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Molecular dynamics study of the effect of grain size of nanocrystalline titanium on the intensity of its dissolution in aluminum

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Using molecular dynamics simulation, the effect of the grain size of nanocrystalline titanium on the intensity of its dissolution in aluminum was studied. It was shown that in the case of grains of the order of several nanometers in size in titanium, due to the high density of grain boundaries, the intensity of mutual diffusion at the interphase boundary is significantly higher than in the case of single-crystal titanium. The high density of grain boundaries in titanium may thus be one of the reasons, along with the energy stored as a result of deformation in defects, for the decrease in the activation energy of the synthesis reaction in the Ti−Al system after mechanical treatment of the initial mixture.

Keywords: molecular dynamics, titanium, nanocrystalline structure, grain size, grain boundary.

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1. Introduction

Intermetallic compounds of the Ti−Al system and alloys based on them have a combination of properties such as high yield strength at elevated temperatures and good resistance to oxidation and corrosion at the same time with relatively low density, which makes them promising for use as high-temperature structural materials, in particular, for aerospace and automotive industries [1–5]. It is known that nonequilibrium processing methods, including, for example, intensive deformation, mechanical alloying, rapid hardening, etc., make it possible to create various unique nonequilibrium microstructures capable of improving the mechanical properties of intermetallic alloys [6–12]. One of the promising methods for obtaining intermetallides, including intermetallides of the Ti−Al system, is the preliminary mechanical processing of initial metal powders before the high-temperature synthesis reaction stage, for example, by grinding them in planetary ball mills [13–19]. So-called mechanocomposites are formed in the process of such mechanical activation. Mechanocomposites constitute a matrix of a more plastic component (in our case, aluminum), in the volume of which there are nanoscale particles of a more fragile component of the mixture (titanium) [18,19]. Mechanical grinding of the initial powders and the nanocomposites obtained in this way are used, in particular, in the currently intensively developing additive manufacturing [18,20]. Such a system is characterized by a high degree of disequilibrium due to the high concentration of defects, interface surfaces, and internal stresses. One of the most interesting properties of such nonequilibrium systems consisting of nanocomposites is a much lower effective activation energy of the synthesis reaction compared to conventional powders: the synthesis reaction (ignition) begins at a temperature significantly lower than the melting point of aluminum [13–19].

Currently, the question remains as to what exactly is the main factor in reducing the ignition temperature and activation energy of the synthesis reaction in mechanically activated mixtures. The following reasons are usually considered: 1) pre-mixing of components and a significant increase in their contact area; 2) accumulation of excess energy as a result of deformation in the form of various structural defects, which can be released as additional heat during relaxation of the structure; 3) decrease in the melting point of aluminum due to the presence of a high concentration of defects or even an amorphous phase; 4) more intensive mutual diffusion due to the high density of channels of facilitated diffusion in the form of grain boundaries, mainly in titanium.

The first mentioned reason, namely an increase in the contact area of the components, is sometimes cited as the main reason for a decrease in the activation energy of the synthesis reaction, often in conjunction with the second, that is, with the accumulation of excess energy in the form of defects, as, for example, in [21,22], where molecular dynamic modeling of the deformation of round metal particles and the initial stage of mutual diffusion. However, strictly speaking, an increase in the contact area of the components alone cannot lead to a decrease in the activation energy of the synthesis reaction and, consequently, the ignition temperature. This only leads to an increase in

the dissolution rate, which, in particular, was shown by us when studying the dissolution of a round titanium particle in aluminum [23], as well as when modeling mutual diffusion in the case of a flat interfacial boundary [24].

The second reason mentioned above should be considered separately, namely, the accumulation of excess energy during deformation in the form of the formation of nonequilibrium defects in the structure of components: grain boundaries, dislocations and disclinations, point defects and their complexes. This reason for the decrease in the activation energy of the synthesis reaction is indicated as the main one, for example, in Refs. [25–27]. Indeed, excessive or accumulated potential energy can be released during heating due to partial filling of the structure and a decrease of the density of defects. For instance, we showed in Refs. [28,29] that energy release and temperature increase can be significant and significantly affect diffusion processes during recrystallization of a metal with a nanocrystalline structure characterized by a very high density of grain boundaries compared to conventional polycrystals.

