Short Notes

phys. stat. sol. (b) **178**, K1 (1993)

Subject classification: 61.50; 61.55; S1.2

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Concentration Dependence of Al–Mn Microstructures

By

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Introduction A quasi-crystalline state is characterized by a long-range icosahedral order [1, 2]. In numerous investigations [3 to 6] it was demonstrated that in some particular situations a structure with icosahedral symmetry point group may be energetically more favourable than a structure with translational invariance. The local atomic arrangement of the alloy and so the probability of icosahedral clustering depends on the concentration of the components.

In Al–Mn alloys not only a quasi-crystalline phase can occur, but the f.c.c. aluminium phase can appear as well. It was pointed out [7] that the icosahedral phase is experimentally found to be most emphasized at 22.5% concentration of Mn in Al–Mn alloys.

An investigation of phase transitions between amorphous and quasi-crystalline phases in Al–Mn films has been carried out [8], showing that these transitions were frequently accompanied by ordering of icosahedra.

Description of the model For solving these problems we used a molecular dynamics (MD) computer simulation of 256 atoms of Al and Mn. The obtained results are representing an average of several computer runs (at least 10). Increasing the number of investigated atoms up to 500 does not change the results within the repeating error, which is denoted in the figures by squares. The interaction between the given atoms is described by the Morse potential [9]. Parameters of the potential were obtained by the pseudopotential method using the Heine-Abarenkov-Animalu form factor with Vashista-Singwi screening [10, 11].

Melts of the alloy at different concentrations of Mn (7%, 14%, 18%, 22.5%, and 25%) were rapidly quenched from 2000 to 300 K by 1700 steps of 1 K. Then the samples were stabilized during 10^4 time steps at 300 K. (One time step was 10^{-15} s.)

All obtained structures were analyzed by the Voronoi polyhedra statistics at the temperature of 300 K.

Results and discussion The most characteristic configurations of Voronoi polyhedra around the Al and Mn atoms are the f.c.c. and icosahedral ones, respectively, and also the Archimedian antiprism and other configurations are observable.

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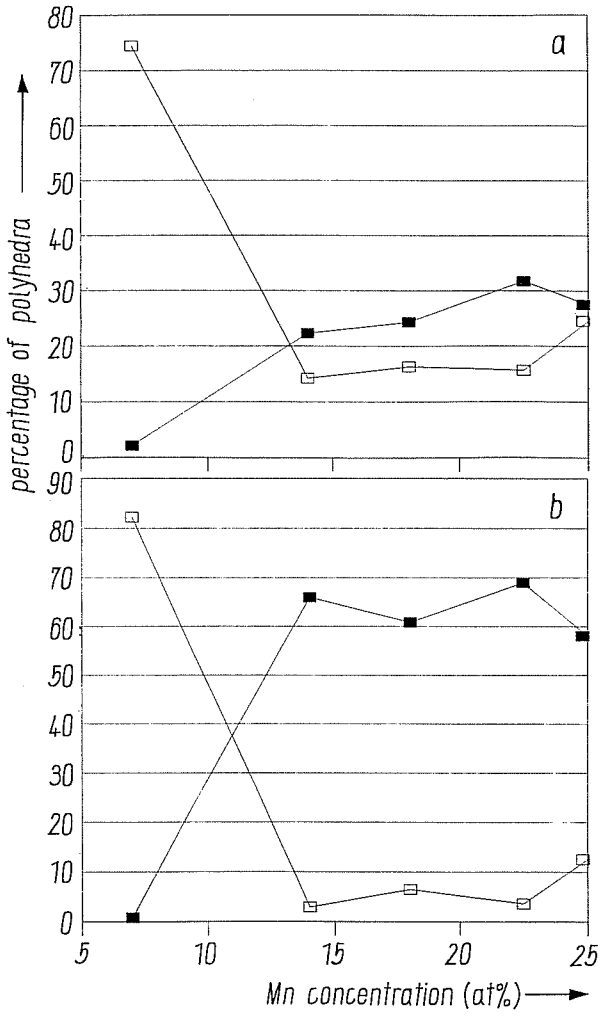

Fig. 1. Distribution of the icosahedral (■) and f.c.c. (□) arrangements in Al–Mn alloys; a) Al and b) Mn

The differences in the number of icosahedral clusters for each of the Mn concentrations are observable. A slight maximum at 22.5% of Mn appears (see Fig. 1), which becomes more obvious in examining the so-called pentagonal dominance, which is the ratio of the polyhedra having pentagons and the polyhedra which are free from these polygons (Fig. 2). The preferred coordination number (CN) of Al and Mn depends on the composition of the alloy (Fig. 3), and at the favoured concentration of Mn (22.5 at %) 13 and 15 are the most characteristic coordination numbers (CN) for Al and Mn, respectively (Fig. 3). The change of the CN against the concentration (Fig. 4) is also interesting: in the case of Al CN = 12 and 13, in Mn CN = 15 and 16 compete with each other. It is remarkable that the highest concentration of the icosahedra takes place at a concentration which has not

