MATERIALS PHYSICS AND MECHANICS RESEARCH ARTICLE

Submitted: February 10, 2025 **Revised: April 22, 2025** **Accepted: May 12, 2025**

Influence of grain size of nanocrystalline titanium on its dissolution intensity in aluminum

G.M. Poletaev [1] ✉, **Y.V. Bebikhov** [2], **A.S. Semenov** [2]

[1] Polzunov Altai State Technical University, Barnaul, Russia

[2] Polytechnic Institute of North-Eastern Federal University, Mirny, Russia

✉ gmpoletaev@mail.ru

ABSTRACT

Using molecular dynamics simulations, this study investigates the influence of grain size of nanocrystalline titanium on its dissolution intensity in aluminum at various temperatures, compared to the dissolution of monocrystalline titanium. It is shown that the grain size in nanocrystalline titanium significantly affects the intensity of mutual dissolution of the components. This is explained by the fact that grain boundaries act as channels for accelerated diffusion, and as the average grain size decreases, the density of grain boundaries increases. In the case of grains on the order of several nanometers, the density of grain boundaries and the contribution of grain boundary diffusion are relatively high. For example, at a temperature of 800 K, which is significantly below the melting point of aluminum, dissolution in the model occurred more intensely for grain sizes smaller than 9 nm than for monocrystalline titanium at 1100 K – this temperature is not only 300 K higher but also corresponds to liquid aluminum. Thus, the nanocrystalline structure and high density of grain boundaries in titanium may be one of the reasons, alongside the energy stored in defects due to deformation, for the reduction in activation energy for the synthesis reaction in the Ti–Al system following mechanical processing of the initial mixture.

KEYWORDS

molecular dynamics • titanium • intermetallide • diffusion • grain boundary

***Funding**. The study was funded by the Russian Science Foundation (project No. 24-22-00092, https://rscf.ru/project/24-22-00092/).*

Citation: Poletaev GM, Bebikhov YV, Semenov AS. Influence of grain size of nanocrystalline titanium on its dissolution intensity in aluminum. *Materials Physics and Mechanics*. 2025;53(2): 13–24.
http://dx.doi.org/10.18149/MPM.5322025_2

Introduction

Intermetallic compounds of the Ti–Al system and their alloys possess a combination of properties such as high yield strength at elevated temperatures and good oxidation and corrosion resistance, along with relatively low density, making them promising for use as high-temperature structural materials, particularly in the aerospace and automotive industries [1–5]. It is known that non-equilibrium processing methods, including intensive deformation, mechanical alloying, rapid quenching, etc., allow for the creation of various unique non-equilibrium microstructures capable of enhancing the mechanical properties of intermetallic alloys [6–9]. One promising method for producing intermetallics, including those in the Ti-Al system, is pre-treatment before the high-temperature synthesis reaction stage through mechanical processing of the initial metal powders, such as by milling in planetary ball mills [10–16]. During this mechanochemical activation process, so-called mechanocomposites are formed, consisting of a matrix made from a more ductile component (in this case, aluminum), within which nanosized particles

Publisher: Peter the Great St. Petersburg Polytechnic University

of a more brittle component (titanium) are located [15,16]. Mechanical milling of the initial powders and the resulting nanocomposites are used, in particular, in the rapidly developing field of additive manufacturing [15,17]. This system is characterized by a high degree of non-equilibrium due to the high concentration of defects, interfaces, and internal stresses. One of the most interesting properties of such non-equilibrium systems consisting of nanocomposites is a significantly lower effective activation energy for the synthesis reaction compared to conventional powders: the synthesis reaction (ignition) begins at a temperature substantially lower than the melting point of aluminum [10–16].

Currently, the question remains open regarding what exactly is the main factor in the reduction of ignition temperature in mechanically activated mixtures. Among the reasons typically considered are the following: 1) preliminary mixing of components and a significant increase in their contact area; 2) accumulation of excess energy due to deformation in the form of various structural defects, which can be released as additional heat during structural relaxation; 3) a decrease in the melting point of aluminum due to the presence of a high concentration of defects or even an amorphous phase; 4) more intense mutual diffusion due to the presence of a high density of diffusion channels in the form of grain boundaries, predominantly in titanium.

The first reason mentioned, namely the increase in the contact area of the components, is sometimes cited as the main reason for the decrease in the activation energy of the synthesis reaction, often in combination with the second one, i.e. the accumulation of excess energy in the form of defects, as, for example, in [18,19], where molecular dynamics simulation of the deformation of round metal particles, their subsequent deformation and the initial stage of mutual diffusion was carried out. However, strictly speaking, an increase in only the contact area of the components cannot lead to a decrease in the activation energy of the synthesis reaction and, accordingly, the ignition temperature. This only leads to an increase in the intensity of dissolution, which, in particular, was shown by us in the study of the dissolution of a round titanium particle in aluminum [20], as well as in the simulation of mutual diffusion in the case of a flat interphase boundary [21].

The second mentioned reason is the accumulation of excess energy during deformation in the form of non-equilibrium defects in the structure of the components, such as grain boundaries, dislocations, disclinations, point defects, and their complexes. This cause for the reduction of activation energy for the synthesis reaction is identified as a primary factor in works such as [22–24]. Indeed, excess or accumulated potential energy can be released upon heating due to partial healing of the structure and a reduction in defect density. For instance, in [25,26], we demonstrated that during the recrystallization of metals with a nanocrystalline structure, characterized by a very high density of grain boundaries compared to conventional polycrystals, the release of energy and temperature increase can be significant and substantially influence diffusion processes.