Sometimes, a possible decrease in the melting point of nanocrystalline aluminum compared to conventional coarse-grained aluminum is considered as another reason for a decrease in the ignition temperature of mechanically activated powders. It is known that the temperature at which the high-temperature synthesis reaction begins in systems such as Ti−Al and Ni−Al coincides with the melting point of aluminum in the case of conventional powders. In numerous studies performed mainly using modeling, it has indeed been shown that nanomaterials are characterized by the so-called „the size-dependent melting point depression phenomenon“, that is, the dependence of the melting point of nanomaterials on their effective size: grain size, film thickness, and nanoparticle diameter. As for materials with a nanocrystalline structure, it was shown in the works of [30–35] using molecular dynamic modeling that melting in them is not a homogeneous process, it begins, as a rule, with free surfaces and grain boundaries. A decrease in the average grain size led to a decrease in the melting point of nanocrystalline Ag [31,32] and Al [33,34]. In Refs. [28.29] we also observed a decrease in the melting point for Ni nanoparticles with a nanocrystalline structure compared to single-crystal particles. Nevertheless, in our other paper in Ref. [23], devoted to the study of the dissolution of titanium nanoparticles in aluminum, it was shown that the state of the titanium structure has a much greater effect on the intensity of mutual diffusion than the state of the aluminum structure, and therefore the reason is related to a possible decrease in the melting point of aluminum, does not seem to be of primary importance in the case of a decrease in the temperature of the start of the synthesis reaction in powders subjected to mechanical activation.

The fourth possible reason, which is the subject of this work, is the formation of high concentration of accelerated diffusion channels in the form of grain boundaries, dislocations, and pores due to intense deformation in titanium. We see the role of these additional channels (mainly grain boundaries) as one of the main ones, along with the energy accumulated in the defects. It is known that diffusion along grain boundaries proceeds orders of magnitude more intensively than diffusion in the volume of grains, and the activation energy of grain-boundary diffusion is significantly lower than the activation energy of vacancy diffusion [36–38]. Moreover, in nanocrystalline materials, the contribution of grain boundaries and triple junctions to their properties, including diffusion properties, is crucial, and increases as the average grain size decreases [39,40]. The presence of a high density of grain boundaries in titanium, at a certain grain size, can lead to a sufficiently high rate of mutual diffusion commensurate with diffusion at the temperature of the reaction onset, at which the phase of self-propagating synthesis is initiated. This study is aimed at verifying this assumption and is devoted to studying, using the method of molecular dynamics, the effect of the grain size of nanocrystalline titanium on the intensity of its dissolution in aluminum at different temperatures compared with the dissolution of single-crystal titanium.

Various authors performed modeling by the method of molecular dynamics of mutual diffusion in the Ti−Al system, as well as in other similar systems. For example, an attempt was made in Refs. [21,22] to simulate the intense deformation of initially round particles Al and Ti, and subsequent mutual diffusion at different temperatures. These studies contain interesting results, but it has proved difficult to identify individual factors that affect the rate of dissolution of the components. In Refs. [23,24], using molecular dynamic modeling, we sought to separately study the effect on the intensity of mutual diffusion in the Ti−Al system of such factors as the orientation of the interfacial boundary relative to the crystal lattices of the components, the size of titanium particles in the aluminum matrix, and the state of the titanium particle structure (crystalline or amorphous). We will focus on studying the effect of the average grain size in this paper and, consequently, the density of grain boundaries in nanocrystalline titanium on the intensity of mutual diffusion.

2. Model description

The interatomic interactions in the Ti−Al system were described by using EAM potentials from Ref. [41] where they were obtained based on comparison with experimental data and *ab initio* calculations for various properties and structures of metals Ti, Al and intermetallides Ti_3Al and TiAl. This potentials have been proved in various studies and have been successfully tested in a wide range of mechanical and structural-energy properties of the system alloys Ti−Al [41–44].

