Peculiarities of primary nanocrystallization of Al-V and Al-Hf alloys

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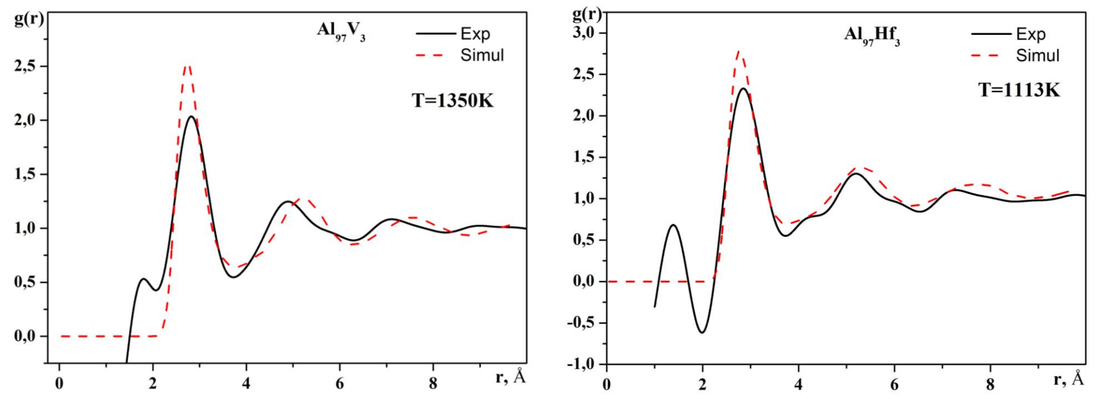
Motivation

The progress of the aerospace industry stimulates the search for new metal alloys with both large plasticity and durability. It is known, these properties depend both on the phase composition of the alloys and on the grain size. As it was shown in many works [1-3], reduction of the grain of aluminum and aluminum alloys occurs after adding a small amount of vanadium, hafnium, zirconium, chromium. As it was established, the reduction of grains is due to the heterogeneous crystallization of aluminum on the crystal nuclei, which are the Al_3V, $Al_{10}V$, Al_3Hf compounds. However, in most cases, only the resulting effect of impurities on grain size has been investigated, without studying the process of formation of crystallization nanocenters, which affect the final grain size distribution.

