

# The role of the atom-atomic interactions depth on the metallic nanofilms structure evolution

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**Abstract.** Stochastic methods of modeling slow-moving processes controlled by diffusion make it possible to analyze the order-disorder phase transitions. The features of the kinetics of these transformations can also be identified due to these methods. Most of the investigations were made for binary alloys, taking into account the interaction of atoms in the first two coordination spheres. There is evidence that in real alloys the influence of the interatomic potential trimming radius is significant. The computer simulation results from the process of isothermal annealing of a binary metal nanofilm by a vacancy mechanism at various temperatures and the extent of the interatomic potential are presented. It has been established that with an increase in the extent of interatomic interaction potential, effects similar to those of temperature disordering a ear.

## 1 Introduction

The possibilities that open up when studying, within the framework of a computer experiment, the processes of a rearrangement of the atomic structure of various materials under the influence of different factors: temperature, stoichiometric composition, vacancy concentration, degree of deformation, laser irradiation and plasma, attract many researchers today [1-27]. Of particular interest are nanostructured surface inclusions, thin-film materials, nanofiber filaments and carbon nanotubes, which have physical and chemical properties that differ from massive materials [8, 14-18, 27-38]. The choice of computer modeling for solving such problems is not accidental. In a real experiment, whether it is electron microscopic studies, autoion microscopy or X-ray diffraction analysis, it is difficult to interpret data on local atomic distributions near and on structural features. The analysis of the results of computer modeling simplifies the explanation of experimental data, provides an understanding of the kinetics of processes and allows determining the contribution and significance of each of the factors at the atomic level.

One of the ways to solving problems of this kind is statistical [1, 21-36]. Within the framework of the statistical theory of atomic ordering, it is possible to determine the parameters either as the average of the statistical ensemble, or as the most probable. In quantum theory, the forces acting between atoms decrease faster than the distance between

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them [1, 31-43], therefore, models most often consider interaction only in the nearest coordination sphere, and the influence of long-range contributions on the process of atomic ordering and the order-disorder phase transition practically has not been studied.

At the same time, in [23, 30-35] it is shown that taking into account two or more coordination spheres in the interatomic interaction significantly affects the nature of the order-disorder phase transformation and leads to features in both short- and long-range ordering. It was shown in [32, 33] that when long-range contributions are included in the ordering energy, the phase with a long-range order in the arrangement of atoms becomes unstable at lower temperatures.

In [33], when studying the structure of an unordered  $AyB_{1-y}$  solid solution, the atoms of which are distributed over the nodes of a square lattice, it was proven that induced correlations arise in the crystal in the presence of a short-range order, which fade in the square lattice when the ninth coordination sphere is reached.

In the presented work, the process of thermally activated migration of atoms by a vacancy mechanism in solid-state thin films of binary composition are modeled and the influence of the "extension" of the interatomic interaction potential on the patterns of atomic distribution in the sample and the structural and energy parameters characterizing its equilibrium state is analyzed.

The choice of thin metal films is not accidental. Firstly, in the entire temperature range of the phase transformation, an order-disorder transition is possible on the surface of the alloy without a presence of such in the bulk [41-44], accompanied by abrupt changes in the parameters characterizing the short- and long-range order on the surface [32,33, 45-48]. Secondly, the type of phase transformations occurring on the surface and in the bulk of binary alloys is also different, and there is also a difference in ordered superstructures in the near-surface layers [24-26, 50-54].

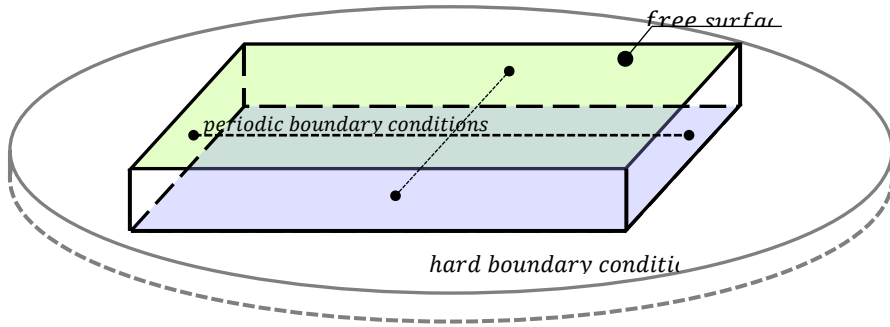
Local order heterophase fluctuations [55-60] are observed in the near-surface layers, preceding the order-disorder phase transitions: nanosized up to 2.5 nm disordered clusters and atomic segregations coexist for a long time with relatively large microdomains (characteristic sizes do not exceed 500 nm) of the ordered phase.

