# FEATURES OF INTERFACE FORMATION IN CRYSTALLITES UNDER MECHANICALLY ACTIVATED DIFFUSION. A MOLECULAR DYNAMICS STUDY.

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**Abstract.** In this paper, we carried out investigation of behavior of the material under loading condition identical those used in FSW using molecular dynamic method. The loading was modelled by a rigid rotating “tool” that movies along boundary between two grains. We considered pairing of two crystallites of copper, crystallites of copper and iron, and two crystallites of aluminum 2024. Analysis of the structure of the sample showed the intermixing and stirring of dissimilar atoms as a result the FSW tool pass at the inter-crystallite boundary. It was shown, that under certain condition of loading when tool passes there a region where atoms can occupying the original position of the crystal lattice. We also show influence of an additional oscillating impact applied to the moving tool on the structure of the resulting weld. The simulation results obtained can be used for understanding the processes realized under mechanically activated diffusion.

## 1 INTRODUCTION

Mechanical acceleration technology is widely used in modern science and industry to improve the efficiency of chemical reactions and physical and mechanical processes under conditions of combining of normal pressure and shear strain. An example of practical application of the acceleration effect of diffusion processes due to mechanical activation is the technology of friction stir welding (FSW) [1]. Using a rotary instrument at the junction of two

metal plates transforms the state of their surface layers to the plastic flow mode. It is found that such loading allow to reach large compared with the volume deformation degrees of plastic deformation with the formation of the structural conditions characterized by a high density of lattice defects. Investigation of mechanisms and identify the physical regularities of formation of the structural state and the factors leading to the formation of structural inhomogeneities and discontinuities in the weld, depending on the loading parameters, is an important task of physics of plasticity and strength.

In spite of the active use of technology of friction stir welding to obtain high-strength inextricable connection between different metals and alloys, many features of the process are still poorly studied. The difficulties of the theoretical and experimental study caused by great diversity, interconnectivity and transience of mechanisms realized in place of loading. This is especially relevant when studying the physics of the process at the atomic scale, when the spatial and temporal scales largely limit the set of used experimental techniques. Due to this, the methods of computer simulation can be considered as an effective tool for solving this type of problems. When choosing a method of numerical study should take into account that mechanical activated processes are inextricably linked to the intensive formation of discontinuities, the generation of the structure defects of different levels and mass transfer. From this viewpoint, the most preferred is using a method of discrete description of a simulated medium [2, 3].

Thus, the purpose of this paper is to analyze at the atomic scale the basic laws and mechanisms of formation of the structural state of the material subjected to severe plastic deformation on the loading scheme simulating the conditions of friction stir welding.

## 2 NUMERICAL MODEL OF THE PROCESS

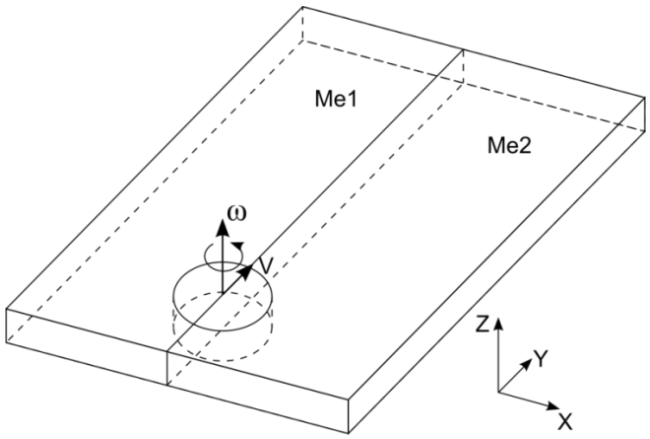



**Figure 1:** Schematic representation of the simulated sample.

The study was conducted in the framework of molecular dynamics method using the software package LAMMPS [4]. The interaction between atoms is described within the embedded atom method [5,6]. In order to study the implementation of possible atomic mechanisms in the loading conditions identical to those used in FSW, we carried out modeling the FSW by a rotating tool in the form of rigid cylinder that moves along the boundary between two grains. Schematic representation of the simulated sample is shown in

Figure 1. The two metal crystallites' sizes (Me1 and Me2) were 10.8 × 21.7 × 3.6 nm. The part of atoms shaped in 3.6 nm diameter cylinder was simulating a tool rotating at constant angular velocity ω. In addition, this cylinder was moved along the boundary at feeding rate V. Modeled sample was considered as NVE ensemble that maintains the number of particles, the occupied volume and the energy of the system. Velocity-Verlet integrator was used. The equations of motion were integrated with a time step $\Delta t = 0.001$ ps.

