

THE CONCENTRATION DEPENDENCE OF MICROSTRUCTURE IN Al-Mn ALLOYS

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Al-Mn alloys with Mn concentrations 14%, 18%, 22.5%, and 25% were modeled by the method of molecular dynamics. The microstructure of these alloys with different concentrations of Mn were found to differ substantially. The structure of all the alloys contained a high percentage of icosahedral microclusters, and the maximum number of the icosahedron-like structures was observed at a concentration of 22.5%.

The quasicrystalline state is characterized by the long-range orientation ordering of icosahedrons [1, 2]. Some investigations [3-6] carried out within the phenomenological approach of the Landau phase transition theory have shown that under certain conditions a structure with an icosahedron point symmetry group can be energetically more advantageous than a structure with translational invariance. The local structure of the alloy and the ability to form an icosahedral structure are governed by both the specific features of the electron structure and the concentration of components. Both factors determine the possibility of occurring of icosahedrons in the alloy and their ordering.

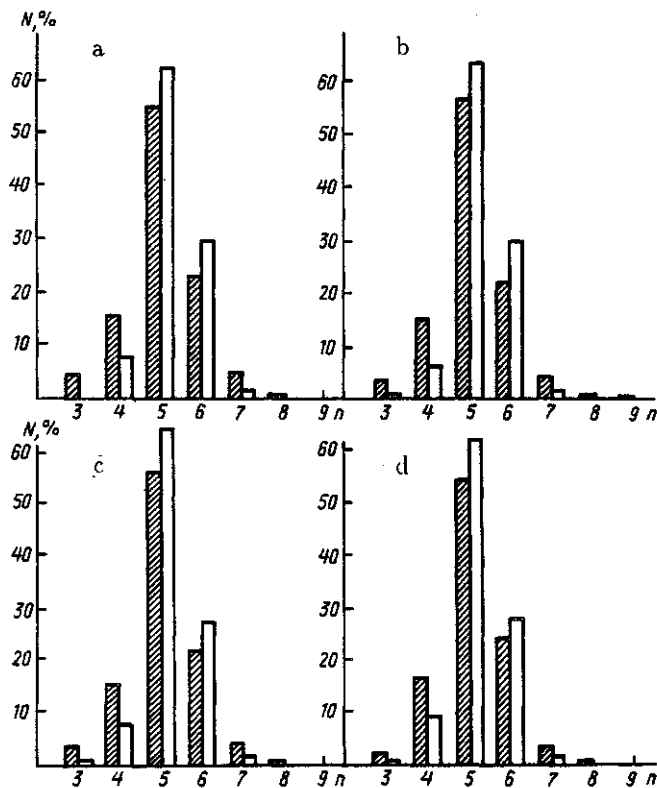


Fig. 1

Table 1

Percentages of the Voronoy Type Polyhedrons Obtained by Computer
Simulation for $Al_{86}Mn_{14}$, $Al_{82}Mn_{18}$, $Al_{77.5}Mn_{22.5}$, and $Al_{75}Mn_{25}$ at the Temperature 300 K

Mn concentration	The atom at the polyhedron center	Polyhedrons		
		Icosahedron-like	Prisms	f. c. c.-type structures
14%	Al	22.3	17.2	14.2
	Mn	66	14.4	2.9
	Weighted mean value	28	16.8	12.5
18%	Al	24.3	20.1	16.3
	Mn	60.8	13	6.5
	Weighted mean value	30.9	18.8	14.5
22.5%	Al	31.7	13.5	15.6
	Mn	69	12.3	3.6
	Weighted mean value	39.8	13.3	12.9
25%	Al	27.5	16.6	24.5
	Mn	58.1	14.4	12.5
	Weighted mean value	35.1	16	21.5

As a rule, the Al-Mn alloys contain, in addition to the quasicrystalline phase, the remains of the Al f. c. c. phase. It was noted in [7] that in experiments the icosahedral phase is pronounced most clearly in the $Al_{77.5}Mn_{22.5}$ alloy. In [8], phase transitions from the amorphous to the quasicrystalline state have been studied in Al-Mn films and it has been established that the transition is accompanied by ordering of the icosahedrons. So, it was necessary to determine the type of microstructure in amorphous Al-Mn alloys of different concentrations and to find the concentration of the components at which microclusters with the icosahedron symmetry are most pronounced. The answer to the second question will clarify which composition of the alloy makes icosahedral ordering more advantageous.