For solid-phase film nanostructures of Cu-Zn, Cu-Au, etc. systems [62-68], it is shown that both the temperature of phase transformations and the nature of the order-disorder phase transformation change compared with those in the bulk of alloys.

## 2 The model

Two-dimensional films previously considered by the authors [31-33, 65] do not allow us to assess the degree of reliability of the results obtained and extend the conclusions drawn to real materials, therefore, within the framework of a stochastic model of the diffusion mechanism of atomic migration through vacant nodes [65,66], a transition to 3D nanofilms was carried out. In the study of equilibrium structures, Monte Carlo methods give results that are in good agreement with experimental data and theoretical predictions, therefore, the choice of this method for solving the tasks set is quite justified.

In a computer experiment, a crystalline nanofilm of an alloy of stoichiometric composition AB with a BCC lattice corresponding to the Ising model was considered, the thickness of which did not exceed 10-12 atomic layers with a size of 100x100 atoms, and the initial structure was completely disordered. The boundary conditions were imposed as shown in Figure 1.



**Fig. 1.** Schematic representation of the calculation block

The sample was subjected to isothermal annealing, with a uniform temperature distribution over the entire bulk of the crystallite, vacancies, the concentration of which was assumed to be equal to equilibrium ( $c_v \sim 10^{-5}$ ) and maintained constant during the modeling process were randomly "thrown" into the sample.

The variable parameters in this computer experiment were the annealing temperature  $T$  and the number of coordination spheres  $L$  taken into account in the interaction of atoms (the radius of action of the interatomic potential). The annealing temperature was set the same throughout the sample and varied during the experiment in the range from 0 to  $1.2 T_c$ , where  $T_K$  is the temperature of the order-disorder phase transformation (Kurnakov point).

The "extent" of the interatomic interaction potential changed during modeling, so that  $L = 1, \dots, 9$ . That means that any lattice atom interacts with atoms lying in  $L$  coordination spheres ( $L$  is the maximum number of the coordination sphere taken into account in the interaction).

The state of the system in the process of thermally activated structural restructuring of the alloy changed only at discrete points in time, while the "transitions" of atoms to vacant nodes were limited to the first two coordination spheres, and when the material reached an equilibrium state, the experiment was stopped.

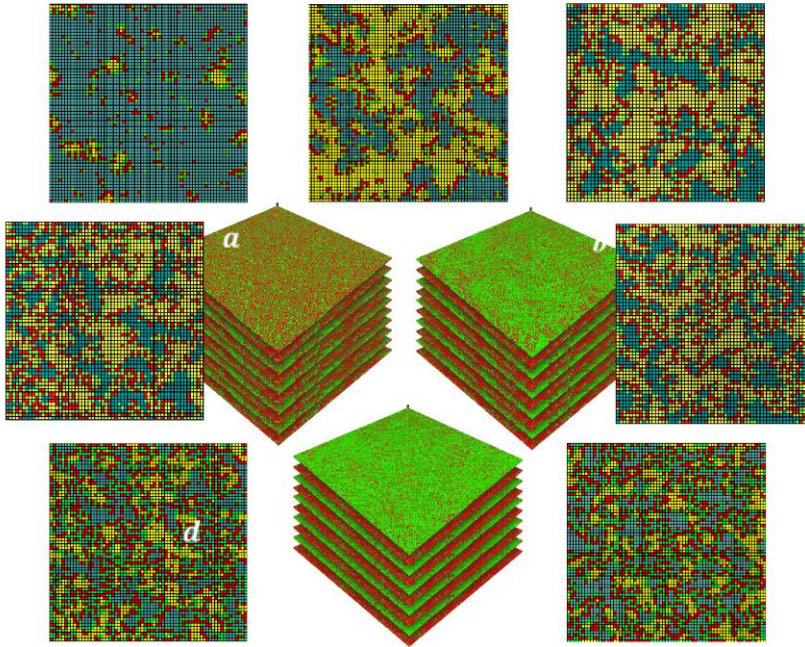
### 3 Results and discussion

The presence of any order in the system implies the presence of certain patterns in the distribution of special points of the system in space and time, corresponding to the minimum entropy in this system [1, 23, 31-33]. The main parameters characterizing the degree of ordering are the short-range order, which determines the order in some selected local area [31-41], and the long-range order, which characterizes the order in the arrangement of atoms in a sufficiently large volume [35,39,64,65]. The short-range ordering can be considered as a local order, which is shown by several mechanisms. Firstly, in the effect of blurring the boundaries separating completely ordered antiphase domains; secondly, in the form of a large number of completely ordered small antiphase domains separated by interlayers with a change in the correct alternation of atoms at their boundaries, and in the form of microdomains "floating" in the disordered phase. [31-34].