The interfacial boundary Ti−Al was created in the center of the simulated calculation cell along the plane xy, as shown in Figure 1, *a*. The number of Ti atoms was approximately equal to the number of Al atoms. Periodic

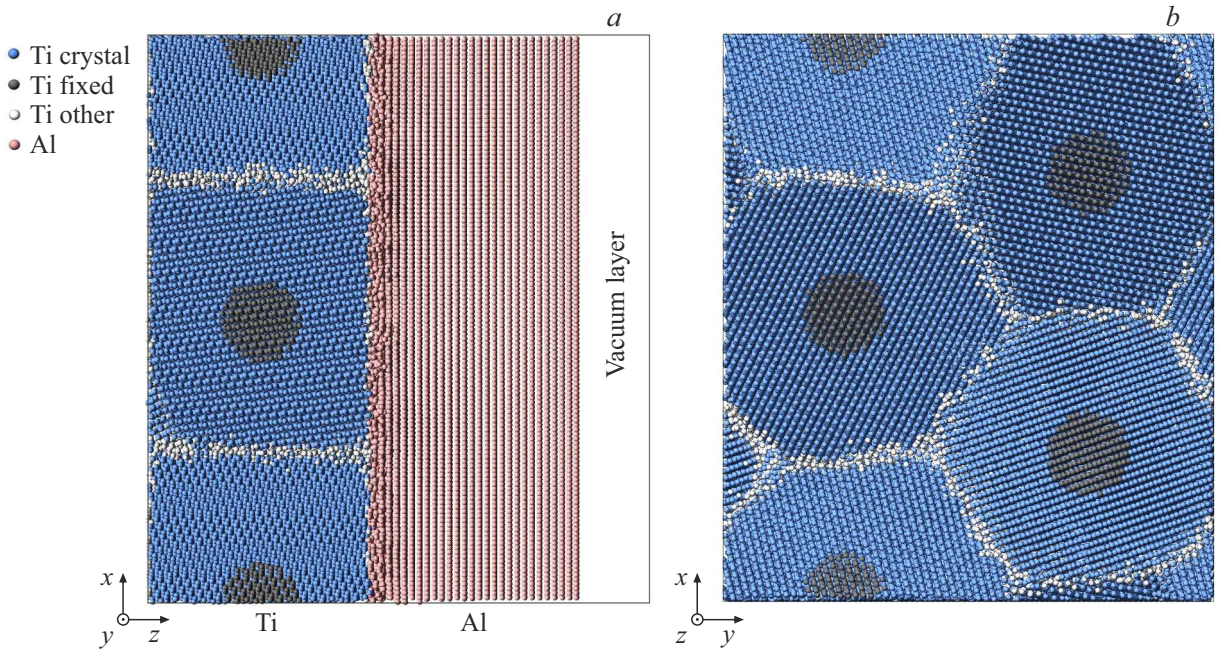

Figure 1. Example of a computational cell containing an interface between aluminum and nanocrystalline titanium with an average grain size of 8.8 nm: *a*) section in the plane xz; *b*) titanium cross section in the plane xy.

boundary conditions were imposed along all axes. At the same time, a vacuum layer was created along the Z axis, that is, parallel to the interphase boundary (Figure 1, *a*), designed so that the bimetal could freely change volume during the simulation of mutual diffusion. The thermal expansion of metals was taken into account when the temperature varied, and the dimensions of the calculation cell were adjusted accordingly. The dimensions along the X and Y axes were selected in such a way that they were multiples, with the minimum possible deviation, of the periods of simultaneous recurrence of the Ti and Al crystal lattices. Thereat, we also took into account the different thermal expansion of metals for each specific temperature at which simulation was performed. The cell dimensions along all axes were approximately 20−25 nm, and the total number of atoms was approximately 300 thousands. Thus, the NPT canonical ensemble was used in the model. A Nose−Hoover's thermostat was used to maintain the constant temperature. The step of time integration in the molecular dynamics method was equal to 2 fs.

Earlier, we found in Refs. [23,24] that the intensity of mutual diffusion at the interface of Ti−Al is mainly influenced by the structure of titanium: the presence of defects, the orientation of the interfacial boundary relative to the titanium lattice, etc. The structure of aluminum transforms much more easily and tends, as a rule, to adjust to the orientation of the titanium lattice near the interface [24]. When aluminum had a nanocrystalline or amorphous structure, at temperatures close to its melting point (which are considered in this paper), rapid recrystallization occurred, or crystallization in the case of the original amorphous structure, and therefore the creation of a nanocrystalline structure, in addition to titanium, did not make sense in aluminum.

