Original paper

On the problem of observing contact melting in a molecular dynamics experiment in Ni-Al bimetallic nanolayer

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Abstract: Using a bimetallic *Ni-Al* nanolayer as an example, molecular dynamics simulations of contact melting during annealing at 900 K were performed. The open-source LAMMPS software and embedded atom potential were used for this study. The interest in this research object stemmed from the complexity of the phase diagram, while the choice of temperature for the molecular dynamics experiment (900 K) was determined by considering the contact melting temperature for the macroscopic *Ni-Al* system and the potential size effect. Furthermore, this temperature is lower than the melting point of the lower-melting element, i.e. aluminum. During annealing for up to 100 ns, several characteristic temperatures were identified, corresponding to different stages of the diffusion process in the bimetallic *Ni-Al* nanolayer. The evolution of the local structure was observed using the open-source Ovito software with a modifier corresponding to the Ackland-Jones method. This approach analyzes the geometry of the angles between the bond vectors of a selected atom with its nearest neighbors. Over the selected time interval (100 ns), interface movement was identified in the *Ni-Al* system, but the crystalline transition layer «prevents» further «activation» of contact melting. This effect is observed for the first time for contact melting in nanoscale metallic systems.

Keywords: contact melting, bimetallic Ni-Al nanolayer, LAMMPS, molecular dynamics simulation, embedded-atom potential, local structure, Ackland-Jones method.

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О проблеме наблюдения контактного плавления в молекулярно-динамическом эксперименте на биметаллическом нанослое Ni-Al

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Аннотация: На примере биметаллического налослоя *Ni-Al* проведено молекулярно-динамическое моделирование контактного плавления в ходе отжига при температуре 900 К. С этой целью использовалось открытое ПО LAMMPS и потенциал погруженного атома. Интерес к выбранному объекту исследования обусловлен сложностью фазовой диаграммы, в то время как выбор температуры для молекулярно-динамического эксперимента (900 К) определен с учетом температуры контактного плавления для макроскопической системы *Ni-Al* и возможного размерного эффекта. Кроме того, данная температура ниже температуры плавления более легкоплавкого элемента, т.е. алюминия. В процессе отжига в течение 100 нс выделены несколько характерных температур, отвечающих различным этапам диффузионного

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процесса в биметаллическом нанослое *Ni-Al*. Эволюцию локальной структуры наблюдали с использованием открытого программного комплекса Ovito с модификатором, отвечающим использованию метода Экленда-Джонса. При данном подходе для выбранного атома анализируется геометрия углов между векторами связей с его ближайшими соседями. На выбранном временном интервале (100 нс) было идентифицировано движение границы раздела в системе *Ni-Al*, однако кристаллический переходный слой «мешает» дальнейшей «активации» контактного плавления. Такой эффект наблюдается впервые для контактного плавления наноразмерных металлических систем.
Ключевые слова: контактное плавление, биметаллический налослой Ni-Al, LAMMPS, молекулярно-динамическое моделирование, потенциал погруженного атома, локальная структура, метод Экленда-Джонса.

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1. Introduction

The use of bimetallic materials in modern industrial technologies is driven, among other things, by the potential to combine the unique properties of both metals (e.g., high strength and corrosion resistance). Furthermore, studying processes at the phase interface allows for control over the thickness and structure of the transition zone. Contact melting is a physicochemical phenomenon in which the formation of a liquid phase at the interface of dissimilar materials occurs at a temperature below the melting point of each component. With the transition to nanoscale bimetallic systems, specific features of contact melting emerge [1], which are due to the size effect of the contact melting temperature [2]. This fact, in turn, determines the relevance of studies of contact melting in binary nanolayers, in particular with the use of atomistic simulation [3-5], which allows us to predict the temperature ranges of stability (the absence of destruction of the local structure and the manifestation of segregation processes under thermally induced influence) when they work as active and passive elements in nanodevices of a wide range of applications: from electronics to aircraft construction.