The long-range order is established as a rule, in atomic systems in a solid crystalline state and is disrupted by various kinds of defects. Similarly, in multicomponent alloys in the crystalline state, the order can be disrupted locally by the distribution of components across the nodes of the crystal lattice, while generally maintaining a high degree of order. The long-range order in a solid solution occurs during phase transformations at temperatures below critical [1, 41, 47].

The analysis of the atomic configurations of the model nanofilm obtained as results of isothermal annealing at different lengths of interatomic interaction showed a significant change in its equilibrium structure.

Figure 2 shows the patterns of atomic distributions in a model nanofilm ( $T/T_c \sim 0.28$ ) at different lengths of the interatomic interaction potential. For clarity, two-dimensional slices in which ordered antiphase domains are highlighted are shown next to the patterns. A significant change in the local order in the film is observed up to  $L=6$  and "fades" in the rigid Ising lattice to the ninth coordination sphere.



**Fig. 2.** Atomic distribution patterns obtained for different lengths of interatomic interaction at a temperature of  $0.3 T_c$ : (a)  $L=1$ ; (b)  $L=2$ ; (c)  $L=3$ ; (d)  $L=5$ ; (e)  $L=7$ ; (f)  $L=8$ ; (g)  $L=9$

At temperatures far from  $T_c$ , taking into account the nearest neighbors leads to the formation of predominantly point substitution defects (PSD). The introduction of long-range connections into the energy of ordering leads to the consistent appearance of new structural formations - clusters and segregation, microdomains (MCD), antiphase boundaries (APB). The grinding of the domains structure of the material is accompanied by an increase in the extent and density of antiphase and interphase boundaries. APBs are faceted, their structure becomes labyrinthine.

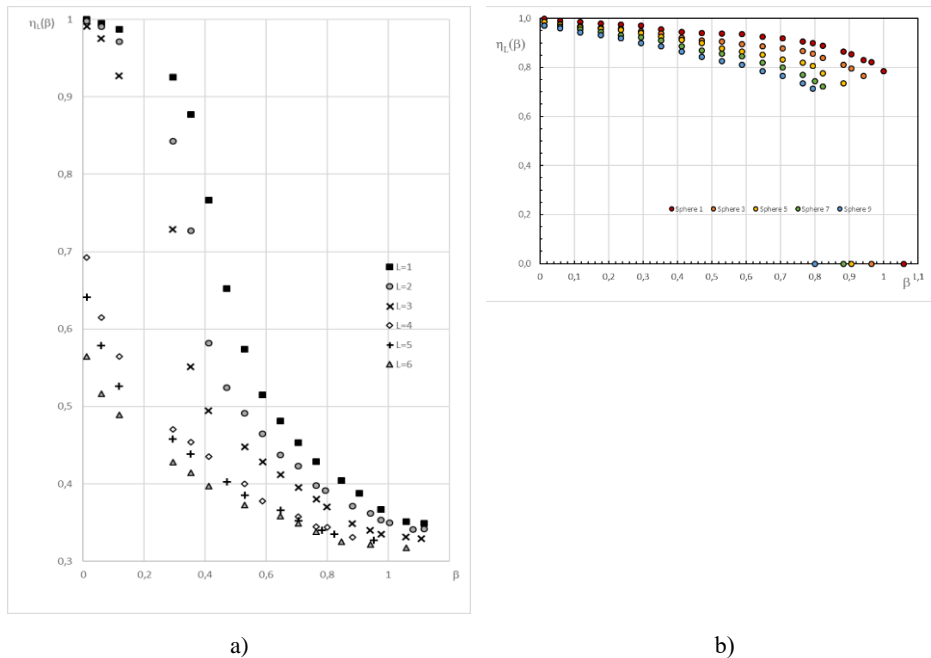
The degree of order decreases near APBs, they "blur" due to the "sticking" of structural features and the formation of structures with a different order in the alternation of atoms near them, which is in good agreement with [31-33, 62-66]. At the same time, significant regions of the phase with a near-order in the arrangement of atoms are formed both inside the ordered domains and at their boundaries. This leads to the sequential activation of the mechanisms of disordering the alloy, which are characteristic of increasing the annealing temperature. This behavior of the ordering alloy agrees well with the data [57-63], where it is shown that in alloys of the Cu-Au system, contributions to the energy of ordering interactions of pairs of atoms up to the fifth coordination sphere are significant.