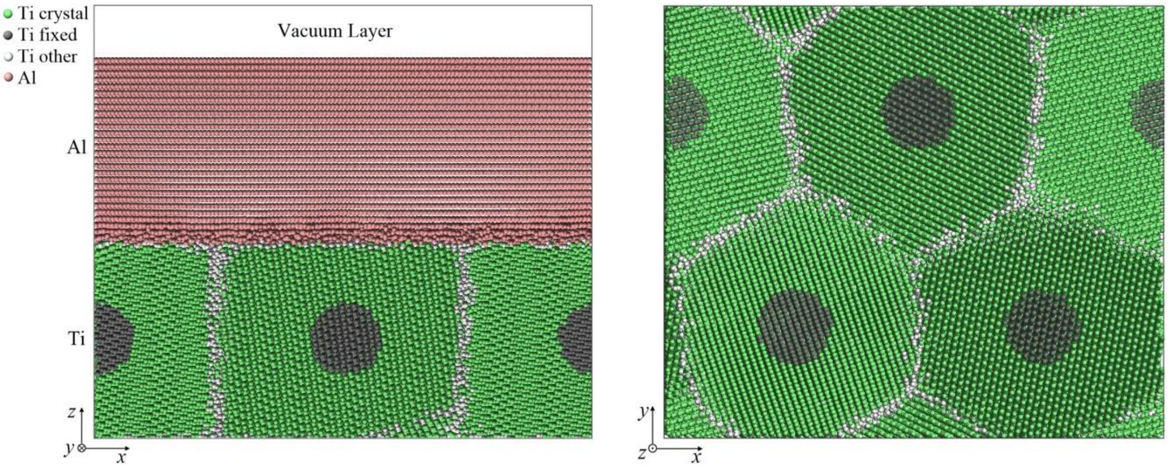
Sometimes, another reason for the reduction of ignition temperature in mechanically activated powders is considered to be the possible decrease in the melting point of nanocrystalline aluminum compared to conventional coarse-grained aluminum. It is known that the onset temperature for the high-temperature synthesis reaction in systems such as Ti–Al and Ni–Al, in the case of conventional powders, coincides with the melting point of aluminum. Numerous studies, primarily conducted through simulations, have indeed shown that nanomaterials exhibit what is known as the "size-dependent melting point depression phenomenon", meaning that the melting temperature of nanomaterials depends on their effective size: grain size, film thickness, and nanoparticle diameter. Regarding materials with a nanocrystalline structure, works [27–32] have demonstrated through molecular dynamics simulations that melting in these materials is not a homogeneous process; it typically begins at free surfaces and grain boundaries. A reduction in average grain size led to a decrease in the melting point of nanocrystalline Ag [28,29] and Al [30,31]. In [25,26], we also observed a decrease in the melting point for Ni nanoparticles with a nanocrystalline structure compared to monocrystalline particles. However, in another of our studies [20], dedicated to investigating the dissolution of a titanium nanoparticle in aluminum, it was shown that the structural state of titanium has a much greater influence on the intensity of mutual diffusion than the structural state of aluminum. Therefore, the reason related to a possible decrease in the melting point of aluminum does not seem to be primary in the case of reducing the onset temperature for the synthesis reaction in powders subjected to mechanical activation.

The fourth possible reason, which this work addresses, is the formation of a high concentration of accelerated diffusion channels in titanium due to intensive deformation, manifested as grain boundaries, dislocations, and pores. The role of these additional channels (primarily grain boundaries) is seen as one of the main factors, alongside the energy accumulated in defects. It is known that diffusion along grain boundaries is orders of magnitude more intense than diffusion in the bulk involving conventional point defects, and the presence of a high density of grain boundaries can lead to a sufficiently high rate of mutual diffusion, comparable to diffusion at the onset temperature of the reaction. This work aims to test this hypothesis and is dedicated to investigating, using molecular dynamics methods, the influence of grain size of nanocrystalline titanium on its dissolution intensity in aluminum at various temperatures compared to the dissolution of monocrystalline titanium.

Description of the model

To describe the interatomic interactions in the Ti–Al system, EAM potentials from [33] were used, which were derived based on comparisons with experimental data and *ab initio* calculations for various properties and structures of the metals Ti, Al, and the intermetallic compounds Ti_3Al and TiAl. These potentials have proven effective in various studies and have undergone successful validation across a wide range of mechanical and structural-energy properties of Ti-Al alloy systems [33–36].

The interphase boundary between Ti and Al was created at the center of the simulated computational cell along the XY plane, as shown in Fig. 1(a). The number of Ti atoms was approximately equal to the number of Al atoms. Periodic boundary conditions were applied along all axes. A vacuum layer was created along the Z-axis, parallel to the interphase boundary (Fig. 1(a)), allowing the bimetal to freely change volume during the simulation of mutual diffusion. When varying the temperature, thermal expansion of the metals was taken into account, and the dimensions of the computational cell were adjusted accordingly. The dimensions along the X and Y axes were chosen to be multiples, with minimal possible deviation, of the periodicity of both Ti and Al crystal lattices. Additionally, the unequal thermal expansion of metals was also considered for each specific temperature at which the simulation was conducted. The dimensions of the cell along all axes were approximately 20−25 nm, and the total number of atoms was around 300 thousand. Thus, an NPT canonical ensemble was used in the model. To maintain a constant temperature, a Nose-Hoover thermostat was applied. The time integration step in the molecular dynamics method was set to 2 fs.