Along with the size effect noted above, nanoscale bimetallic systems are characterized by a change in phase diagrams [6]. Moreover, as an analysis of modern Russian [7, 8] and foreign [9] sources shows that phase diagrams for macro-samples also have some features for the temperature ranges of formation of intermetallic compounds in the $Ni-Al$ system (see Fig. 1).

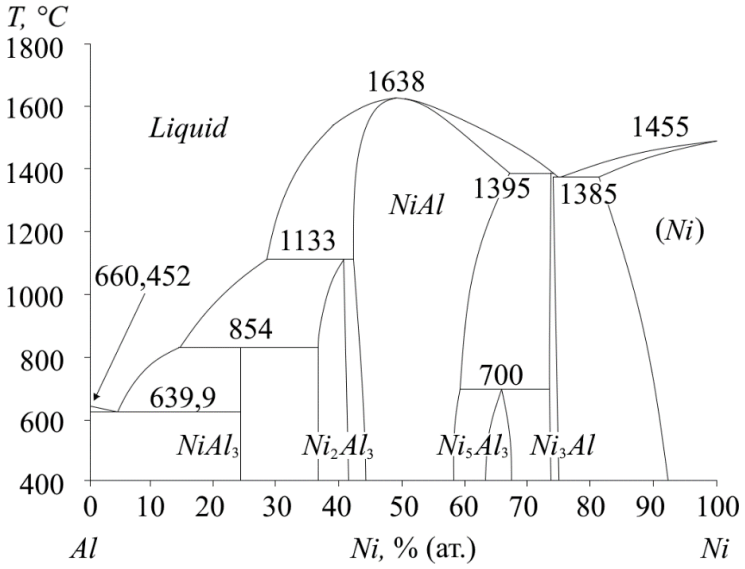

Fig. 1. Phase diagram of the nickel-aluminum system [8].

It is obvious that difficulties may arise in interpreting the phase diagram of the binary $Ni-Al$ system due to the presence of a large number of phase states. Information on the crystal structure of the compounds formed in the $Ni-Al$ system is given in Table 1. It should also be noted that, according to [10], despite the fact that the phase diagram of the nickel-aluminum system has been well studied for macroscopic samples, discrepancies still exist regarding the concentration range of 70-80 at.% nickel.

Thus, in this work, the object of study is a bimetallic nanoscale layer of $Ni-Al$, and the interpretation of the results will be carried out on the basis of the phase diagram presented in Fig. 1, which was obtained for macroscopic samples.

Table 1. Crystal structure of compounds of the $Ni-Al$ system [10].

Compound	Aluminum content, at. %	Prototype	Lattice parameters, Å		
			a	*b*	*c*
$NiAl_3$	75	$NiAl_3$	6,611	7,366	4,812
Ni_2Al_3	60	Ni_2Al_3	4,036	-	4,90
$NiAl$	50,2	$CsCl$	2,887	-	-
Ni_5Al_3	34,9	Pt_5Ga_3	7,475	6,727	3,732
Ni_3Al	25	Cu_3Au	3,589	-	-

2. Statement of the problem and results of molecular dynamics experiments

A distinctive feature of this work, compared to the approach proposed earlier [11] for binary and multicomponent metallic nanoparticles, is the use of the Ackland-Jones method [12] as a basic modifier for the analysis of the local structure in a molecular dynamics experiments. Unlike other methods used for the analysis of the local structure [13-15] in the Ovito software [16], the Ackland-Jones method does not use structural parameters based on interatomic distances (which can be strongly distorted by thermal vibrations during

thermally induced exposure), but analyzes the geometry of the angles between the bond vectors of the selected atom with its nearest neighbors.

