpha)).$$

For all forms of clusters — $\alpha = S \cdot L$, d is between plane distance.

The computational program within the framework of the cluster model was developed according to the following scheme:

1. Input of the experimental structure factor a(S), where S is the magnitude of the wavevector change during scattering.
2. Calculation of the radial distribution function (RDF) based on the type of diffraction peak. The apodization method, as described in [6,7], was used, which involves applying a weighting function during the computation of the RDF using Tikhonov regularization to solve diffraction problems for macroscopically isotropic structures. This method significantly reduces oscillatory components caused by measurement errors and the finite upper limit of the wavevector change. In the absence of a weighting function, the procedure results in broadening of the RDF peaks.

$$G(r) = (4\pi\tau)^{-\frac{1}{2}}\int_{-\infty}^{\infty} 4\pi x\rho(x)\exp\left(-\frac{(r-x)^2}{4\tau}\right)dx = 4\pi r\rho_0 + \frac{2}{\pi}\int_0^{S_m} S[a(S)-1]e^{-\tau S^2}\sin(\mathrm{Sr})\cdot dr,$$

where τ is a constant of apodization, $\rho(x)$ is a local atomic closeness. Thus

$$4\pi r\rho(r) = \sum_k \frac{z_k}{r_{k\sqrt{2\pi\sigma^2}}}\exp\left(-\frac{(r-r_k)^2}{2\sigma^2}\right).$$

In right part of equalization $G(r)$ can be found minimization of quadratic form

$$Q = \int_{r_1}^{r_2}\{G(r)-G_e(r)\}^2 dr. \tag{8}$$

A system of nonlinear transcendental equations was solved using the gradient descent method. The procedure was as follows:

Initial values of the parameters z_k, r_k, σ^2 were estimated based on assumptions about the short-range order, corresponding to the position of the diffraction peak. The parameter σ^2, related to the speed of sound propagation and the nearest interatomic distances, was determined accordingly. The values of z_k were estimated based on the average effective cluster sizes in the melt and their shapes. By selecting a specific effective cluster shape, its average size was adjusted to minimize the deviation between the theoretical and experimental diffraction peak profiles.

The peak profile was approximated by the expression:

$$i(S) = \frac{B}{d_{nk1}}\int_0^{\infty} g(L)dL\int_{-L}^{L} V\left(\left|\frac{x}{L}\right|\right)\cos Sxdx, \tag{9}$$

where model function of distribution of clusters for to the sizes:

$$g(L) = AL^{\frac{3n}{2}}\exp\left(-\beta L^m\right). \tag{10}$$

m=2-3 (the best approximation answers m=3, n=1).

Coefficient A it is determined from the condition of setting of norms

$$\int_0^{\infty} g(L)dL = 1$$

Minimization (9) is determine $z_k, r_k, \sigma^2$are the specified values for 30 co-ordinating spheres.

The following structural parameters were obtained from the approximation results:

- Average interatomic distance,
- Average distance between clusters,
- Optimal cluster size.

For the investigated object, as reported in [4], results were obtained for temperatures ranging from near the melting point of 40°C (Tm=38.9°C T_m = 38.9°C Tm=38.9°C) to 60°C, 240°C, and 360°C. This range includes the interval of 250—300°C, where anomalies in the temperature dependence of viscosity and density are observed, along with a significant change in the first peak of the structure factor a(S), indicating a substantial change in the short-range order structure of liquid rubidium [1, 2].

Tabl. 1 presents the values of the structural parameters for the aforementioned temperatures. As shown in Fig. 2, at 240°C, an anomalous decrease in the average interatomic distance is observed, accompanied by a sharp increase in the average distance between clusters, followed by a decrease at 360°C.