(a) (b)

Fig. 1. Example of a computational cell containing the interface between aluminum and nanocrystalline titanium with an average grain size of 8.8 nm: (a) section in the XZ plane; (b) section of titanium in the XY plane

In works [20,21], we previously established that the intensity of mutual diffusion at the Ti–Al interface is primarily influenced by the structure of titanium: the presence of defects, the orientation of the interphase boundary relative to the titanium lattice, etc. The structure of aluminum is much more easily transformed and tends to adapt to the orientation of the titanium lattice near the interphase boundary [21]. When aluminum has a nanocrystalline or amorphous structure, rapid recrystallization or crystallization (in the case of an initially amorphous structure) would occur at temperatures close to its melting point (which are considered in this work). Therefore, creating a nanocrystalline structure not only in titanium but also in aluminum does not make sense.

The nanocrystalline structure of titanium with initially uniform grain sizes was created as follows. In the ideal titanium crystal, prior to the stage of bonding with aluminum, the centers of future grains were determined based on the specified average grain size. These centers were located in the computational cell at the nodes of a superlattice with hexagonal packing in the XY plane, parallel to the interphase boundary (Fig. 1(b)). The structure around each center was rotated in space at random angles within spheres with a diameter of 0.8 times the specified grain size (the nearest distance between centers). With the structure inside the spheres fixed, the remaining structure was melted and then subjected to crystallization simulation by holding it for 500 ps at a temperature of 1500 K. In the final stage, the structure was cooled to 0 K. The rotation of grains when creating their arbitrary orientation in space was performed around two axes by random angles. In this regard, the boundaries were generally of a mixed type and mostly high-angle. Boundaries of a special type were not observed in the model.

To prevent the influence on the results of recrystallization and grain growth during the simulation, especially for small grains, the structure at the centers of the grains within spheres with a diameter of 0.3 times the average grain size remained fixed throughout the simulation. The fixed regions at the centers of the grains are highlighted in dark gray in Fig. 1(b). This was done to conduct the study of mutual diffusion under conditions of unchanged grain size.

The average grain size varied from 2.7 to 8.8 nm. In Fig. 1(b), sections of the computational cells with grains sized 8.8 nm are shown using a crystal phase visualizer based on the Common Neighbor Analysis (CNA) method [37]. Green Ti atoms are those whose nearest environment corresponds to the HCP crystal structure, white atoms indicate that the crystal lattice is either undefined or corresponds to an amorphous structure, and dark gray atoms are those that remained stationary during the simulation. The grains in the model had a shape close to that of an icosahedron. In most cases, the grain boundaries were of a mixed type.

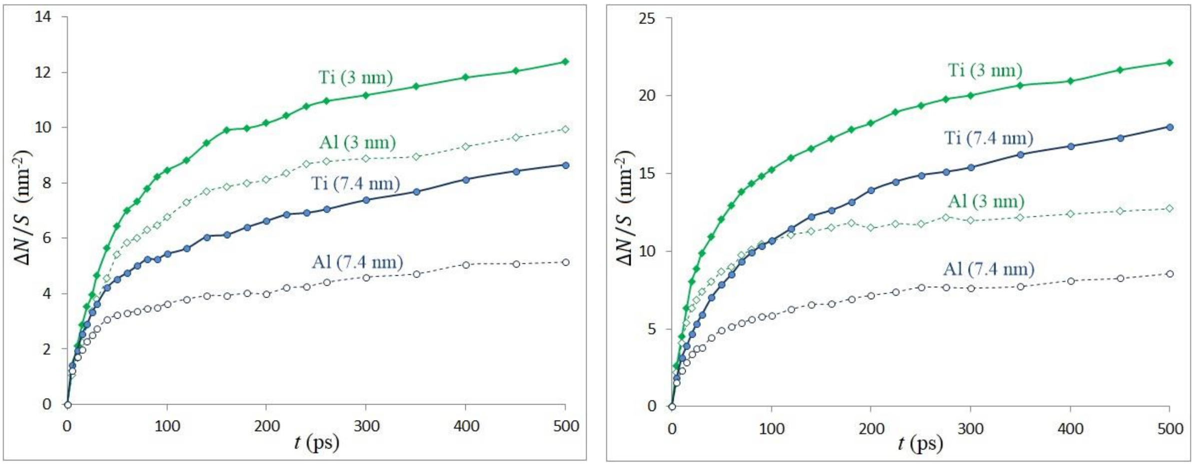
After the stage of creating the nanocrystalline titanium structure, the next step was to create a layer of aluminum with approximately the same number of atoms as that of titanium and to bond it with titanium. Following this, the structure was relaxed once more, but at a low starting temperature, with subsequent cooling to a temperature close to 0 K.

In addition to the interfaces between nanocrystalline titanium and aluminum, the boundaries between monocrystalline titanium and aluminum were also considered for comparison. Two orientations of the boundary relative to the crystal lattices of Ti (HCP) and Al (FCC) were examined: (0001):(111) and (0011):(001).