Molecular dynamics simulations were performed in the open-source LAMMPS software [17] using the embedded atom potential [18]. The simulations were performed at a temperature of 900 K, which is below the melting point of the lower-melting element, aluminum [19], and also below the contact melting temperature for the macrosample of 640°C (913 K) [20], and for the films of 650°C (923 K) [21]. Periodic boundary conditions were used, the simulation cell sizes at the initial time were: (32,4×120,7×32,4 Å), 0,2 ns (34,7×120,6×34,8 Å), 10 ns (34,6×120,4×34,6 Å), 100 ns (35,1×117,0×35,2 Å), in the initial state an fcc cell was used. The first 0,1 ns of the simulation were performed in the NPT ensemble, the rest of the simulation time in the NVT ensemble, respectively. An example of the initial configuration is shown in Fig. 2.

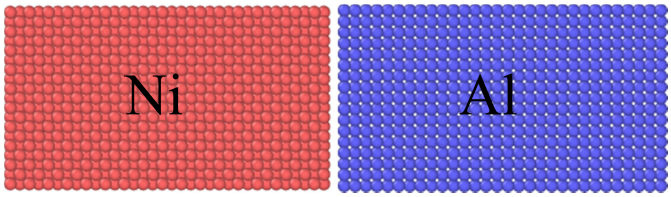

Fig. 2. Initial configuration of the $Ni-Al$ bimetallic nanolayer.

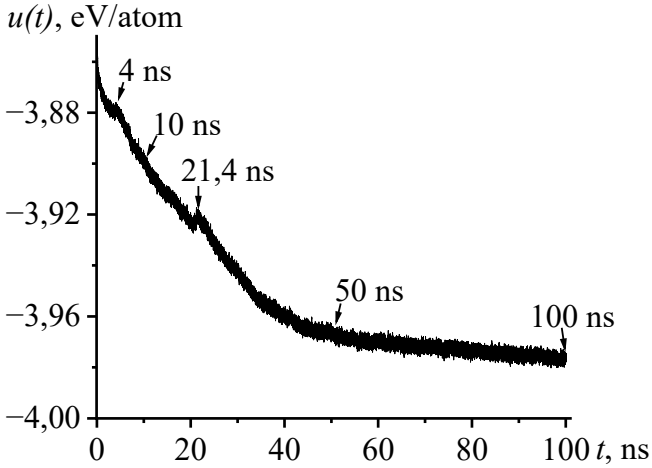

Fig. 3. Time dependence of the specific potential energy of the bimetallic $Ni-Al$ nanolayer.

For a preliminary analysis of structural transformations in the $Ni-Al$ bimetallic nanolayer, it is necessary to examine the dependence of the specific potential energy of the system on annealing time (see Fig. 3). Arrows indicate the characteristic time points studied in this study, at which a change in the behavior of the kinetic dependence occurs (the presence of a jump or some stabilization of the specific potential energy). For the time points shown in Fig. 3, it is of interest to visualize the displacement of nickel and aluminum atoms during annealing (see Fig. 4). At the selected time interval (100 ns), nickel atoms reach the outer boundary of the bilayer, represented by aluminum. At the same time, aluminum atoms do not move throughout the entire volume of

the nickel bilayer (only about a third of the distance over which the presence of aluminum atoms is identified), i.e., the interface of the $Ni-(Ni-Al)$ system is clearly identified.