Originally, we modeled the process which reproduced at the atomic scale the loading conditions used in FSW of two ideal copper crystallites. The rotation rate and feeding rate of the tool were chosen V=50 m/s and $\omega$=0,1 $ps^{-1}$, respectively. Heat removal from the sample was realized by introducing the artificial viscosity of atoms belonging to two buffer layers on the edges of both fragments. Periodic boundary conditions were set in all directions to account for extended sizes of the simulated sample. In what follows, we have considered loading materials with different crystal lattices and two similar solid solutions.

## 3 SIMULATION RESULTS

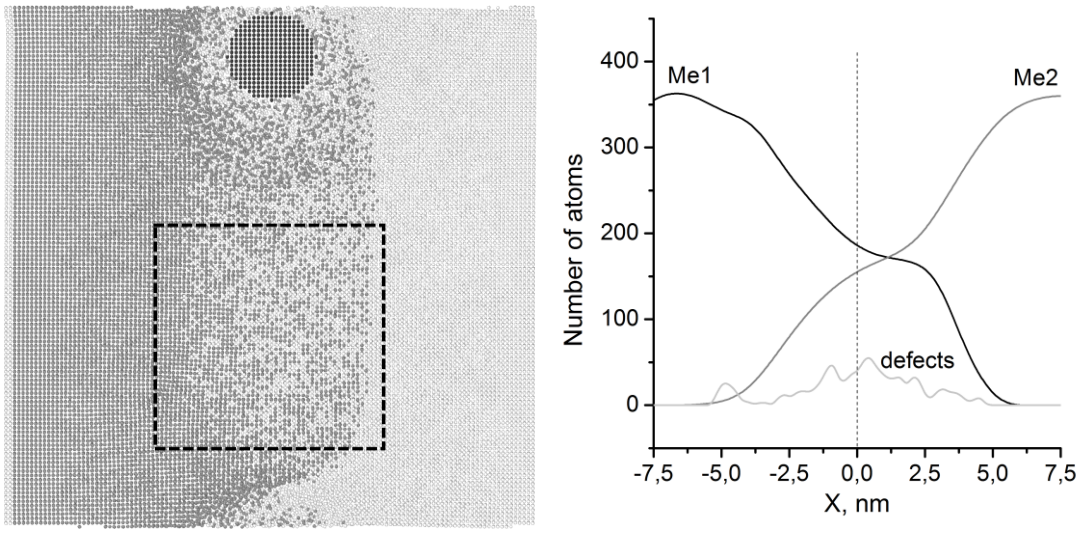
### 3.1 Conjugation of two identical metals

Analysis of the structure of the sample showed the intermixing and stirring of dissimilar atoms as a result the FSW tool pass at the inter-crystallite boundary. Figure 2a shows the mapping of atoms on the plane X0Y for a moment of time corresponding to the working tool pass along the entire length of the boundary between two metals. Atoms originally belonged to either Me1 or Me2 crystallites are marked by different shade of the gray. It is seen that the trace of passing instrument consists of two parts. The area with the crystal lattice irregularities has been found directly behind the tool. Atoms of Me1 and Me2 fragments present in it in approximately equal proportions. The thickness of this area is comparable with the size of the rotating tool. When tool passes far along the boundary at a distance comparable with its diameter, there formed a region where atoms start occupy the original position of the crystal lattice due to relaxation in the nodes. The specificity of this area is the gradient distribution of atoms belonging to grains Me1 and Me2. The spatial distribution of the atoms of the two metals near the interface is shown in Figure 2b.