The nanocrystalline structure of titanium with grains of the same size was initially created as follows. In an ideal titanium crystal, even before the stage of bonding with aluminum, depending on a given average grain size, the centers of future grains were determined, located in the computational cell at the nodes of the superlattice with hexagonal packing in the plane xy parallel to the plane of the interfacial boundary (Figure 1, *b*). The structure around each center in spheres with a diameter of 0.8 of a given grain size (the closest distance between the centers) was rotated in space at random angles. The structure inside the spheres was fixed and the rest of the structure was subjected to melting followed by modeling of crystallization at a temperature of 1500 K for 500 ps. The structure was cooled to 0 K at the final stage.

The structure in the grain centers in spheres with a diameter of 0.3 of the average grain size remained fixed throughout the modeling to prevent any impact on the results of recrystallization and grain growth during the modeling, especially for small grains. The fixed areas in the grain centers are highlighted in Figure 1, *b* in dark gray. This was done to ensure that the grain size initially set did not change during the simulation.

The average grain size ranged from 2.7 to 8.8 nm. The sections of calculated cells with grains of 8.8 nm are visualized in Figure 1 using the crystal phase visualizer based on the CNA (Common Neighbor Analysis) method [45]. Blue atoms of Ti are atoms with the immediate environment

corresponding to the HCP crystal structure, white atoms are atoms with unidentified crystal lattice or with an amorphous structure, gray atoms are atoms that were stationary during the modeling. The grains in the model had a shape close to an icosahedron. Grain boundaries in most cases were of a mixed type.

The stage of creating the nanocrystalline structure of titanium was followed by the stage of creating an aluminum layer and combining it with titanium. After that, the structure was relaxed again, but at a low starting temperature, followed by cooling to a temperature close to 0 K. The number of aluminum atoms was approximately equal to the number of titanium atoms.

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

3. Results and discussion

The use of a traditional diffusion coefficient has a number of disadvantages for quantifying the mutual diffusion at the interface in a molecular dynamic model, mainly related to the need and difficulty of isolating only the mutual component of diffusion, along with, for example, self-diffusion and other possible atomic displacements in the model. In the case of computer modeling, it is possible to use more precise and specific characteristics. A special characteristic was used in our study to evaluate the dissolution of atoms of one metal in another — 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, S is the area of the interfacial boundary. A dissolved atom of the metal in question was considered if the number of atoms of another metal in its immediate environment exceeded 50 %. The closest environment was considered to be a volume within a radius of 0.37 nm, that is, including only the first coordination sphere.

Figure 2 shows examples of the dependence of the value $\Delta N/S$ on the time of computer simulation for the cases of average grain size in titanium 3 and 7.4 nm at a constant temperature below and above the melting point of aluminum: 800 K (Figure 2, *a*) and 1100 K (Figure 2, *b*). In all cases, as can be seen in the figures, the dissolution initially proceeded intensively, then the rate decreased and subsequently remained approximately constant. The same dissolution pattern was observed by other researchers, for example, in Refs. [46,47], as well as by us in Ref. [23] when studying the dissolution of titanium nanoparticles in aluminum, and is explained by the formation of a diffusion zone saturated with atoms of both components at the first stage.

As can be seen from the above dependencies, titanium diffuses into aluminum significantly more intensively than aluminum into titanium. This difference only increases as the temperature increases, and especially after aluminum melting (Figure 2, *b*). This is a well-known phenomenon, which in the case of solid-phase contact is explained by the comparatively lower mobility of atoms in the titanium lattice, mainly due to the greater depth of potential wells in which titanium atoms are located. When aluminum melts, diffusion in it, both self-diffusion and diffusion of titanium atoms in liquid aluminum, increase significantly, while titanium remains in its crystalline state.

According to the graphs shown in Figure 2, it is also seen that the diffusion of both titanium atoms into aluminum and aluminum atoms into titanium proceeds significantly more intensively in the case of grain size 3 nm than in the case of size 7.4 nm. This is already a qualitative evidence of the fact that the grain size, or rather the density of grain boundaries, in titanium affects the intensity of mutual diffusion.