Table 1. Parameters of structure

	Middle between atomic distance, a_1(Å)	Optimal size of cluster, L_{opt}, Å	Middle distance is between clusters, D_1, Å
Rb -40°C, ρ_0=0,01037			
bipyramid	5,7411	13,9595	0,13565
tripyramid	5,7443	13,296	0,1189
prism	5,7458	13,5846	0,1155
Rb - 160°C, ρ_0=0,00988			
bipyramid	5,761	13,295	0,323
tripyramid	5,772	12,333	0,267
prism	5,76	12,605	0,3123

Continue of the table 1

Rb - 240°C, ρ_0=0,00971			
bipyramid	5,7399	12,674	0,567
tripyramid	5,755	12,756	0,518
prism	5,732	11,982	0,567
Rb - 360°C, ρ_0=0,00934			
bipyramid	5,902	11,379	0,264
tripyramid	5,894	10,494	0,271
prism	5,899	10,653	0,259

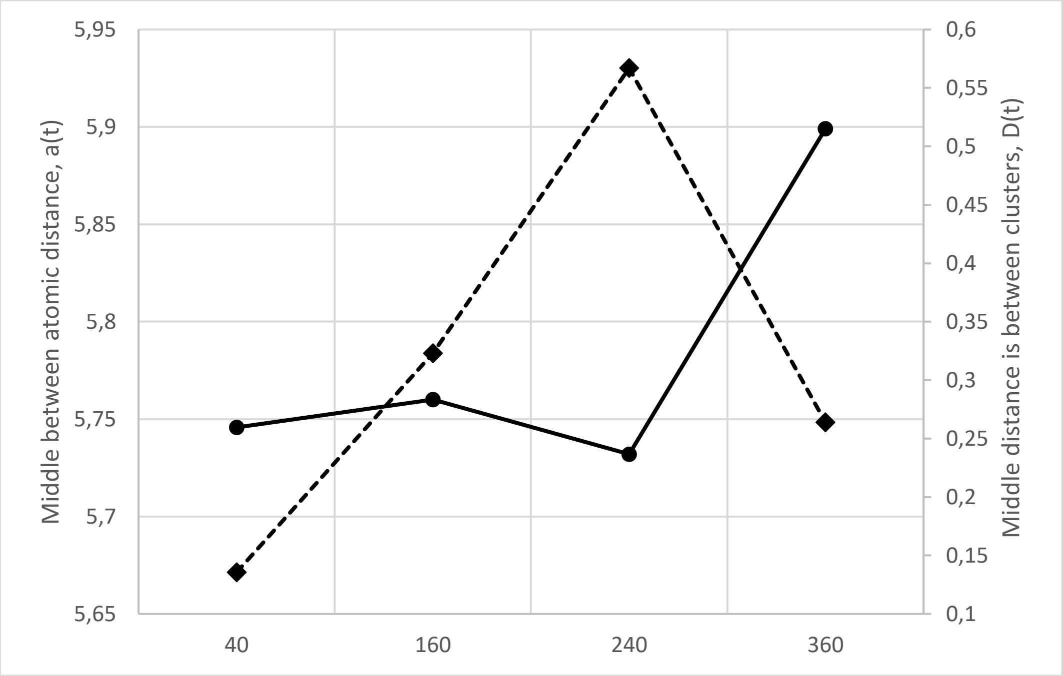

Fig. 2. Dependences of parameters of structure to the rubidium from a temperature

As shown in Fig. 3, the dependence of optimal cluster size on temperature in the range of 40°C to 160°C clearly corresponds to the bipyramid shape, which has a volume-to-surface-area ratio of 0.17, the highest among the considered shapes and thus the most stable. This is further supported by the observed decrease in cluster size with increasing temperature in this range.

For higher temperatures (240°C and 360°C), the values obtained for the bipyramid do not correspond to experimental observations, as they do not correlate with the changes in the average interatomic distance a(t) and the average distance between clusters D(t) in this range, nor do those for the prism (with a volume-to-surface-area ratio of 0.15). Significant correlation in this temperature range is observed only for the tripyramid, which has the lowest volume-to-surface-area ratio of 0.14 and the highest total surface energy of the clusters. These results indicate the presence of a second-order phase transition at approximately 240°C, driven by a change in cluster shape from bipyramid to tripyramid. This process is accompanied by an increase in the total surface area of the clusters and, consequently, their surface energy.