Analysis of the crystal lattice structure by using the common neighbor analysis [7] revealed the structural defects. However, their volume fraction relative to the total number of atoms is negligible. A small number of atoms with a local topology bond, other than an fcc structure is observed only in the vicinity of the original position of the line interface of the two metals (see. Figure 2b). According to the represented dependence point of intersection of concentration curves of metals Me1 and Me2 is shifted to the right relative to the original position of the interface, which can be explained by the direction of rotation of the tool. Presence of points of inflection on both curves at their intersection indicates that there is a layer thickness of ~2.5 nm (0 to 2.5 nm along the X-axis), wherein the concentration of atoms opposing fragments varies slightly.

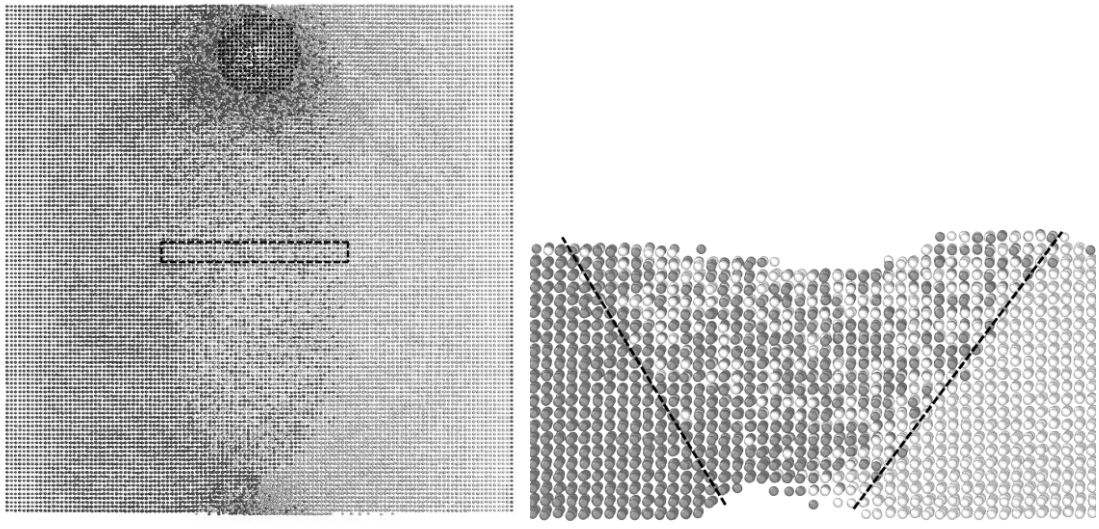
In this paper, we investigated the influence of an additional oscillating impact applied to the indenter in the vertical direction (axis Z) on the features of implementation of possible atomic mechanisms under loading conditions, identical to process of friction stir welding. Since the cylindrical indenter in case of vertical movements will only slightly change the resulting stress, in these studies the shape indenter was changed to a cone. Originally, we

modeled movement of indenter without vibration impact. This allowed us to compare the simulation results with previous studies, when indenter has a cylindrical shape. In the next stage of research, we simulate cyclical movement along the axis Z in addition to move in direction Y (see. scheme in Figure 1). The amplitude of oscillatory motion of the indenter A = 0.1 nm, and the frequency $\omega' = 2$ ps$^{-1}$.




a) b)

**Figure 2:** a) Projection of atoms on the plane X0Y after the passage tool in conjugate pair Cu - Cu; б) the spatial distribution of the atoms of the two metals and structural defects in the selection marked by a dotted line in the figure (a). Hereinafter the vertical dotted line indicates the original position of the interface between two metals.



a) b)

**Figure 3:** The resulting structure of the sample of conjugate pair of Cu-Cu after the passage of the conical tool excluding additional vibration exposure: a) projection of atoms on the plane X0Y; b) a fragment of the central region of the sample, oriented parallel to the plane X0Z. The dashed lines show the approximate boundaries of the position of the interstitial atoms.