For a more detailed study of this issue, we obtained the dependences of the specific number of dissolved atoms

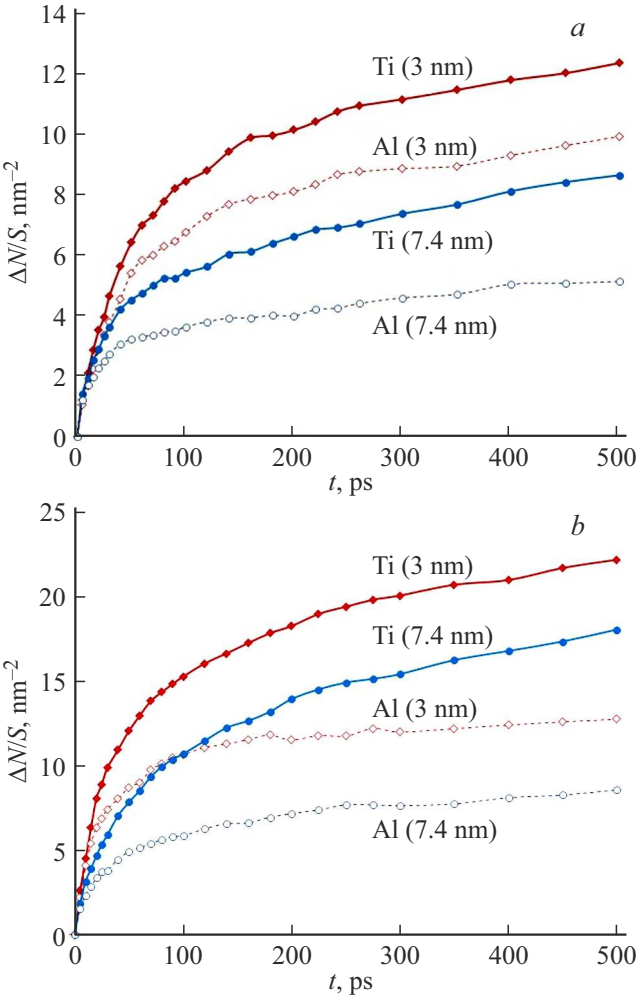

Figure 2. Dependences of the specific number of dissolved atoms $\Delta N/S$ on the computer simulation time for cases of average grain size in titanium 3 and 7.4 nm at constant temperature: *a*) 800 K, *b*) 1100 K.

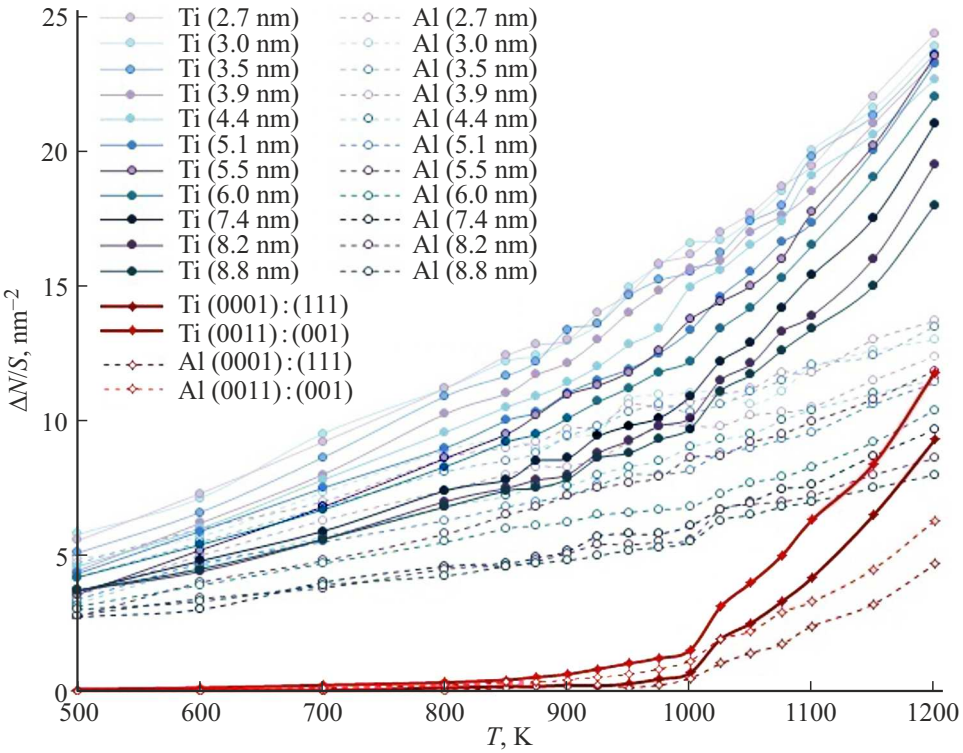

Figure 3. Dependences of the specific number of dissolved atoms $\Delta N/S$ from temperature after computer simulation for 300 ps for different grain sizes in titanium. Solid curves show titanium dissolution in aluminum, dashed curves show aluminum in titanium.