Results and Discussion

For a quantitative assessment of mutual diffusion at the interphase boundary, we found the use of a traditional diffusion coefficient, derived from real experiments, to be inconvenient and fraught with several drawbacks, primarily related to the necessity and complexity of isolating only the mutual component of diffusion alongside, for example, self-diffusion and other possible atomic movements in the model. In a computer model, it is possible to utilize more precise and specific characteristics. In our case, to evaluate the dissolution of atoms of one metal in another, a special characteristic was used – the specific number of dissolved atoms $\Delta N/S$, where ΔN is the difference in the number of dissolved atoms of the metal in question at the current and initial time points, and S is the area of the interphase boundary. An atom of the metal in question was considered dissolved if the number of atoms of the other metal in its immediate vicinity exceeded 50 %. The immediate vicinity was defined as a volume within a radius of 0.37 nm, which includes only the first coordination sphere. At the initial stage of mutual diffusion, that is, when one of the metals contains a relatively low concentration of the second metal, which is considered in the present work, the mutual diffusion coefficient of titanium atoms is linearly proportional to the specific number of dissolved atoms.

Figure 2 shows examples of the dependence of the quantity $\Delta N/S$ on the time of computer simulation for cases with average grain sizes in titanium of 3 and 7.4 nm at constant temperatures below and above the melting point of aluminum: 800 K (Fig. 2(a)) and 1100 K (Fig. 2(b)). In all cases, as seen in the figures, dissolution initially occurred rapidly, then the rate decreased and subsequently remained approximately constant. A similar dissolution behavior was observed by other researchers, for example in [38,39], as well as by us in [20] during the investigation of the dissolution of titanium nanoparticles in aluminum. This behavior is explained by the formation of a diffusion zone saturated with atoms of both components during the initial stage.



(a) (b)

Fig. 2. Dependencies of the specific number of dissolved atoms Δ*N/S* on the time of computer simulation for average grain sizes in titanium of 3 and 7.4 nm at constant temperatures: (a) 800 K, (b) 1100 K

As can be seen from the provided dependencies, titanium diffuses into aluminum significantly more intensively than aluminum diffuses into titanium. With increasing temperature, and especially after the melting of aluminum (Fig. 2(b)), this difference only increases. This is a well-known phenomenon that, in the case of solid-state contact, is explained by the relatively lower mobility of atoms in the titanium lattice, primarily due to the greater depth of the potential wells in which titanium atoms are located. Upon melting aluminum, both self-diffusion in aluminum and the diffusion of titanium atoms in liquid aluminum significantly increase, while titanium remains in a crystalline state.

The graphs presented in Fig. 2 also show that the diffusion of both titanium atoms into aluminum and aluminum atoms into titanium occurs significantly more intensively for a grain size of 3 nm compared to a grain size of 7.4 nm. This already serves as qualitative evidence that grain size, or more precisely, the density of grain boundaries in titanium, affects the intensity of mutual diffusion.

To investigate this issue in more detail, we obtained the dependencies of the specific number of dissolved atoms Δ*N/S* on temperature after computer simulations lasting 300 ps for all considered grain sizes in titanium (Fig. 3). The temperature was maintained constant during the simulation, with values ranging from 500 to 1200 K. For comparison, similar dependencies were also obtained for the cases of the interphase boundary between monocrystalline titanium and aluminum with boundary orientations relative to the crystal lattices of Ti and Al (0001):(111) and (0011):(001) (the lower graphs in Fig. 3, highlighted in red).

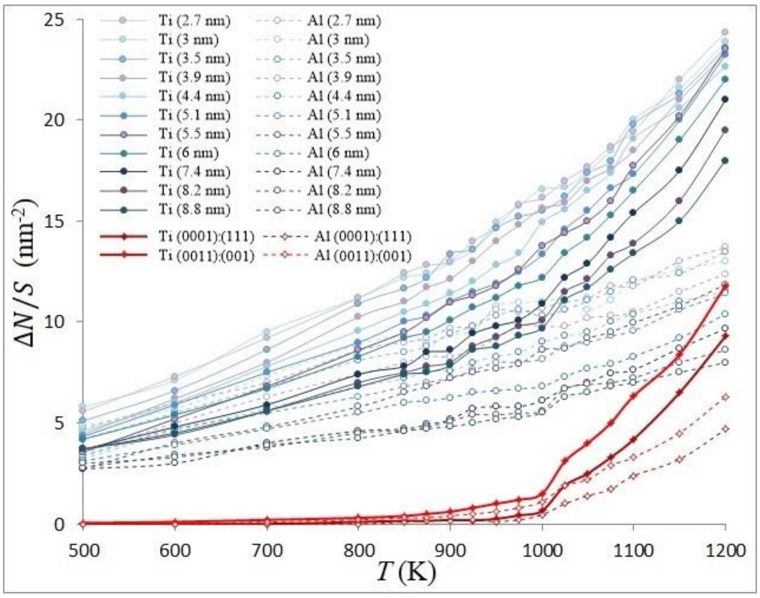


Fig. 3. Dependencies of the specific number of dissolved atoms Δ*N/S* on temperature after computer simulation for 300 ps for various grain sizes in titanium. Solid curves represent the dissolution of titanium in aluminum, while dashed curves represent the dissolution of aluminum in titanium

As the temperature increases, the intensity of diffusion also increases, which is consistent with the classical Arrhenius equation for diffusion, according to which the probability of elementary diffusion events exponentially rises with temperature. However, it should be understood that the classical Arrhenius equation is intended to describe steady-state diffusion, meaning that the diffusion flux and diffusion coefficient remain constant over the time interval considered. In our case, however, the diffusion process is more complex: as shown above (Fig. 2), it involves at least two stages characterized by different diffusion rates of the components. A third stage is also to be expected – gradual slowing of diffusion due to the equalization of component concentrations in the mixture.