A comparison of the patterns of the equilibrium distribution of atoms with the behavior features of the parameters of the far and near order, the average energy and entropy of a

crystalline nanofilm allows us to describe the nature of the order-disorder phase transformation (ODPT) in the entire temperature range under consideration, depending on  $L$ .

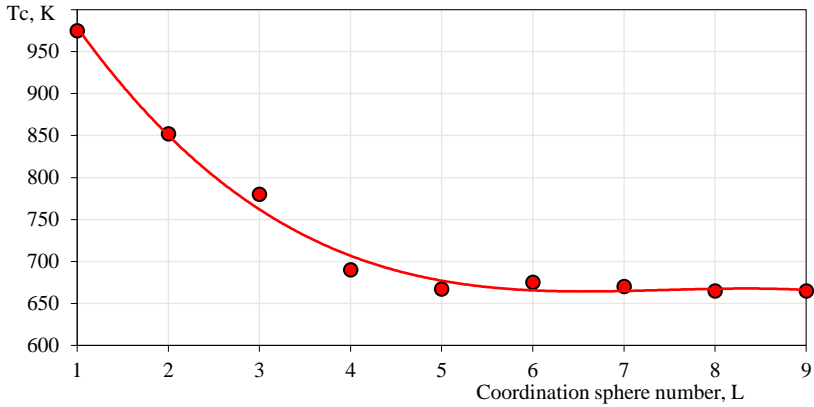
For this model material, the ODPT passes through a two-phase region. The temperature dependences of the long-range parameter  $\eta_L(\beta)$ , where  $\beta = T/T_c$  for a different number of  $L$  taken into account in the interaction of coordination spheres, are shown in Figure 3 (a, b). The nonlinear sections of the graphs, which illustrate the dependencies  $\eta_L(\beta)$  in ordered domains, correspond to the two-phase state of the alloy in this temperature range. To characterize the stability of an ordered phase with respect towards the near-order phase, the lowest value of the order parameter  $\eta$  and the slope of the tangent  $\frac{\partial \eta}{\partial \beta}$  at  $\beta \rightarrow 1$  are usually used. Obviously,  $\Delta \eta \sim 0.25 \div 0.47$ , at  $\frac{\partial \eta}{\partial \beta} \sim 0.07$ . The smallness of the latter characteristic means that the ordered state is close to loss of stability.

A nanofilm of a metal alloy of stoichiometric composition AB passes through a two-phase region during the ODPT process, revealing features of a blurred phase transition of the first kind. The temperature range of the existence of two phases in the material - an ordered phase with a long-range order (antiphase domains) and a phase with a short-range order (microdomains, clusters and segregation) - shifts to the region of lower temperatures.



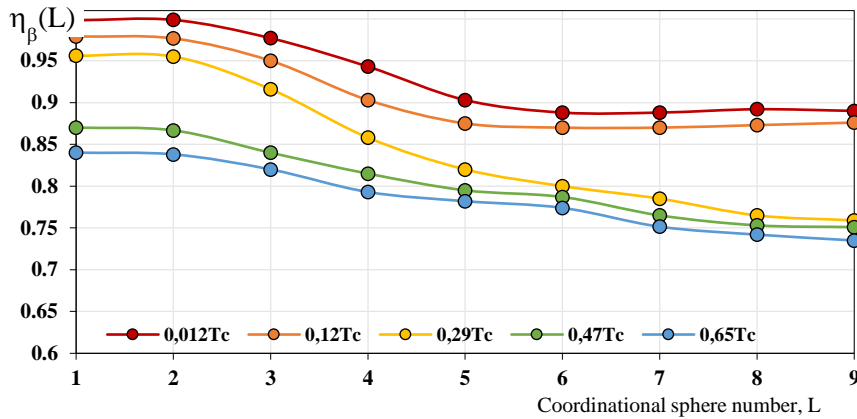
**Fig. 3.** Dependence of the average of the sample (a) and within the domain (b) long-range order parameters on the temperature of the order-disorder phase transformation at different values of the number of coordination spheres  $L$  taken into account in the interaction

As  $L$  increases, the area of stability loss by the ordered phase becomes wider, and the temperature corresponding to the Kurnakov point decreases up to the sixth coordination sphere (Figure 4). At the same time, the near-order phase, becoming more and more likely, has a high local order (Figure 5).