$\Delta N/S$ on temperature after computer simulation for 300 ps for all considered grain sizes in titanium (Figure 3). The temperature was kept constant during the simulation. Values from 500 to 1200 K were considered. For comparison, similar dependences were also obtained for the cases of the interfacial boundary between single-crystal titanium and aluminum with the orientation of the boundary relative to the crystal lattices of Ti and Al $(0001):(111)$ and $(0011):(001)$ (the lower graphs in Figure 3, highlighted in red).

The diffusion intensity increases as the temperature increases, which is consistent with the classical Arrhenius equation for diffusion, according to which, as the temperature increases, the probability of elementary diffusion acts increases exponentially. At the same time, however, it should be understood that the classical Arrhenius equation is intended to describe well-established diffusion, that is, when the diffusion flux and the diffusion coefficient remain unchanged during the time period under consideration. The diffusion process is more complicated in our case: as shown above (Figure 2), it includes at least two stages, differing in the rate of diffusion of the components. The third stage should also be expected — a gradual slowdown in diffusion due to the equalization of the concentration of components in the mixture.

As the temperature increases, as can be seen from Figure 3, the dissolution rate of titanium in aluminum increases faster than aluminum in titanium, especially after melting aluminum. Titanium remained in a solid state over the entire temperature range under consideration. The mobility of atoms in it was significantly lower than the mobility of atoms in aluminum.

After aluminum melting (in the model, the melting point of aluminum was approximately 1016 K), a hop can be seen on the graphs, which became more pronounced as the average grain size increased. The sharpest step was observed in the case of single-crystal titanium (lower graphs in Figure 3). This clearly demonstrates the effect of the aggregate state of aluminum on the diffusion rate: in the case of the single-crystal state of titanium, this effect is decisive, however, in the case of a nanocrystalline structure with a grain size of the order of several nanometers, this effect is significantly weaker, and for grain sizes less than about 6 nm, it is almost not observed at all.

It should be noted that the authors of the potential for Al obtained the value of its melting point of 1042 K [48]. However, this value was found in Ref. [48] for calculation cells that do not contain any defects, including the surface. We showed in Ref. [35] that in the case of grain boundaries or a free surface, melting proceeds heterogeneously and starts from them, and the melting temperature in the model is lower than that calculated by the authors of the potential for a defect-free crystal. It was shown in Ref. [35], for example, that the melting point depends on the crystallographic orientation of the surface. The following values were obtained for aluminum in Ref. [35]: (110) — 990 K, (100) — 1004 K, (111) — 1016 K.

Earlier, we showed in Ref. [24] that the orientation of the interfacial boundary relative to the titanium lattice (to a much lesser extent relative to the aluminum lattice) affects the intensity of mutual diffusion and, for example, for the orientations considered in this paper, it is greater in the case of orientation $(0011):(001)$ and less in case of orientation $(0001):(111)$, this is clearly visible from the graphs in Figure 3 (lower graphs). This is explained by the density of atoms in the near-surface layer of titanium, or rather by the difference in the depths of the potential pits in which they are located. In the case of different orientations, different energies are required to detach them from the plane and carry them into the aluminum phase.

The main conclusion to be drawn from the graphs in Figure 3 is the critical effect of the grain size in titanium on the intensity of mutual dissolution of the components. Indeed, as can be seen from Figure 3, as the average grain size and, consequently, the density of grain boundaries in titanium decrease, the specific number of dissolved atoms $\Delta N/S$ significantly increases. This is especially noticeable when comparing the values of $\Delta N/S$ obtained for single-crystal titanium (lower red graphs in Figure 3) and for the nanocrystalline structure (upper graphs). It is known that grain boundaries are a kind of channels of accelerated diffusion, diffusion along grain boundaries proceeds orders of magnitude faster than in the volume of grains [36–38]. The density of grain boundaries increases as the average grain size decreases. In our case, the grains are only a few nanometers in size, which is why the density of grain boundaries and the contribution of grain-boundary diffusion are comparatively very high.