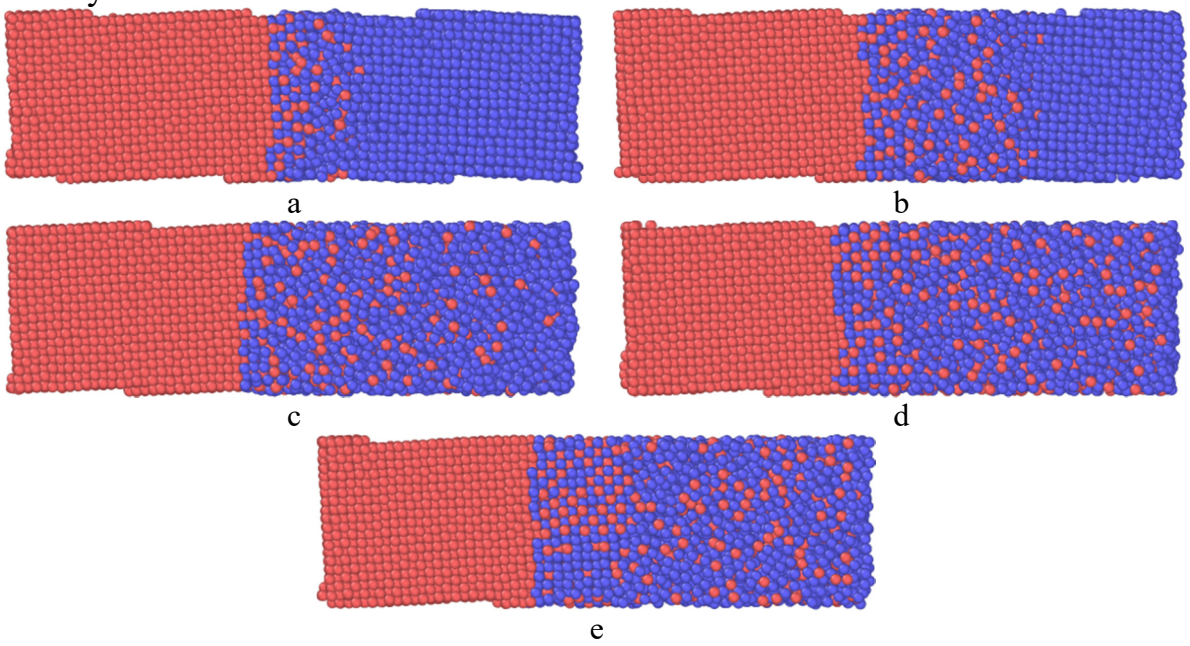

Fig. 4. Visualization of the diffusion process in the bimetallic $Ni-Al$ nanolayer: a – 4 ns, b – 10 ns, c – 21.4 ns, d – 50 ns, e – 100 ns.