Analysis of the sample structure showed that mixing of atoms, initially belonging to different fragments, was observed in the sample at the junction of two crystallites as a result of the passage of the rotating tool. This result is identical to what was obtained for the cylindrical indenter (Figure 3a). The difference from the results obtained for the cylindrical indenter is the distribution of embedded atoms along the axis of rotation of the tool. Figure 3b shows a projection of the atoms of the central fragment on a plane X0Z. It can be seen that the width of the layer with mutual introduction of atoms, originally belonging to the opposite crystallites is much wider at the top of the sample. This is due to cone-shaped tool. Common neighbor analysis of the crystal lattice showed that, as before, the volume fraction of structural defects in relation to the total number of atoms is negligible. Thus, the use of the conical indenter leads to irregular distribution of embedded atoms in the transverse direction along the interface in comparison with the results obtained using a cylindrical tool.

In order to make the distribution of embedded atoms more uniform in the next phase of research we specify additional oscillating load directed along the axis Z to indenter. The result of the impact of additional oscillating movement of the tool is a more uniform distribution of embedded atoms throughout the depth of the sample in the interface area, where there is a mixing of atoms, originally belonging to different crystallites (ref. Figure 3b and Figure 4).

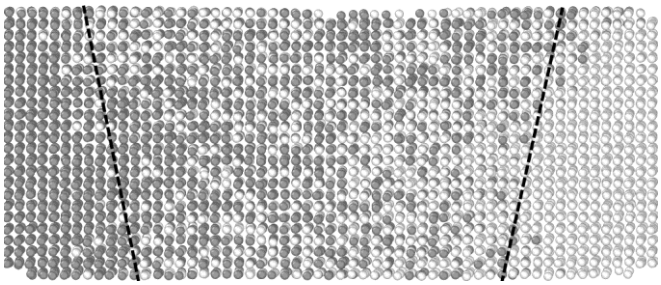


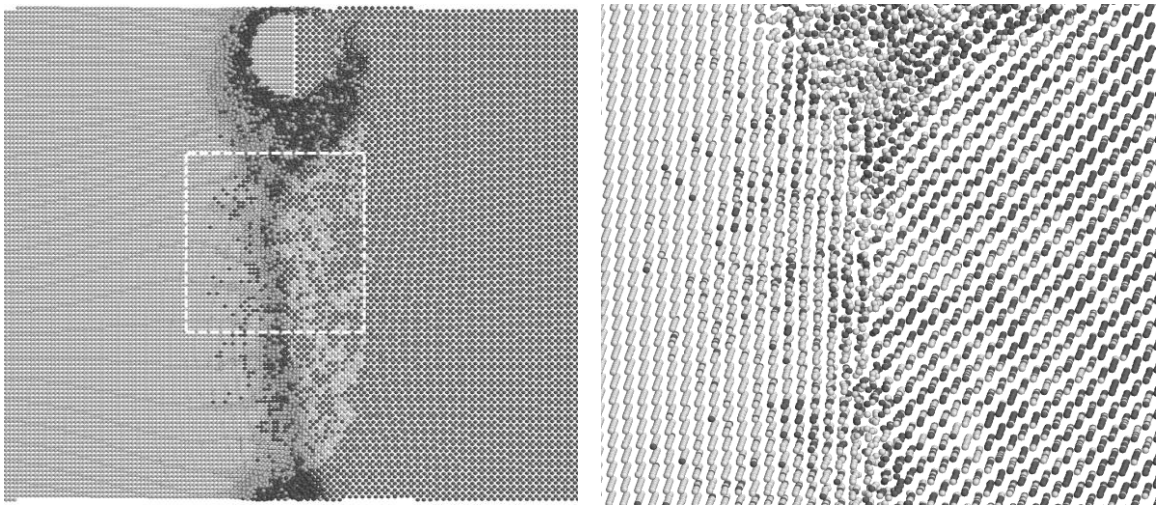
**Figure 4:** Projection of atoms of structure fragment near “trace” on the plane X0Z after the passage conical tool with additional vibration impact in conjugate pair Cu-Cu. The dashed lines show the approximate boundaries of the position of the interstitial atoms.