For clarity, to show that a sufficiently high density of grain boundaries in titanium can significantly reduce the activation energy of the synthesis reaction, see Figure 4 shows the dependences of the value of $\Delta N/S$ on the average grain size of d in titanium. Three pairs of graphs for the dissolution of titanium and aluminum are shown: for temperatures of 800 and 1100K, as well as for comparison, the dotted lines show the values of $\Delta N/S$ for the case of single-crystal titanium with the initial orientation of the interface $(0011):(001)$ at a temperature of 1100 K (aluminum is liquid at this temperature, so its initial orientation doesn't matter). In the case of orientation (0011), dissolution proceeds faster than in the case of orientation of the boundary (0001), therefore, the first option was chosen for comparison.

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

To demonstrate that the grain boundaries in the model were indeed channels of facilitated diffusion for both

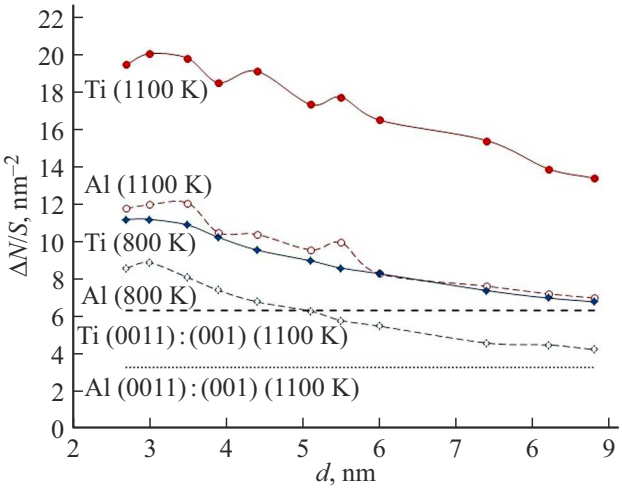

Figure 4. Dependences of the specific number of dissolved atoms $\Delta N/S$ from average grain size d in titanium during simulation for 300 ps at temperatures of 800 and 1100 K. For comparison, the dashed lines also show the values of $\Delta N/S$ for the case of single-crystal titanium with the initial orientation of the interfacial boundary. $(0011):(001)$ at temperature 1100 K.

aluminum atoms that diffused into the titanium phase and titanium atoms that migrated more intensively into aluminum from the grain boundaries, Figure 5 provides an example of the distribution of titanium atoms (Figure 5, a) and aluminum atoms (Figure 5, b) in a layer of another metal near the interface. These figures were obtained for an average grain size of 7.4 nm and modeling after 500 ps at a temperature of 900 K, that is, below the melting point of aluminum.

In the figures, especially in the case of aluminum diffusion into titanium (Figure 5, b), it is clearly seen that diffusion actually proceeds mainly along grain boundaries (the position of the boundaries in the figures is shown by wide blue lines). The intensity of diffusion along different boundaries, as can be seen, was different. Obviously, this was attributable to the characteristics of the boundaries affecting the diffusion permeability, in particular, their energy and specific free volume [36–38].

A greater blurring is observed in the case of diffusion of titanium atoms into the aluminum phase (Figure 5, a) which is probably attrubutable to the relatively „looser" structure of aluminum and the relatively greater mobility of titanium atoms in aluminum than vice versa.

Thus, it can be concluded based on the results obtained in this study, as well as based on the results of our previous study in Refs. [23,24,28] and the papers of other authors in Refs. [25–27] that the main contribution is made by two of the four possible factors listed in the introduction that may affect the reduction of the activation energy of the synthesis reaction in the Ti–Al system after mechanical treatment of the initial mixture: the energy stored in defects and the high density of grain boundaries in titanium. In the first case, part of the energy stored in defects created during