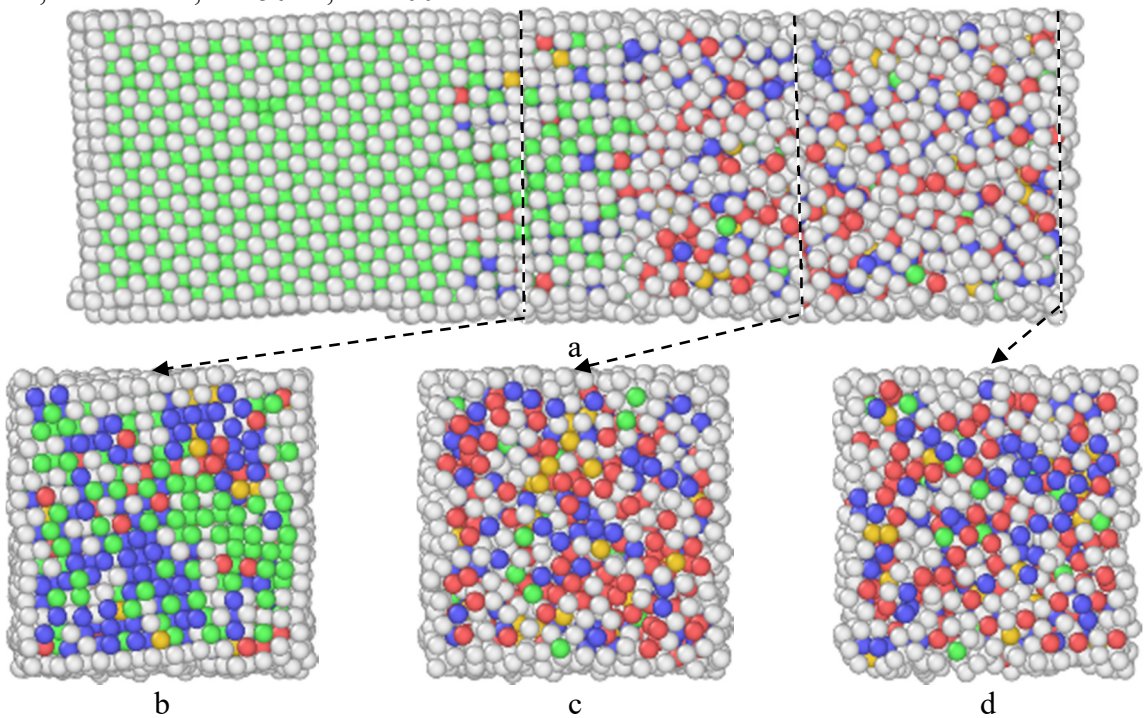

Fig. 5. Spatial distribution of local phases in the bimetallic $Ni-Al$ nanolayer at 100 ns: a – profile, b-d – corresponding sections (location indicated by dotted lines). The local fcc environment is colored green, hcp is red, bcc is blue, and icosahedral symmetry cores are yellow; gray corresponds to atoms with an unidentified local environment.

This fact is of particular scientific interest from the standpoint of the

patterns of local structure formation in different regions of the bilayer (see Fig. 5), which is why it is necessary to trace the evolution of the local structure using the Ackland-Jones method in the Ovito software [16].

3. Conclusion

Even at a sufficiently high temperature (900 K), a noticeable time is required to «initialize» the contact melting process in the $Ni-Al$ bimetallic layer. Despite the fact that the interface motion in the $Ni-Al$ system is identifiable on the studied time scale (see Fig. 4), it is the crystalline transition layer that «hinders» further «activation» of contact melting. According to our preliminary estimates, this effect was observed on time scales up to 300 ns. Thus, using a binary $Ni-Al$ nanolayer as an example, it is shown that the structure formation in the transition contact layer (its recrystallization) can slow down the contact melting process, which is a particular problem for a molecular dynamics experiment (see Fig. 5, panels b-d). We also note that the annealing procedure at the contact melting temperature was carried out experimentally for one hour to observe eutectic structures in $Ni-Al$ films [21]; such time intervals are clearly inaccessible in molecular dynamics experiments.

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References:

1. Akhkubekov A.A., Orkvasov T.A., Sozaev V.A. *Kontaktnoe plavlenie metallov i nanostruktur na ikh osnove: monografiya* [Contact melting of metals and nanostructures based on them: monograph]. M.: Fizmatlit Publ., 2008. – 152 p. (In Russian).
2. Korotkov P.K., Orkvasov T.A., Sozaev V.A. The size effect in contact melting of metals, *Technical Physics Letters*, 2006, vol. 32, issue 1, pp. 61-63. DOI: 10.1134/S1063785006010202.
3. Samsonov V.M., Kuzmin N.B., Talyzin I.V. et al. Application of fractal analysis to characterize the contact melting process in a bimetallic Cu–Ag nanolayer, *Theoretical Foundations of Chemical Engineering*, 2025, vol. 59, issue 3, pp. 549-554. DOI: 10.1134/S0040579525601773.
4. Samsonov V.M., Kuz'min N.B., Sdobnyakov N.Yu. et al. Contact melting in bimetallic Cu-Ag nanolayer: Molecular dynamics simulation and fractal analysis, *Nano-Structures & Nano-Objects*, 2025, vol. 43, art. no. 101496, 10 p. DOI: 10.1016/j.nanoso.2025.101496.
5. Samsonov V.M., Kuzmin N.B., Talyzin I.V. et al. Contact melting effect in a molecular dynamics model of a noneutectic Cu–Ni bilayer, *Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques*, 2025, vol. 19, issue 6, pp. 1691-1697. DOI: 10.1134/S1027451025702374.
6. Guo X., Li S., Wang G. Phase diagram of continuous binary nanoalloys: size, shape and segregation effects, *Scientific Reports*, 2017, vol. 7, art. №0 41990, 10 p. DOI: 10.1038/srep41990.
7. *Diagrammy sostoyaniya dvojnykh metallicheskikh sistem: spravochnik: v 3 tomakh* [Phase diagrams of binary metallic systems: a reference book: in 3 volumes] / ed, by N.P. Lyakishev. M.: Mashinostroenie Publ., 1996-2000, vol. 1, 1996, 992 p.; vol. 2, 1997, 1024 p.; vol. 3, book 1, 2000, 872 p.; vol. 3, book 2, 2000, 448 p. (In Russian).
8. Zhikharev A.V., Bystrov S.G., Bayankin V.Ya. et al. Vliyanie lazera na formirovanie soedinenij Ni-Al v poverkhnostnykh sloyakh nikelevoj fol'gi v zavisimosti ot plotnosti moshchnosti lazernogo izlucheniya [The laser influence on the formation of Ni-Al compounds in the nickel foil surface layers depending on the laser radiation power density], *Khimicheskaya fizika i mezoskopiya [Chemical Physics and Mesoscopics]*, 2023, vol. 25, no. 2, pp. 239-249. DOI: 10.15350/17270529.2023.2.22. (In Russian).