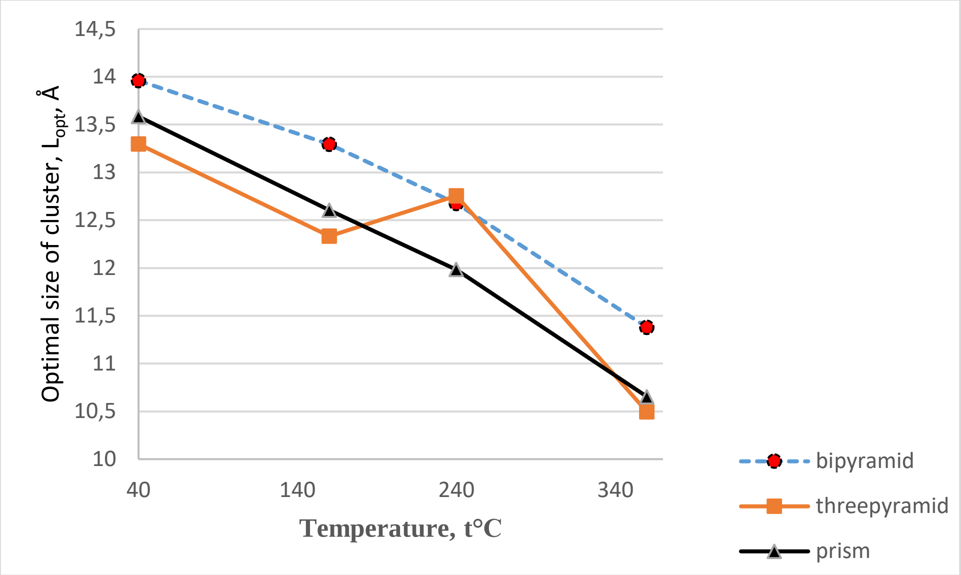

Fig. 3. Dependences of optimal cluster sizes are on a temperature

Conclusions

For the object considered in [4], the following results were obtained: average interatomic distance, optimal cluster size, and average distance between clusters. The temperature dependence of the structural parameters of molten rubidium was studied in the temperature range from just below the melting point 40°C ($t°_{pl}$=38,9°C) to 360°C. The developed computational algorithm, implemented in the utilized software, ensured an approximation accuracy of 0.05 %.

Fig. 3 presents the dependence of optimal cluster size on temperature in the range of 40°C—160°C. These dependencies likely correspond to a bipyramidal form, for which the volume-to-surface-area ratio equals 0.17 — the highest and, hence, the most stable. This is also supported by the observed decrease in cluster size with increasing temperature within this range.

At higher temperatures (240°C and 360°C), the values obtained for the bipyramidal model no longer correspond to reality, as they do not match the observed changes in a(t) and D(t). Similar discrepancies were found for the prism-shaped model (volume-to-surface-area ratio = 0.15), which also does not align with the experimental trends of a(t) and D(t). A significant correlation in this temperature range is observed only for the three-pyramidal model, which has the smallest volume-to-surface-area ratio (0.14) and the highest total surface energy of the clusters.

These findings suggest the occurrence of a second-order phase transition at approximately 240°C, likely associated with a change in cluster geometry from bipyramidal to tripyramidal. This transition is accompanied by an increase in the total cluster surface area and, consequently, their surface energy.

References

[1] Wax, J. F., & Bryk, T. (2017). Analyzing the dynamic structure of liquid metals and alloys. *EPJ Web of Conferences*, *151*, 02005. https://doi.org/10.1051/epjconf/201715102005

[2] Bryk, T., Schirmacher, W., & Ruocco, G. (2022). Comment on “Deformations, relaxation, and broken symmetries in liquids, solids, and glasses: A unified topological field theory”. Physical Review E, 106(3), 036601. DOI 10.1103/physreve.106.036601 https://arxiv.org/pdf/2203.05039

[3] Louzguine-Luzgin, D. V. (2022). Structural changes in metallic glass-forming liquids on cooling and subsequent vitrification in relationship with their properties. *Materials*, *15*(20), 7285. https://doi.org/10.3390/ma15207285