As seen in Fig. 3, with increasing temperature, the intensity of titanium dissolution in aluminum increases faster than that of aluminum in titanium, especially after the melting of aluminum. Titanium remained in a solid state throughout the entire temperature range considered – the mobility of atoms in titanium was significantly lower than that of atoms in aluminum.

After the melting of aluminum (in the model, the melting temperature of aluminum was approximately 1015 K), a noticeable jump can be observed in the graphs, which became more pronounced with increasing average grain size. The most significant step was observed in the case of monocrystalline titanium (the lower graphs in Fig. 3). This clearly demonstrates the influence of the aggregate state of aluminum on the diffusion rate: in the case of monocrystalline titanium, this influence is decisive; however, in the case of a nanocrystalline structure with grain sizes on the order of several nanometers, this influence is significantly weaker, and for grain sizes less than approximately 6 nm, it is almost negligible.

It should be noted that the authors of the potential for Al obtained a melting temperature value of 1042 K [40]. However, this value was found in [40] for computational cells that contained no defects, including surfaces. In [32], we demonstrated that in the presence of grain boundaries or free surfaces, melting occurs heterogeneously and begins at these locations, resulting in a lower melting temperature in the model compared to that calculated by the authors of the potential for a defect-free crystal. For example, it was shown in [32] that the melting temperature depends on the crystallographic orientation of the surface. The following values were obtained for aluminum in [32]: (110) – 990 K, (100) – 1004 K, (111) – 1016 K.

In [21], we previously demonstrated that the orientation of the interphase boundary relative to the titanium lattice (and to a significantly lesser extent, relative to the aluminum lattice) affects the intensity of mutual diffusion. For the orientations considered in this work, diffusion is more intense for the orientation (0011):(001) and less intense for the orientation (0001):(111), as clearly seen in the graphs in Fig. 3 (lower graphs). This is explained by the density of atoms in the near-surface layer of titanium, specifically by the difference in depths of the potential wells in which they are located. Different energies are required to detach them from the plane and draw them into the aluminum phase for different orientations.

The main conclusion that can be drawn from the graphs in Fig. 3 is the critical influence of grain size in titanium on the intensity of mutual dissolution of the components. Indeed, as seen in Fig. 3, as the average grain size decreases, and consequently the density of grain boundaries in titanium increases, the specific number of dissolved atoms $\Delta N/S$ significantly increases. This is particularly evident when comparing the values of $\Delta N/S$ obtained for monocrystalline titanium (the lower red graphs in Fig. 3) and for the nanocrystalline structure (the upper graphs). It is well known that grain boundaries act as channels for accelerated diffusion, with diffusion along grain boundaries occurring orders of magnitude faster than in the bulk of the grains [41]. As the average grain size decreases, the density of grain boundaries increases. In our case, with grains only a few nanometers in size, the density of grain boundaries and the contribution of grain boundary diffusion are relatively very high.

For clarity, to demonstrate that a sufficiently high density of grain boundaries in titanium can significantly reduce the activation energy of the synthesis reaction, Fig. 4 presents the dependencies of $\Delta N/S$ on the average grain size d in titanium. Three pairs of graphs are shown for the dissolution of titanium and aluminum: at temperatures of 800 and 1100 K. For comparison, the values of $\Delta N/S$ for the case of monocrystalline titanium with the initial orientation of the interphase boundary (0011):(001) at 1100 K are indicated by dashed lines (at this temperature, aluminum is liquid, so its initial orientation is irrelevant). In the case of the (0011) orientation, dissolution occurs faster than with the (0001) boundary orientation; therefore, the first option was chosen for comparison.

As the average grain size d decreases, the specific number of dissolved atoms $\Delta N/S$ for both titanium and aluminum increases, which clearly illustrates the influence of grain boundary density in titanium on the intensity of mutual diffusion. Figure 4 also clearly shows that even at a temperature of 800 K, which is significantly below the melting point of aluminum, dissolution is more intense for grain sizes less than 9 nm than for the case of monocrystalline titanium at 1100 K. This latter temperature is not only 300 K higher but also corresponds to aluminum that is already in a liquid state.