**Fig. 4.** Dependence of the temperature of the order-disorder phase transition on the extent of the potential of interatomic interaction

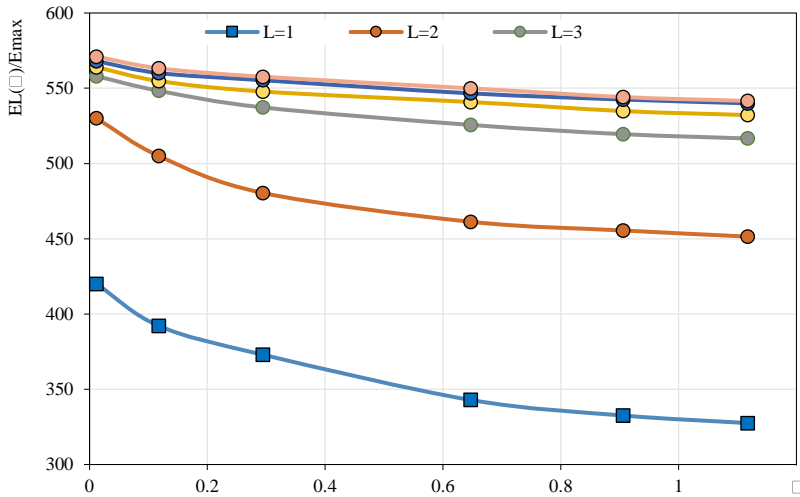
At temperatures a roaching and above the Kurnakov point  $T_c$  the local (near) order turns out to be quite high. This indicates that the disordered structure contains a significant number of ordered domains and microdomains. Conversion of the microdomain model of the near-order parameter into a long-range one gives us a local order in the microdomains structure of at least 0.78 at  $L \leq 6$ .



**Fig. 5.** Dependence of the long-range order parameter inside ordered regions on the radius of the interatomic potential pruning (the number of coordination spheres L).

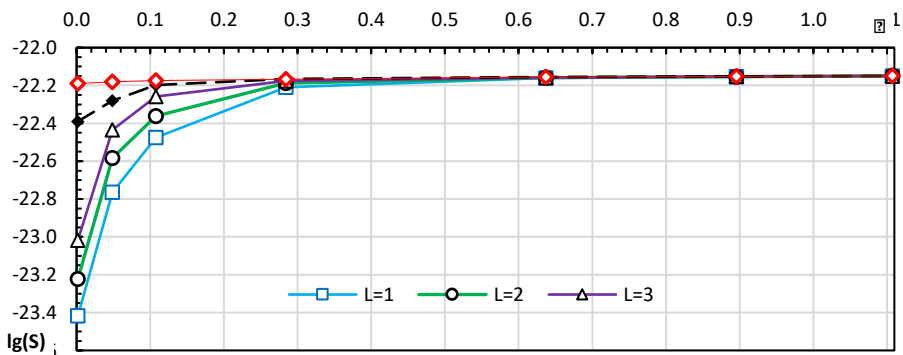
Let's note that the phase with a short-range order in the arrangement of atoms at temperatures above  $T_c$  is sensitive to temperature increase (regardless of long-range contributions). While maintaining a high intra-domain order, the long-range parameter that is average by the sample continues to decrease (Figure 3). This is probably due to the further fragmentation of microdomains while maintaining a high degree of order in them and increasing the concentration of clusters and segregations.

The different rate of change in the in the relative energy  $E_L(\beta)/E_{max}$  per atom of the model metal nanofilm is due to a decrease in characteristic temperatures (Figure 6), when various mechanisms of disordering begin to "turn on" at different lengths of the interatomic interaction potential [31,62-66].