### 3.2 Conjugation of metals with different types of crystal lattice

At the next stage of the research we reproduced on the atomic scale the loading conditions used in FSW of dissimilar material crystallites such as Cu (Me1) and α-Fe (Me2). Along the Y and Z directions periodic conditions were simulated. In the X direction the hard boundary conditions were set up. As in the previous case, the interaction was computed using a model of embedded atom method. Sizes of simulated fragments of Me1 and Me2 were equal to 21,7 × 21,7 × 2,9 nm. Initial crystallographic orientation of both crystallites was chosen as [100] [010] and [001] along the respective axes. Tool speed was V = 50 m/s and $\omega = 0{,}1$ ps$^{-1}$. As before, the removal of heat from the specimen is realized by introducing an artificial viscosity of atoms belonging to the two buffer layers peripheral with respect to the plane of coupling of both crystallites.

Simulation results showed that after the passage of the rotating tool along the boundary, we can see there a complex configuration comprising the intermixing of copper and iron atoms (Figure 5a). The detailed analysis of the resultant structure showed some Cu-atoms substituted Fe ones in the α-Fe bcc lattice in the vicinity of initial joint interface and vice

versa iron atoms substituted copper ones in the fcc lattice. This is clearly seen in Figure 5b, which shows an enlarged image of the area of initial connection of two metals immediately after passage of the instrument. Figure 6, which shows the concentration distribution of the atoms of the two metals along the X axis in the selection area, you can also see a slight movement of the position of the interface (the area where there is a change of crystallographic order) to the side of the crystallite that softer by mechanical properties.



a) b)

**Figure 5:** Projection of atoms on the plane X0Y after the passage tool in conjugate pair Cu - α-Fe. Image (b) corresponds to the fragment framed in (a).

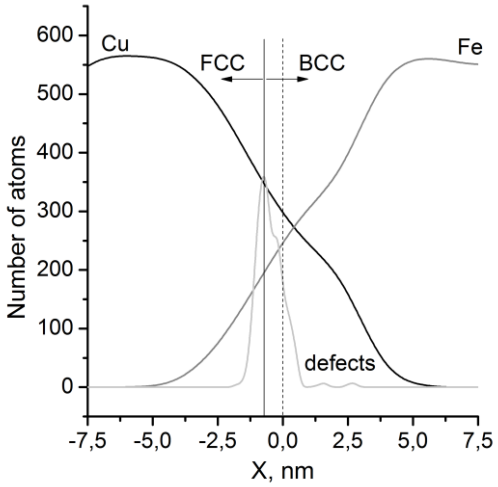



**Figure 6:** The spatial distribution of the atoms of the two metals and structural defects in the selection shown in Figure 5a.

As previously, the gradient character of atom substitution zone in both metals has been observed but the width of this zone is less in comparison with the results obtained for the Cu-Cu interface. This can be explained by the differences in crystal lattice structures. This also

explains the presence of numerous structural defects along the boundary obtained after passing the instrument.

As in the previous example of coupling of two identical metals in the next step of research, the problem of influence of additional oscillating load applied to the cone-shape indenter was solved. Options of oscillating load: amplitude A = 0,1 nm, and the frequency $\omega' = 2$ ps$^{-1}$.

Simulation results showed that, as before, after the passage of the rotating tool at the interface of crystallite formation of complex configuration, wherein there is a mixing of the atoms originally belonging to different metals, is observed. In contrast to the results obtained using a cylindrical indenter without oscillating impact final position is shifted toward the interface of copper by a large amount. Figure 7 shows the spatial distribution of the number of atoms of the two metals, depending on their position along the axis X. A distinctive feature of the presentation of results is an increase in the width of the layer in which the atoms, local topology of atomic bonds that cannot be correlated with both the fcc and bcc metals, are located. Thus, the action of the oscillating impact increases the number of structural defects. The point of intersection of the two curves, reflecting the change in the number of atoms of various metals, as well as the previous case, is shifted toward the crystallite iron.