9. Huang W., Chang Y.A. A thermodynamic analysis of the Ni-Al system, *Intermetallics*, 1998, vol. 6, issue 6 pp. 487-498. DOI: 10.1016/S0966-9795(97)00099-X.
10. Shevtsova L.I. *Struktura i mekhanicheskie svojstva materialov na osnove alyuminida nikelya, poluchennykh po tekhnologii iskrovogo plazmennogo spekaniya poroshkovykh smesej* [Structure and mechanical properties of nickel aluminide-based materials obtained by spark plasma sintering of powder mixtures]. Cand. tech. sci.: 05.16.09. Novosibirsk, NSTU Publ., 2015, 200 p. (In Russian).
11. Sdobnyakov N.Yu. *[Modelirovanie strukturnykh prevrashchenij v odnokomponentnykh i mnogokomponentnykh metallicheskikh nanosistemakh: uchebnik]* Simulation of structural transformations in single-component and multi-component metallic nanosystems: a textbook. Tver, Tver State University Publ., 2025, 408 p. DOI:10.26456/sny.2025.408. (In Russian).
12. Ackland G.J., Jones A.P. Applications of local crystal structure measures in experiment and simulation, *Physical Review B*, 2006, vol. 73, issue 5, pp. 054101-1-054104-7. DOI: 10.1103/PhysRevB.73.054104.
13. Larsen P.M., Schmidt S., Schiøtz J. Robust structural identification via polyhedral template matching modelling, *Modelling and Simulation in Materials Science and Engineering*, 2016, vol. 24, no. 5, art. № 055007, 18 p. DOI: 10.1088/0965-0393/24/5/055007.
14. Polak W.Z. Efficiency in identification of internal structure in simulated monoatomic clusters: Comparison between common neighbor analysis and coordination polyhedron method, *Computational Materials Science*, 2022, vol. 201, art. № 110882, 8 p. DOI: 10.1016/j.commatsci.2021.110882.
15. Tsuzuki H., Branicio P.S., Rino J.P. Structural characterization of deformed crystals by analysis of common atomic neighborhood, *Computer Physics Communications*, 2007, vol. 177, issue 6, pp. 518-523. DOI: 10.1016/j.cpc.2007.05.018.
16. Stukowski A. Visualization and analysis of atomistic simulation data with OVITO – the open visualization tool, *Modelling and Simulation in Materials Science and Engineering*, 2010, vol. 18, issue 1, pp. 015012-1-015012-7. DOI: 10.1088/0965-0393/18/1/015012.
17. LAMMPS Molecular Dynamics Simulator. Available at: www.url: http://lammps.sandia.gov. (accessed 02.05.2026).
18. Purja Pun G.P., Mishin Y. Development of an interatomic potential for the Ni-Al system, *Philosophical Magazine*, 2009, vol. 89, issue 34-36, pp. 3245-3267. DOI: 10.1080/14786430903258184.
19. *Svoystva elementov. Spravochnik* [Properties of elements. Handbook], ed. M.E. Drits, Moscow, Metallurgiya Publ., 1985, 672 p. (In Russian).
20. Shmorgun V.G., Trykov Yu.P., Bogdanov A.I. et al. Kinetika vzaimodejstviya alyuminiya i nikelya pri zhidkofaznom formirovanii diffuzionnoj zony [Kinetics of interaction between aluminum and nickel during liquid-phase formation of a diffusion zone], *Vestnik Sibirskogo gosudarstvennogo industrial'nogo universiteta [Bulletin of the Siberian State Industrial University]*, 2014, no. 2 (8), p. 3-6. (In Russian).
21. Lajpanov M.Z. *Kontaktnoe plavlenie i fazoobrazovanie makro-, mikrorazmernykh sistem med'-alyuminij, nikel'alyuminij, nikel'-olovo* [Contact melting and phase formation of macro- and micro-sized systems of copper-aluminum, nickel-aluminum, nickel-tin]. Cand. fiz.-mat. nauk: 01.04.07. Nal'chik: KBSU Publ., 2019, 103 p. (In Russian).