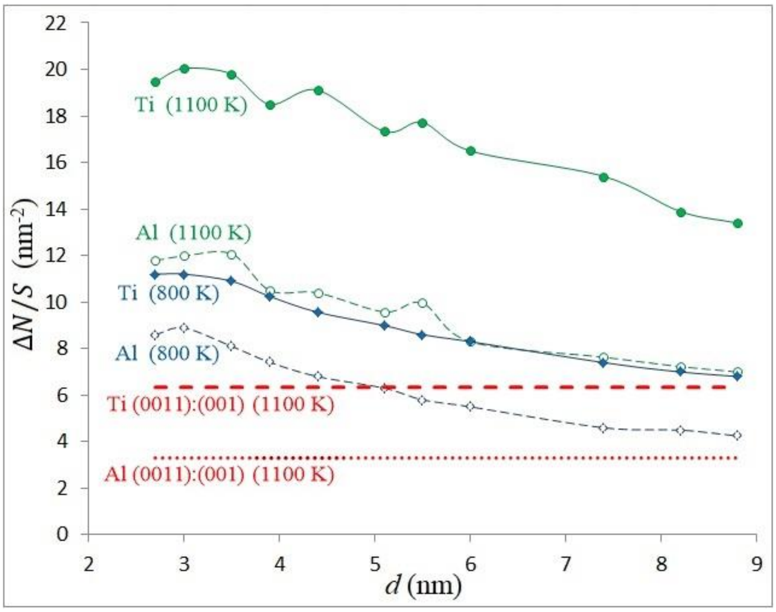


Fig. 4. Dependencies of the specific number of dissolved atoms Δ*N/S* on the average grain size *d* in titanium during simulation for 300 ps at temperatures of 800 K and 1100 K. For comparison, the values of Δ*N/S* for the case of monocrystalline titanium with the initial orientation of the interphase boundary (0011):(001) at 1100 K are also shown as dashed lines

To demonstrate that the grain boundaries in the model indeed served as channels for facilitated diffusion for both aluminum atoms diffusing into the titanium phase and titanium atoms migrating more intensively into aluminum from the grain boundaries, Fig. 5 presents an example of the distribution of titanium atoms (Fig. 5(a)) and aluminum atoms (Fig. 5(b)) in a layer of the other metal near the interphase boundary. These images were obtained for an average grain size of 7.4 nm and after 500 ps of simulation at a temperature of 900 K, which is below the melting point of aluminum.

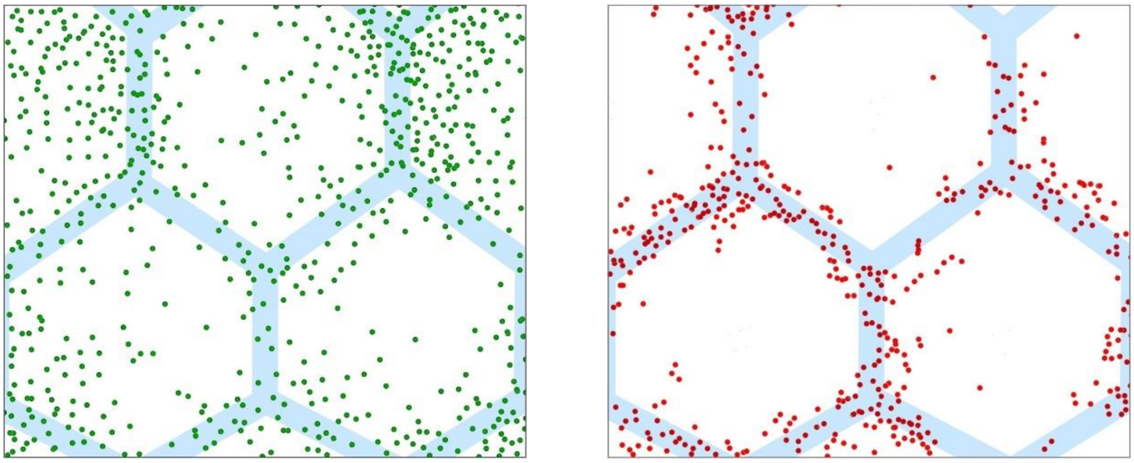

(a) (b)

Fig. 5. Distributions of titanium (*a*) and aluminum atoms (*b*) in a layer of the other metal near the interphase boundary after simulation at a temperature of 900 K for 500 ps. Average grain size is 7.4 nm. Atoms of the second metal, into which the atoms have diffused, are not shown. The positions of the grain boundaries in titanium are indicated by wide blue lines

In the figures, especially in the case of aluminum diffusion into titanium (Fig. 5(b)), it is clearly visible that diffusion predominantly occurs along the grain boundaries (the positions of the boundaries are indicated by wide blue lines in the images). The intensity of diffusion along different boundaries, as can be observed, varied. This is evidently related to the characteristics of the boundaries that affect diffusion permeability, particularly their energy and specific free volume [41].

In the case of titanium atoms diffusing into the aluminum phase (Fig. 5(a)), a greater blurring is observed compared to the diffusion of aluminum atoms into titanium. This is apparently related to the relatively "looser" structure of aluminum and the comparatively greater mobility of titanium atoms in aluminum than vice versa.

Thus, based on the results obtained in this study, as well as on the findings of our previous works [20,21,25] and works of other authors [22–24], we can conclude that among the four potential factors mentioned in the introduction that may influence the reduction of the activation energy of the synthesis reaction in the Ti–Al system after mechanical treatment of the initial mixture, two factors make the primary contribution: the energy stored in defects and the high density of grain boundaries in titanium. In the first case, as a result of structural transformations, part of the energy stored in defects created during intense deformation is released upon heating and "healing" of the structure. This additional energy reduces the amount of energy required to initiate the synthesis reaction. In the second case, grain boundaries in titanium serve as channels for accelerated or facilitated diffusion. As their density increases, the intensity of mutual diffusion also increases proportionally, while the activation energy for diffusion and, consequently, the activation energy for the synthesis reaction also decrease.

Conclusions

Using molecular dynamics simulations, this study investigates the influence of grain size of nanocrystalline titanium on its dissolution intensity in aluminum at various temperatures, compared to the dissolution of monocrystalline titanium.