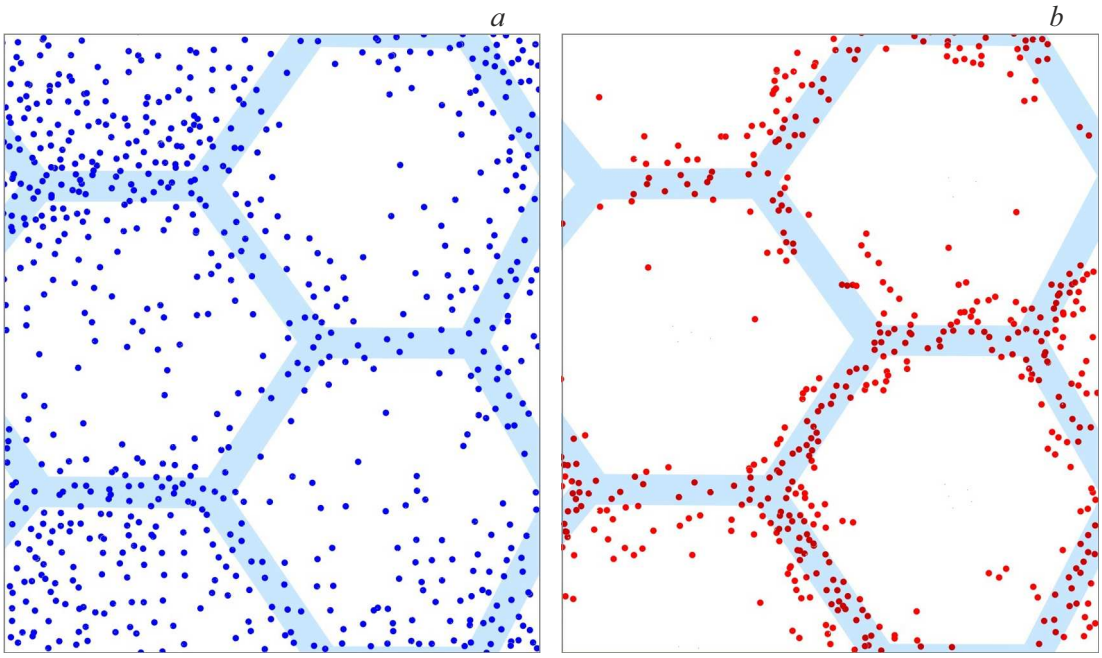

Figure 5. Distributions of titanium atoms (a) and aluminum atoms (b) in a layer of another metal near the interface after simulation at 900 K for 500 ps. The average grain size is 7.4 nm. The atoms of the second metal, into which the atoms diffused, are not shown. The position of the grain boundaries in titanium is shown by wide blue lines.

intense deformation is released upon heating and healing of the structure as a result of structural transformations. This additional energy reduces the amount of energy needed to initiate the fusion reaction. In the second case, the grain boundaries in titanium constitute channels of accelerated or facilitated diffusion. An increase in their density leads to a decrease in the effective (i. e., average) activation energy of mutual diffusion. The synthesis reaction of intermetallides is exothermic in nature, with a certain intensity of mutual dissolution of the components and sufficient heat generation, the stage of spontaneous combustion of the mixture (self-propagating high-temperature synthesis) begins, after which additional heat supply is not needed. In this regard, a decrease in the activation energy of diffusion due to an increase in the density of grain boundaries in titanium can also lead to an actual decrease in the ignition temperature.

4. Conclusion

The influence of the grain size of nanocrystalline titanium on the intensity of its dissolution in aluminum at different temperatures compared with the dissolution of single-crystal titanium has been studied using molecular dynamic modeling.

When modeling mutual diffusion, it was shown that, regardless of the grain size in titanium, the diffusion process included two stages. At first, the dissolution of the components proceeded intensively, then the dissolution rate decreased and subsequently remained approximately constant. This type of dissolution is explained by the formation of a diffusion zone saturated with atoms of both components at the first stage. The third stage should also be expected, which remained outside the time frame of the model, a gradual slowdown in diffusion due to the equalization of the concentration of components in the mixture.

Our work has 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 are a kind of channels of accelerated diffusion, diffusion along grain boundaries proceeds orders of magnitude faster than in the bulk of grains. The density of grain boundaries increases as the average grain size decreases. In the case of grains of 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, that is, significantly lower than the melting point of aluminum, for grain sizes less than 9 nm, dissolution in the model proceeded more intensively than for the case of single-crystal titanium at a temperature of 1100 K, which is not only 300 K higher, but also corresponds to liquid aluminum.

As the density of the grain boundaries in titanium increases, the effective activation energy of mutual diffusion decreases, which leads to a decrease in the activation energy of the synthesis reaction. Thus, the nanocrystalline structure and high density of grain boundaries in titanium may be one of the reasons, along with the energy stored as a result of deformation in defects, for a decrease in the activation

energy of the synthesis reaction in the Ti–Al system after mechanical processing of the initial mixture.

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Conflict of interest

The authors declare no conflict of interest.

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