Библиографический список:

1. **Ахкубеков, А.А.** Контактное плавление металлов и наноструктур на их основе: монография / А.А. Ахкубеков, Т.А. Орквасов, В.А. Созаев. – М.: Физматлит, 2008. – 152 с.
2. **Коротков, П.К.** Размерный эффект контактного плавления металлов / П.К. Коротков, Т.А. Орквасов, В.А. Созаев // Письма в Журнал технической физики. – 2006. – Т. 32. – Вып. 2. – С. 28-32.
3. **Samsonov, V.M.** Application of fractal analysis to characterize the contact melting process in a bimetallic Cu–Ag nanolayer / V.M. Samsonov, N.B. Kuzmin, I.V. Talyzin et al. // Theoretical Foundations of Chemical Engineering. – 2025. – V. 59. – I. 3. – P. 549-554. DOI: 10.1134/S0040579525601773.
4. **Samsonov, V.M.** Contact melting in bimetallic Cu-Ag nanolayer: Molecular dynamics simulation and fractal analysis / V.M. Samsonov, N.B. Kuz'min, N.Yu. Sdobnyakov et al. // Nano-Structures & Nano-Objects. – 2025. – V. 43. – Art. № 101496. – 10 p. DOI: 10.1016/j.nanoso.2025.101496.
5. **Samsonov, V.M.** Contact melting effect in a molecular dynamics model of a noneutectic Cu–Ni bilayer / V.M. Samsonov, N.B. Kuzmin, I.V. Talyzin et al. // Journal of Surface Investigation: X-ray, Synchrotron and Neutron Techniques. – 2025. – V. 19. – I. 6. – P. 1691-1697. DOI: 10.1134/S1027451025702374.
6. **Guo, X.** Phase diagram of continuous binary nanoalloys: size, shape and segregation effects / X. Guo, S. Li, G. Wang // Scientific Reports. – 2017. – V. 7. – Art. №0 41990. – 10 p. DOI: 10.1038/srep41990.
7. Диаграммы состояния двойных металлических систем : справочник : в 3 томах / под общей редакцией Н. П. Лякишева. – М.: Машиностроение, 1996-2000. – Т. 1. – 1996. – 992 с.; – Т. 2. – 1997. – 1024 с.; – Т. 3.