In the modeling of mutual diffusion, it was shown that, regardless of the grain size in titanium, the diffusion process involved two stages. Initially, the dissolution of the components occurred intensely, then the dissolution rate decreased and subsequently remained approximately constant. This pattern of dissolution is explained by the formation of a diffusion zone saturated with atoms of both components during the first stage. A third stage is also to be expected, which lies beyond the time frame of the model – gradual slowing of diffusion due to the equalization of component concentrations in the mixture.

In our work, it has been shown that the grain size in nanocrystalline titanium significantly affects the intensity of mutual dissolution of the components. This is explained by the fact that grain boundaries act as channels for accelerated diffusion, with diffusion along grain boundaries occurring orders of magnitude faster than in the bulk of the grains. As the average grain size decreases, the density of grain boundaries increases. In the case of grains on the order of several nanometers, the density of grain boundaries and the contribution of grain boundary diffusion are relatively very high. For example, at a temperature of 800 K, which is significantly below the melting point of aluminum, dissolution in the model was more intense for grain sizes less than 9 nm than for the case of monocrystalline titanium at 1100 K, which is not only 300 K higher but also corresponds to aluminum that is already in a liquid state.

Thus, the nanocrystalline structure and high density of grain boundaries in titanium may be one of the reasons, alongside the energy stored in defects due to deformation, for the reduction in activation energy for the synthesis reaction in the Ti–Al system following mechanical processing of the initial mixture.

CRediT authorship contribution statement

Gennady M. Poletaev **:** conceptualization, writing – review & editing, writing – original draft; **Yuriy V. Bebikhov** **:** investigation, data curation; **Alexander S. Semenov** **:** investigation, data curation.

Conflict of interest

The authors declare that they have no conflict of interest.

References

1. Kim YW. Ordered intermetallic alloys, part III: gamma titanium aluminides. *The Journal of The Minerals, Metals & Materials Society.* 1994;46: 30–39.
2. Appel F, Beaven PA, Wagner R. Deformation processes related to interfacial boundaries in two-phase γ-titanium aluminides. *Acta Metallurgica et Materialia.* 1993;41(6): 1721–1732.
3. Lapin J. TiAl-based alloys: Present status and future perspectives. In*: Proceedings of the Metal; Tanger: Ostrava, Czech Republic.* 2009;19(21.5): 2019–2031.
4. Tetsui T. Manufacturing technology for gamma-TiAl alloy in current and future applications. *Rare Metals.* 2011;30: 294–299.
5. Voisin T, Monchoux J-P, Couret A. Near-net shaping of titanium-aluminum jet engine turbine blades by SPS. In: *Spark Plasma Sintering of Materials.* Cham: Springer; 2019. p.713–737.
6. Morris MA, Leboeuf M. Grain-size refinement of γ-Ti-Al alloys: effect on mechanical properties. *Materials Science and Engineering: A.* 1997;224(1–2): 1–11.
7. Bohn R, Klassen T, Bormann R. Mechanical behavior of submicron-grained γ-TiAl-based alloys at elevated temperatures. *Intermetallics.* 2001;9(7): 559–569.
8. Kambara M, Uenishi K, Kobayashi KF. Nano-structured intermetallic compound TiAl obtained by crystallization of mechanically alloyed amorphous TiAl, and its subsequent grain growth. *Journal of Materials Science.* 2000;35: 2897–2905.
9. Kimura H. High-strength intermetallic TiAl synthesized via high-temperature crystallization of the amorphous alloy. *Philosophical Magazine A.* 1996;73(3): 723–737.
10. Boldyrev VV, Tkacova K. Mechanochemistry of Solids: Past, Present, and Prospects. *Journal of Materials Synthesis and Processing.* 2000;8: 121–132.
11. Rogachev AS, Shkodich NF, Vadchenko SG, Baras F, Chassagnon R, Sachkova NV, Boyarchenko OD. *International Journal of Self-Propagating High-Temperature Synthesis.* 2013;22: 210–216.
12. Rogachev AS, Shkodich NF, Vadchenko SG, Baras F, Kovalev DY, Rouvimov S, Napapushev AA, Mukasyan AS. Influence of the high-energy ball milling on structure and reactivity of the Ni+Al powder mixture. *Journal of Alloys and Compounds.* 2013;577: 600–605.
13. Shuck CE, Mukasyan AS. Reactive Ni/Al Nanocomposites: Structural Characteristics and Activation Energy. *The Journal of Physical Chemistry A.* 2017;121(6): 1175–1181.
14. Rogachev AS. Mechanical activation of heterogeneous exothermic reactions in powder mixtures. *Russian Chemical Reviews.* 2019;88(9): 875–900.
15. Nepapushev AA, Moskovskikh DO, Buinevich VS, Vadchenko SG, Rogachev AS. Production of rounded reactive composite Ti/Al powders for selective laser melting by high-energy ball milling. *Metallurgical and Materials Transactions B.* 2019;50: 1241–1247.