To achieve these purposes, we used the method of molecular dynamics [9]. The interaction between the atoms was described by the Morse potential. The parameters of this potential, i. e., the depth and position of the first minimum, were determined by fitting to the pairwise potentials calculated by the method of pseudopotential using the Heine-Abarenkov-Animalu form factor with the Vashista-Singwi screening [10, 11].

We modeled fast cooling of the melts to the temperature 300 K with a time interval 10^{-15} s (1700 intervals altogether). Afterwards we conducted thermostabilization of the model within 10 000 intervals.

The basic results presented below are obtained for relatively small ensembles consisting of 256 atoms.

The type of Voronoy polyhedrons was determined for every alloy [10]. The results are presented in Figs. 1 and 2 and in Table 1.

Figure 1 shows the number N of n -sided polygons ($n = 3, 4, \dots, 9$), which form the faces of Voronoy polyhedrons circumscribed about Al and Mn atoms (in percent of the total number of faces of polyhedra circumscribed about Al and Mn atoms). The unshaded regions correspond to Al and the shaded regions to Mn. The Mn concentration is 14% (a), 18% (b), 22.5% (c), and 25% (d).

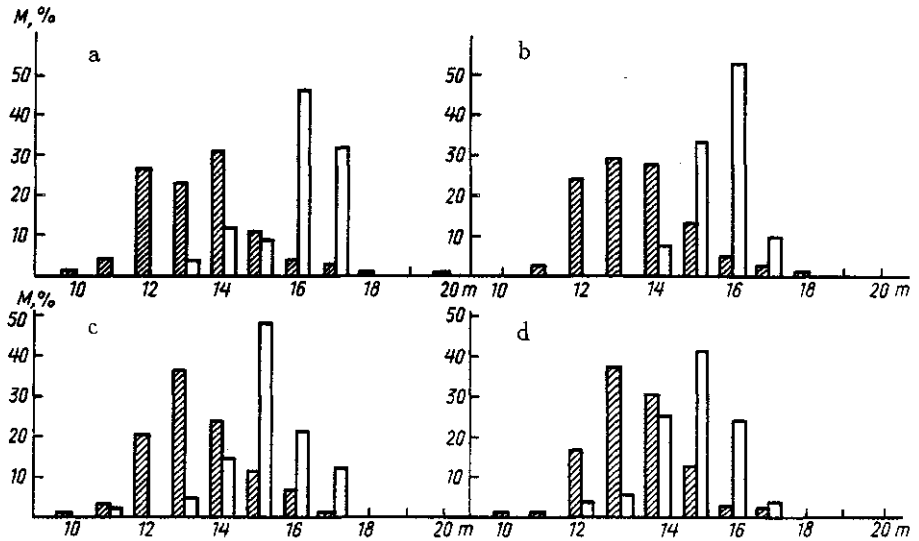


Fig. 2

All the figures show a clearly pronounced maximum at $n = 5$. In the general case this situation corresponds not only to icosahedrons but also to, e.g., Archimedes antiprism, but the percentage for the latter is substantially lower than for icosahedrons, which is also apparent from Table 1.

Table 1 presents the characteristic types of Voronoy polyhedrons circumscribing Al and Mn, in percent of the total number of polyhedrons about the given type of atoms and of the number of polyhedrons on the whole, for different Mn concentrations at the temperature 300 K.

Figure 2 shows the number M of m -sided Voronoy polyhedrons ($m = 10, 11, \dots, 19$) circumscribed about Al and Mn atoms, in percent of the total number of polyhedrons circumscribed about these atoms. The Mn concentrations and notation are the same as in Fig. 1.

Figure 2 and Table 1 demonstrate that the microstructure of these alloys substantially varies for different Mn concentrations, the maximum number of the icosahedron-like structures being observed at the concentration 22.5%.

These results are consistent with the experimental data and show that the concentration of micro-clusters of the icosahedral type first grows with increasing Mn concentration, reaches a maximum at 22.5% concentration, and then starts decreasing.

A more rigorous quantitative analysis will require the use of more realistic interaction potentials (possibly, empirical) and a manifold increase of the number of atoms in an ensemble. Application of supercomputers in this case, will, perhaps, allow us to observe the transition from the amorphous to the quasicrystalline state during a prolonged exposure of the system. As follows from our analysis, these transitions could be controlled by varying the component concentrations.

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