[4] Baglyuk, G. A., Vlasova, O. V., Kartuzov, V. V., Mamonova, A. A., Mogila, N. V., & Rozhenko, N. M. (2016). Features of the application of the Tikhonov regularization method for determining

the parameters of the defective state of mechanically activated iron powder. *Mathematical Models and Computational Experiment in Materials Science*, *18*, 72–79. http://www.materials.kiev.ua/article/2126

[5] Grygoriev, O. M., Kartuzov, V. V., & Rozhenko, N. M. (2017). Improving the accuracy of quantitative estimates of the Hall-Williamson graphical method through digital processing of XRD diffractograms. *Electron Microscopy and Strength of Materials. Series: Physical Materials Science, Structure and Properties of Materials, 23*, 16–35. http://www.materials.kiev.ua/publications/EMMM/2017/1.pdf

[6] Caralampio, D. Z., Martínez, J. M., Pappalardo, R. R., & Marcos, E. S. (2017). The hydration structure of the heavy-alkalines Rb+ and Cs+ through molecular dynamics and X-ray absorption spectroscopy: Surface clusters and eccentricity. *Physical Chemistry Chemical Physics, 19*(42), 28993–29004. https://doi.org/10.1039/C7CP05346K

[7] Gorelli, F. A., De Panfilis, S., Bryk, T., Ulivi, L., Garbarino, G., Parisiades, P., & Santoro, M. (2018). Simple-to-complex transformation in liquid rubidium. *The Journal of Physical Chemistry Letters, 9*(11), 2909–2913. https://doi.org/10.1021/acs.jpclett.8b01094

Список використаної літератури

1. Wax J. F., Bryk T. Analyzing the dynamic structure of liquid metals and alloys. 16th International Conference on Liquid and Amorphous Metals (LAM-16). 2017. Vol. 151. 02005. DOI: https://doi.org/10.1051/epjconf/201715102005.
2. Bryk T., Schirmacher W., Ruocco G. Comment on “Deformations, relaxation, and broken symmetries in liquids, solids, and glasses: A unified topological field theory”. Physical Review E. 2022. Vol. 106, iss. 3. 036601. DOI: https://doi.org/10.1103/physreve.106.036601 URL: https://arxiv.org/pdf/2203.05039
3. Louzguine-Luzgin D. V. Structural changes in metallic glass-forming liquids on cooling and subsequent vitrification in relationship with their properties. Materials. 2022. Vol. 15, № 20. 7285. DOI: https://doi.org/10.3390/ma15207285 URL: https://www.mdpi.com/1996-1944/15/20/7285
4. Баглюк Г. А., Власова О. В., Картузов В. В. та ін. Особливості застосування методу регуляризації Тихонова до визначення параметрів дефектного стану механоактивованого порошку заліза. Математичні моделі і обчислювальний експеримент в матеріалознавстві. Київ: ІПМ ім. І. М. Францевича НАН України, 2016. № 18. С. 72–79. URL: http://www.materials.kiev.ua/article/2126
5. Григор’єв О. М., Картузов В. В., Роженко Н. М. Підвищення точності кількісних оцінок графічного методу Холла-Вільямсона за рахунок цифрової обробки XRD-дифрактограм. Електронна мікроскопія та міцність матеріалів. Серія: Фізичне матеріалознавство, структура та властивості матеріалів. 2017. № 23. С. 16–35. URL: http://www.materials.kiev.ua/publications/EMMM/2017/1.pdf
6. Caralampio D. Z., Martínez J. M., Pappalardo R. R., Marcos E. S. The hydration structure of the heavy-alkalines Rb+ and Cs+ through molecular dynamics and X-ray absorption spectroscopy: surface clusters and eccentricity. Physical Chemistry Chemical Physics. 2017. Vol. 19, № 42. С. 28993–29004. DOI: https://doi.org/10.1039/C7CP05346K
7. Gorelli F. A., De Panfilis S., Bryk T. et al. Simple-to-complex transformation in liquid rubidium. The Journal of Physical Chemistry Letters. 2018. Vol. 9, № 11. С. 2909–2913. DOI: https://doi.org/10.1021/acs.jpclett.8b01094 URL: https://pubs.acs.org/doi/10.1021/acs.jpclett.8b01094

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