16. Filimonov VYu, Loginova MV, Ivanov SG, Sitnikov AA, Yakovlev VI, Sobachkin AV, Negodyaev AZ, Myasnikov AYu. Peculiarities of phase formation processes in activated Ti+Al powder mixture during transition from combustion synthesis to high-temperature annealing. *Combustion Science and Technology.* 2019;192(3): 457–470.
17. Nguyen Q, Huang C, Schoenitz M, Sullivan KT, Dreizin EL. Nanocomposite thermite powders with improved flowability prepared by mechanical milling. *Powder Technology.* 2018;327: 368–380.
18. Fourmont A, Politano O, Le Gallet S, Desgranges C, Baras F. Reactivity of Ni-Al nanocomposites prepared by mechanical activation: a molecular dynamics study. *Journal of Applied Physics.* 2021;129(6): 065301.
19. Baras F, Bizot Q, Fourmont A, Le Gallet S, Politano O. Mechanical activation of metallic powders and reactivity of activated nanocomposites: a molecular dynamics approach. *Applied Physics A.* 2021;127: 555.
20. Poletaev GM, Bebikhov YV, Semenov AS, Sitnikov AA, Yakovlev VI. Molecular dynamics study of the dissolution of titanium nanoparticles in aluminum. *Materials Physics and Mechanics.* 2023;51(5): 9–15.
21. Poletaev GM, Bebikhov YuV, Semenov AS, Sitnikov AA. Molecular dynamics investigation of the effect of the interface orientation on the intensity of titanium dissolution in crystalline and amorphous aluminum. *Journal of Experimental and Theoretical Physics.* 2023;136(4): 477–483.
22. Hoffmann U, Horst C, Kunz E. Reactive Comminution. In: Sundmacher K, Keinle A, Seidel-Morgenstern A. (eds.) *Integrated Chemical Processes*. Wiley; 2005. p.407–436.
23. Khina BB. Effect of mechanical activation on SHS: Physicochemical mechanism. *International Journal of Self-Propagating High-Temperature Synthesis.* 2008;17: 211–217.
24. Mukasyan AS, Khina BB, Reeves RV, Son SF. Mechanical activation and gasless explosion: nanostructural aspects. *Chemical Engineering Journal.* 2011;174(2–3): 677–686.
25. Poletaev GM, Bebikhov YV, Semenov AS. Molecular dynamics study of the formation of the nanocrystalline structure in nickel nanoparticles during rapid cooling from the melt. *Materials Chemistry and Physics.* 2023;309: 128358.
26. Poletaev GM, Gafner YY, Gafner SL. Molecular dynamics study of melting, crystallization and devitrification of nickel nanoparticles. *Letters on Materials.* 2023;13(4): 298–303.
27.Phillpot SR, Lutsko JF, Wolf D, Yip S. Molecular-dynamics study of lattice-defect-nucleated melting in silicon. *Physical Review B.* 1989;40: 2831.
28. Xiao S, Hu W, Yang J. Melting behaviors of nanocrystalline Ag. *The Journal of Physical Chemistry B.* 2005;109(43): 20339–20342.
29. Xiao S, Hu W, Yang J. Melting temperature: from nanocrystalline to amorphous phase. *Journal of Chemical Physics.* 2006;125(18): 184504.
30. Wejrzanowski T, Lewandowska M, Sikorski K, Kurzydlowski KJ. Effect of grain size on the melting point of confined thin aluminum films. *Journal of Applied Physics.* 2014;116(16): 164302.
31. Noori Z, Panjepour M, Ahmadian M. Study of the effect of grain size on melting temperature of Al nanocrystals by molecular dynamics simulation. *Journal of Materials Research.* 2015;30: 1648–1660.
32. Poletaev G, Rakitin R, Bebikhov Y, Semenov A. Molecular dynamics study of melting initiation at tilt grain boundaries depending on their misorientation angle in aluminum. *Physica Scripta.* 2025;100(1): 015988.
33. Zope RR, Mishin Y. Interatomic potentials for atomistic simulations of the Ti-Al system. *Physical Review B.* 2003;68: 024102.
34. Kim Y-K, Kim H-K, Jung W-S, Lee B-J. Atomistic modeling of the Ti-Al binary system. *Computational Materials Science.* 2016;119: 1–8.
35. Pei Q-X, Jhon MH, Quek SS, Wu Z. A systematic study of interatomic potentials for mechanical behaviours of Ti-Al alloys. *Computational Materials Science.* 2021;188: 110239.
36. Poletaev GM, Bebikhov YuV, Semenov AS, Starostenkov MD. Self-diffusion in melts of Ni-Al and Ti-Al systems: molecular dynamics study. *Letters on Materials.* 2021;11(4): 438–441.
37. Tsuzuki H, Branicio PS, Rino JP. Structural characterization of deformed crystals by analysis of common atomic neighborhood. *Computer Physics Communications.* 2007;177(6): 518–523.
38. Levchenko EV, Evteev AV, Lorscheider T, Belova IV, Murch GE. Molecular dynamics simulation of alloying in an Al-coated Ti nanoparticle. *Computational Materials Science.* 2013;79: 316–325.
39. Cherukara MJ, Weihs TP, Strachan A. Molecular dynamics simulations of the reaction mechanism in Ni/Al reactive intermetallics. *Acta Materialia.* 2015;96: 1–9.
40. Mishin Y, Farkas D, Mehl MJ, Papaconstantopoulos DA. Interatomic potentials for monoatomic metals from experimental data and ab initio calculations. *Physical Review B.* 1999;59(5): 3393–3407.
41. Bokstein B., Rodin A. Grain boundary diffusion and grain boundary segregation in metals and alloys. *Diffusion Foundations.* 2014;1: 99–122.