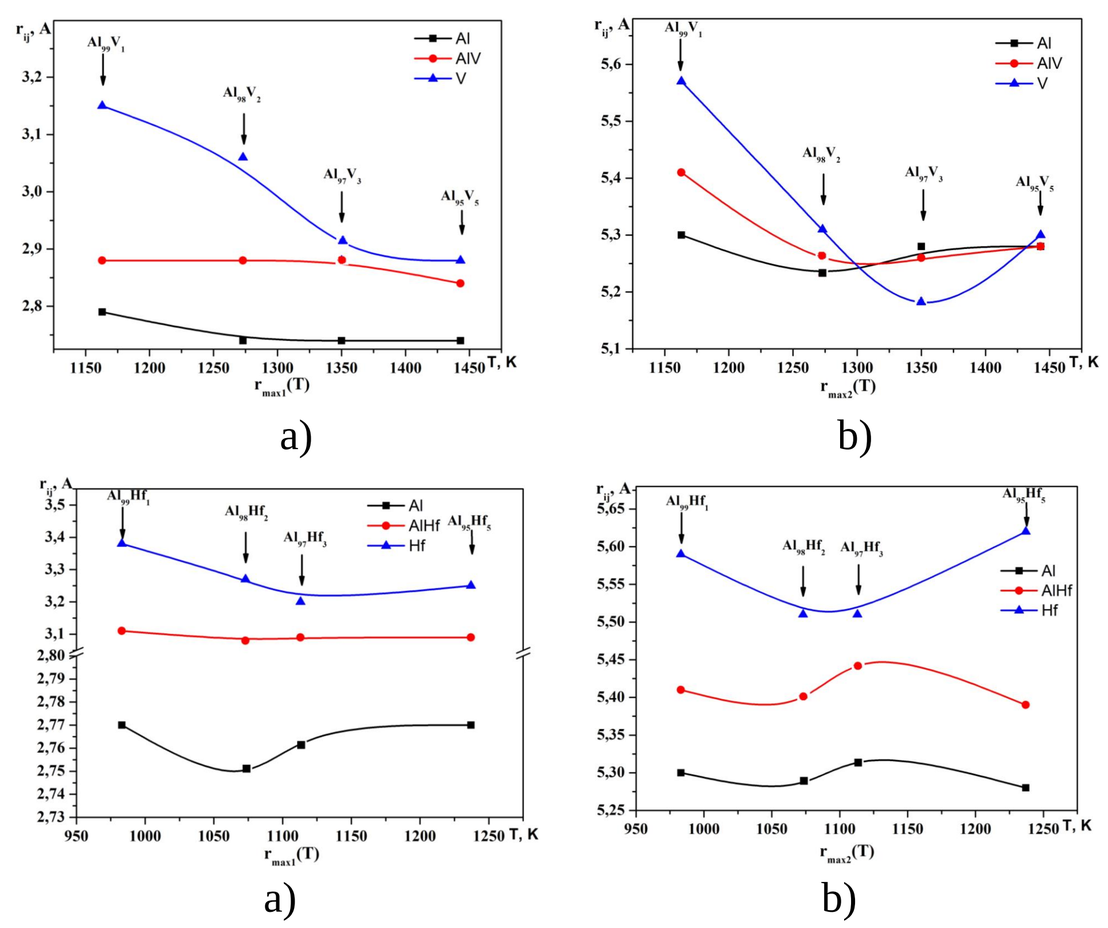
Conclusions

In this work, the mechanism of formation of nanocrystallization centers in Al-Hf and Al-V alloys from the liquid state is investigated. Research on nanocrystallization was studied by the method of molecular dynamic modeling and with the help of experimental methods. As a result of the work, the optimal conditions for the crystallization of alloys to obtain a dispersed structure with improved mechanical properties were established.