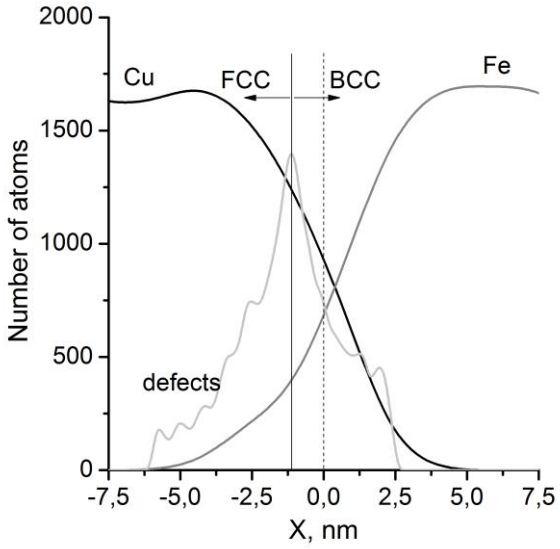


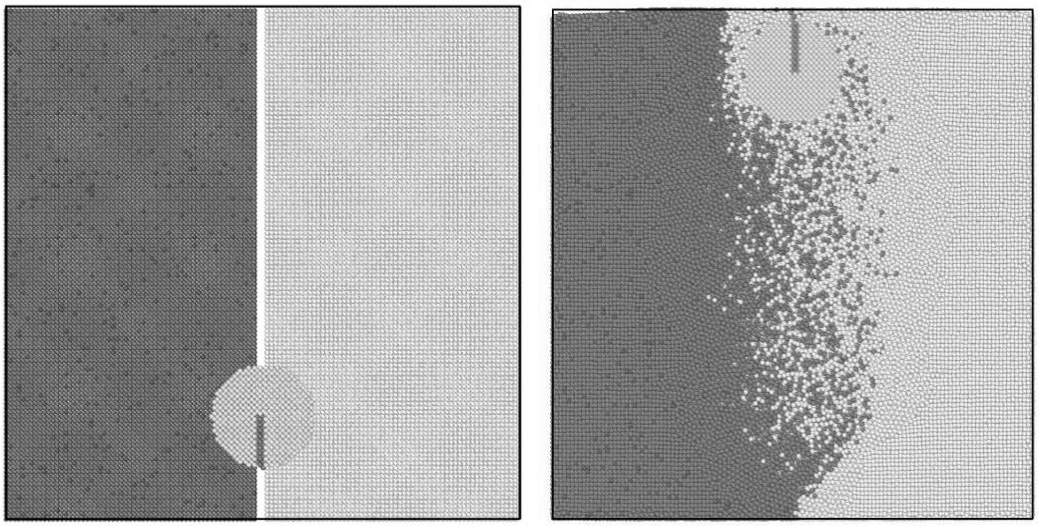

**Figure 7:** The spatial distribution of the atoms of the two metals and structural defects in the selection shown in Figure 5a in case of additional oscillating impact.

### 3.3 Conjugation of two identical solid solutions

The results shown above were obtained for metals having a perfect crystal structure. At the same time, most of the materials used in practice for the manufacture of various components and structures, in particular by using friction stir welding, are metallic alloys that are solid solutions. Their crystal structure may contain a certain amount of different defects, including particles of intermetallic. In this regard, developed numerical model of analysis of atomic mechanisms realized under the loading conditions, identical to process of friction stir welding, can be applied for the study of the behavior of atomic lattices of solid solutions. In the work for this purpose two crystallite atomic structure of which corresponded to the aluminum alloy

2024 have been chosen. Interatomic interaction described by potentials, calculated by the method of the modified embedded atom [8]. To simulate the loading conditions identical to those of the friction stir welding, as in the previous calculations movement of the rotating rigid cone along the area of conjugation of two crystallites was simulated. The contact area the gap is initially created for simulate the influence of end faces roughness of connected crystallites. To create a structure of aluminum alloy 2024 in an ideal fcc lattice of atoms of Al, a random 5% Al atoms are replaced by atoms of Cu, which correspond to intermetallic phase. Each crystallite dimensions were 12,2×24,4×2,03 nm. Along the directions X and Y rigid boundary conditions were simulated. Along the Z-axis direction were set free surface. Initial crystallographic orientation of both the crystallites was selected as the [100], [010] and [001] along the respective axes. Indenter atoms rotates at a constant angular velocity $\omega = 0{,}1$ ps$^{-1}$. Additionally, the indenter atoms is progressively moved as a whole with a velocity V = 50 m/s. As before, removal of heat from the specimen is realized by introducing an artificial viscosity to atoms in buffer layers of both fragments.