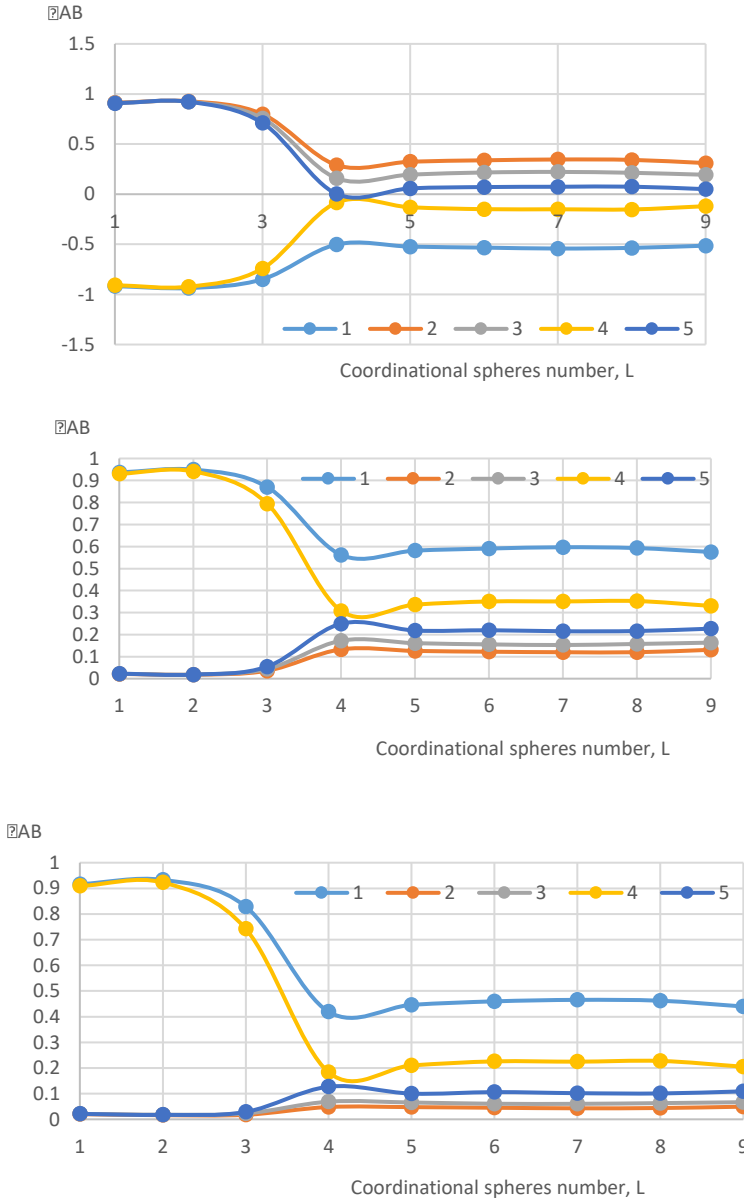
**Fig. 6.** Dependence of the relative configuration energy of a metal nanofilm,  $E_{max}$  is the maximum energy of an ordered thin film

In Figure 7, we have illustrated the configuration entropy as a function of temperature. An increase in the pruning radius of the interatomic interaction potential leads to the fact that during isothermal annealing the degree of disorder in the simulated atomic system reaches saturation faster due to the earlier activation of new disordering mechanisms.



**Fig. 7.** Temperature dependence of the configuration entropy  $S$ , which characterizes the equilibrium distribution of atoms in a metal nanofilm.

The energy characteristics behavior of the metal nanofilm at the various interatomic potential lengths under the different annealing temperature is due not only to the growth of "disorder" in the structure of the material. The influence of correlation effects is also significant, as evidenced by the dependences of paired  $\sigma_{AB}$ , three-particle  $\epsilon_{AB}$  and four-particle  $\xi_{AB}$  correlation functions in the first five coordination spheres (Figure 8). The observed functional features of the correlation coefficients may be related to fluctuations in the potential used in the model [1,41,69].



**Fig. 8.** Dependences of paired  $\sigma_{AB}$ , three-particle  $\epsilon_{AB}$  and four-particle  $\xi_{AB}$  correlation functions in the first five coordination spheres on the range of the interatomic potential at a temperature near  $0,12T_c$

## 4 Conclusion

It has been established that with an increase in the extent of the potential of interatomic interaction, effects similar to those of temperature disordering a ear. For the simulated thin film, the ODPT is close to a phase transition of the first kind, however, due to the blurring of the APB, the phase transformation is not point-like.

The influence of long-range contributions is significant up to the sixth coordination sphere, and then they quickly "fade out". With an increase in the extent of the potential for interatomic interaction, the temperatures at which the ordered phase loses stability shift to lower values, and as a result, the temperature of the ODPT decreases. From the point of view of the statistical theory of atomic ordering, which operates even with a constant ordering energy (independent of the lattice parameter, order state, annealing temperature, etc.), this indicates that for this material the role of three- and four-partial correlations contributes significantly to the ordering energy.

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