– Кн. 1. – 2000. – 872 с.; – Т. 3. – Кн. 2. – 2000. – 448 с.
8. **Жихарев, А.В**. Влияние лазера на формирование соединений Ni-Al в поверхностных слоях никелевой фольги в зависимости от плотности мощности лазерного излучения / А.В. Жихарев, С.Г. Быстров, В.Я. Баянкин и др. // Химическая физика и мезоскопия. – 2023. – Т. 25. – № 2. – С. 239-249. DOI: 10.15350/17270529.2023.2.22.
9. **Huang, W.** A thermodynamic analysis of the Ni-Al system / W. Huang, Y.A. Chang // Intermetallics. – 1998. – V. 6. – I. 6. – P. 487-498. DOI: 10.1016/S0966-9795(97)00099-X.
10. **Шевцова, Л.И.** Структура и механические свойства материалов на основе алюминида никеля, полученных по технологии искрового плазменного спекания порошковых смесей: дис. ... канд. техн. наук: 05.16.09 / Шевцова Лилия Ивановна. – Новосибирск: НГТУ, 2015. – 200 с.
11. **Сдобняков, Н.Ю.** Моделирование структурных превращений в однокомпонентных и многокомпонентных металлических наносистемах: учебник / Н.Ю. Сдобняков. – Тверь: Тверской государственный университет, 2025. – 408 с. DOI:10.26456/sny.2025.408.
12. **Ackland, G.J.** Applications of local crystal structure measures in experiment and simulation / G.J. Ackland, A.P. Jones // Physical Review B. – 2006. – V. 73. – I. 5. – P. 054101-1-054104-7. DOI: 10.1103/PhysRevB.73.054104.
13. **Larsen, P.M.** Robust structural identification via polyhedral template matching modelling / P.M. Larsen, S. Schmidt, J. Schiøtz // Modelling and Simulation in Materials Science and Engineering. – 2016. – V. 24. – № 5. – Art. № 055007. – 18 p. DOI: 10.1088/0965-0393/24/5/055007.
14. **Polak, W.Z.** Efficiency in identification of internal structure in simulated monoatomic clusters: Comparison between common neighbor analysis and coordination polyhedron method / W.Z. Polak // Computational Materials Science. – 2022. – V. 201. – Art. № 110882. – 8 p. DOI: 10.1016/j.commatsci.2021.110882.
15. **Tsuzuki, H.** Structural characterization of deformed crystals by analysis of common atomic neighborhood / H. Tsuzuki, P.S. Branicio, J.P. Rino // Computer Physics Communications. – 2007. – V. 177. – I. 6. – P. 518-523. DOI: 10.1016/j.cpc.2007.05.018.
16. **Stukowski, A.** Visualization and analysis of atomistic simulation data with OVITO – the open visualization tool / A. Stukowski // Modelling and Simulation in Materials Science and Engineering. – 2010. – V. 18. – I. 1. – P. 015012-1-015012-7. DOI: 10.1088/0965-0393/18/1/015012.
17. LAMMPS Molecular Dynamics Simulator. – Режим доступа: www.url: http://lammps.sandia.gov. – 02.05.2026.
18. **Purja Pun, G.P.** Development of an interatomic potential for the Ni-Al system / G.P. Purja Pun, Y. Mishin // Philosophical Magazine. – 2009. – V. 89. – I. 34-36. – P. 3245-3267. DOI: 10.1080/14786430903258184.
19. Свойства элементов. Справочник / под общей ред. проф. М.Е. Дрица. – М.: Металлургия, 1985. – 672 с.
20. **Шморгун, В.Г.** Кинетика взаимодействия алюминия и никеля при жидкофазном формировании диффузионной зоны / В.Г. Шморгун, Ю.П. Трыков, А.И. Богданов и др. // Вестник Сибирского государственного индустриального университета. – 2014. – № 2 (8). – С. 3-6.
21. **Лайпанов, М.З.** Контактное плавление и фазообразование макро-, микроразмерных систем медь-алюминий, никельалюминий, никель-олово: дис. ... канд. физ.-мат. наук: 01.04.07 / Лайпанов Мурат Занарустумович. – Нальчик: КБГУ, 2019. – 103 с.