Simulation results showed that after passing conical tool at the interface of the crystallites formation of complex configuration, which present both mixing atoms crystallites, is observed. At that movement both atoms Cu and atoms Al occurs. The projections of the crystallite atoms on a plane X0Y before and after pass of the indenter shown in Figure 8.



a) b)

**Figure 8:** Projection of atoms on the plane X0Y at different points in time. Darker shades of gray in both the crystallites shown atoms Cu.

Figure 8 shows that after the formation of the weld atoms of both the first and second crystallites are present in both plates. The proportion of atoms of one crystallite in another quite rapidly decreases with distance from the weld and at a distance corresponding to the diameter of the tool becomes zero.

As before, we investigate the influence of additional vibration impact applied to the rotating and linearly moving conical indenter. Periodic movement of the tool was carried out in the Z direction sinusoidal with the angular velocity $\omega = 0{,}1$ ps$^{-1}$ and an amplitude equal to 4.16% of the tool diameter.

Figure 9 shows a diagram of the distribution of atoms in the crystallites after their compounds in the usual way, and with an additional vibration impact. Hereinafter shaded rectangle corresponds to the position initial gap between the crystallites. The figure shows that in the case of a vibration impact the penetration of atoms of one crystallite to another increased by about 20% compared with the same value for the process without vibration impact. Fractures of the distribution curves of the atoms in the area of crystallite conjugation are due to the absence there atoms at the initial time and the subsequent filling of this area during the formation of the joint.

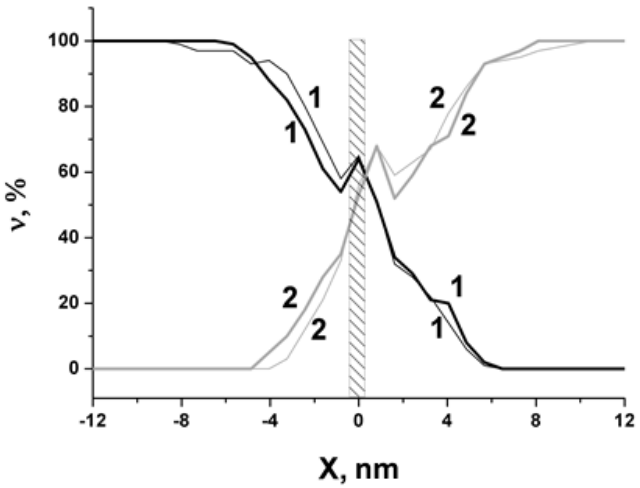



**Figure 9:** The distribution of the atoms along the direction X simulated crystallites. Distribution curves correspond to atoms: 1 - the first crystallite 2 - the second crystallite. The thickness of the curves corresponds to different welding processes: thin – without vibration impact; fat – using the vibration impact.

Results of the analysis of the dynamics of the process of friction stir welding on a scale of 1 to 10 nm show that the use of ultrasonic influence to the operating element in a direction parallel to the axis of rotation of the tool leads to a uniform introduction of the elements of the opposite plate in the weld zone along a vertical cross section, which means increasing the bond strength along weld line.

## 4 CONCLUSIONS

Based on the research results the conclusions can be made as follows. In spite of the fundamental differences in characteristic spatial and temporal parameters, computer simulation results are in good qualitative agreement with those of experimental studies. Computer model may be a test bed serving for better understanding the basic laws of structural inhomogeneity origin in FSW. The simulation results obtained can be those of practical importance. They allow discovering new ways and mechanisms to obtain non-equilibrium states in the crystal lattice due to the initiation of the mechanically activated metal interdiffusion at the atomic level.

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