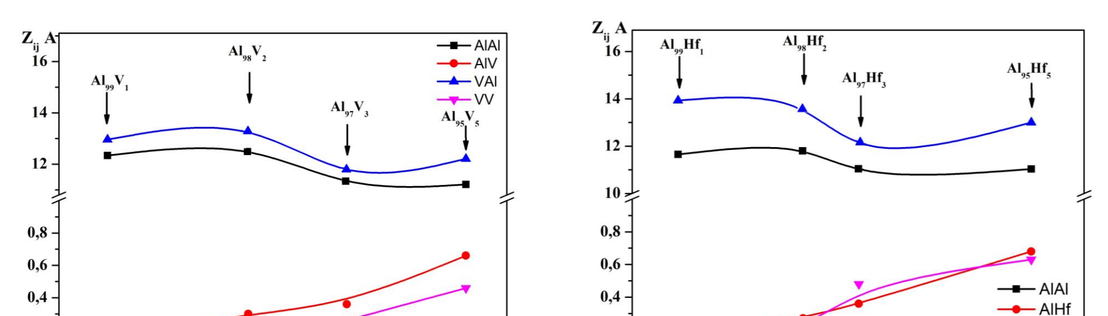
Results



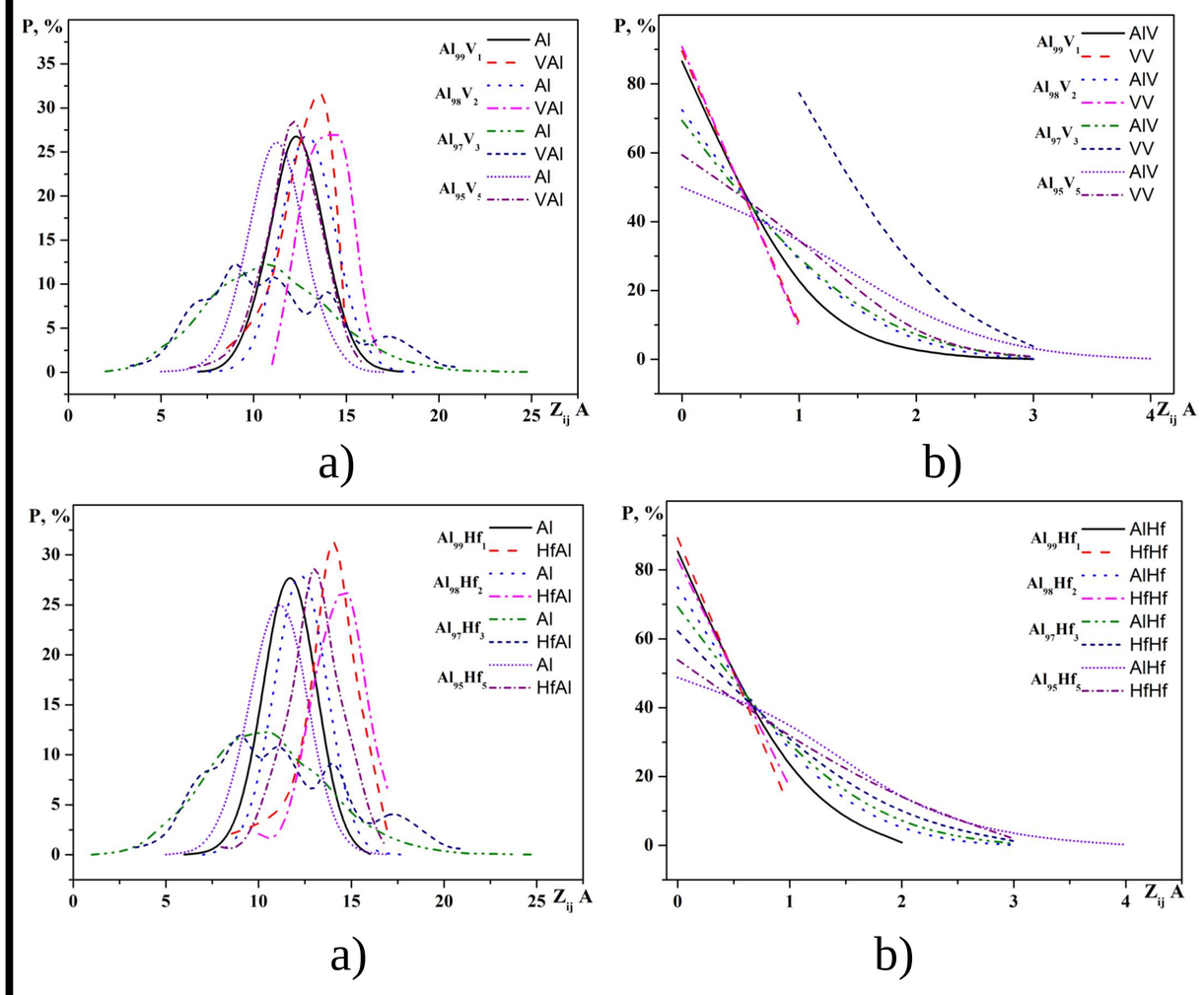
Typical view of pair correlation functions obtained as a result of X-ray difraction studies and simulations



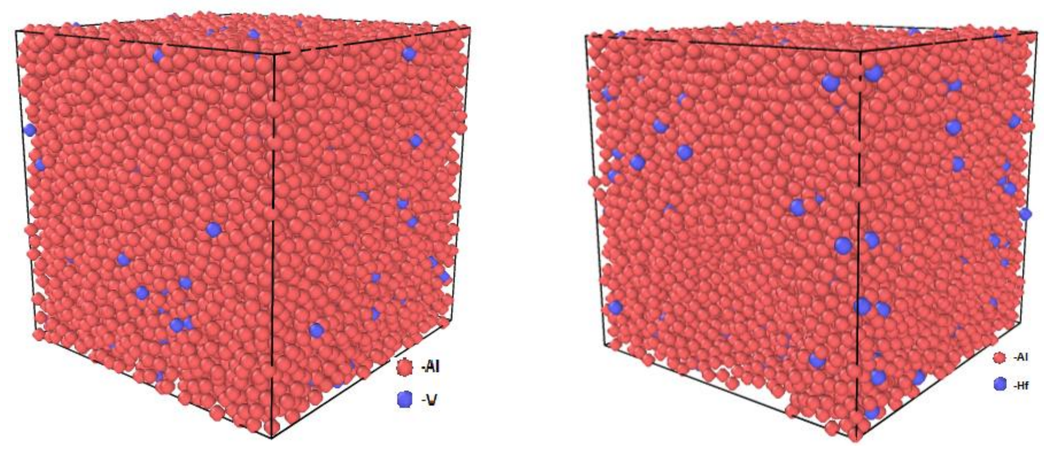
The most probable partial interatomic distances for AlV and AlHf melts at different concentrations.



Temperature dependences of the most probable coordination numbers of AlV and AlHf melts at different concentrations.



Distribution of partial coordination numbers of AlV and AlHf melt at different temperatures and concentrations.



Distribution of atoms in the model cell of the Al97V3 and Al97Hf3 melt at temperatures T =1350K (a) and T = 1113K (b)

References:

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