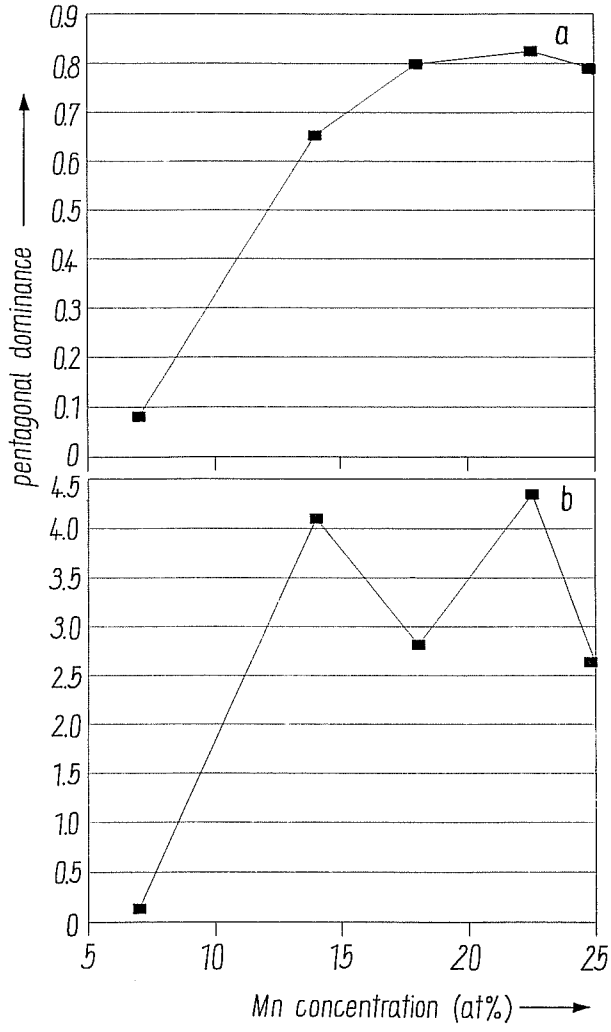

Fig. 2. The pentagonal dominance of the clustering polyhedra around a) Al and b) Mn

the most dominant CN (17 at% and 25 at% for Al and Mn, respectively). The observed difference of the favoured CN's can be one of the sources of the icosahedral preference. At the concentration of 22.5 at% the distributions of Voronoi polyhedra are most independent, having the highest splitting of their CN.

Conclusion The Mn atoms show an unusual behaviour in the micro-arrangement of the aluminium matrix, as they prefer characteristically higher CN, which is usually required for Al. This tendency destroys the f.c.c. lattice and a well harmonized split distribution of CN's appears at 22.5 at% where a maximum of icosahedral polyhedra is observable.

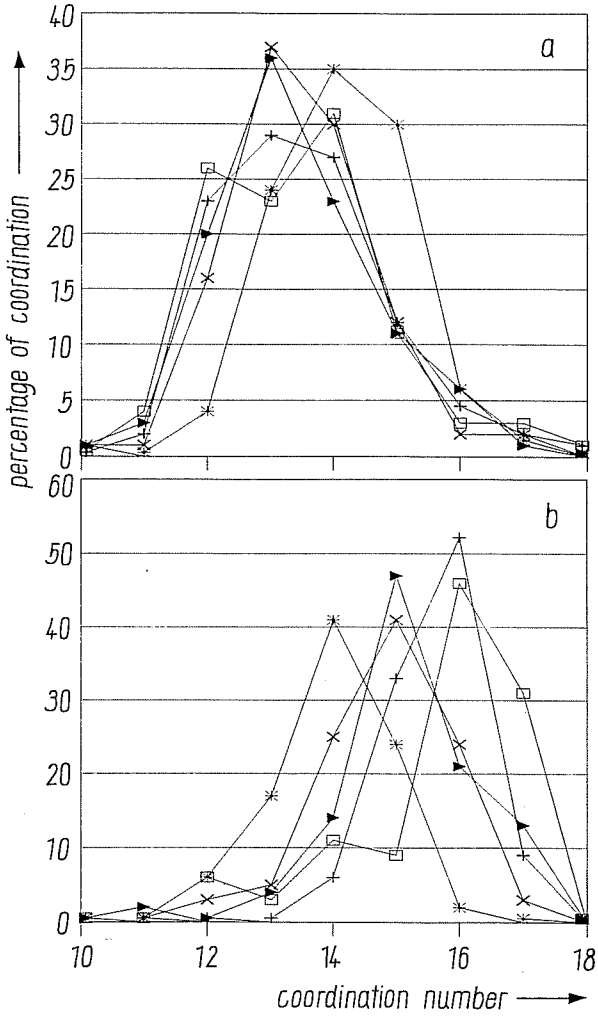

Fig. 3. Distribution of the coordination numbers around a) Al and b) Mn; (*) 7, (□) 14, (+) 18, (►) 22.5, and (×) 25 at% Mn

We guess that the change of the structure is explainable on the basis of the Frank-Kasper phases [12], but we had no direct proof for it yet. Further investigation in this direction is in progress.

This work was partially supported by the Austrian Ministry of Research, 'East-West' Cooperation.

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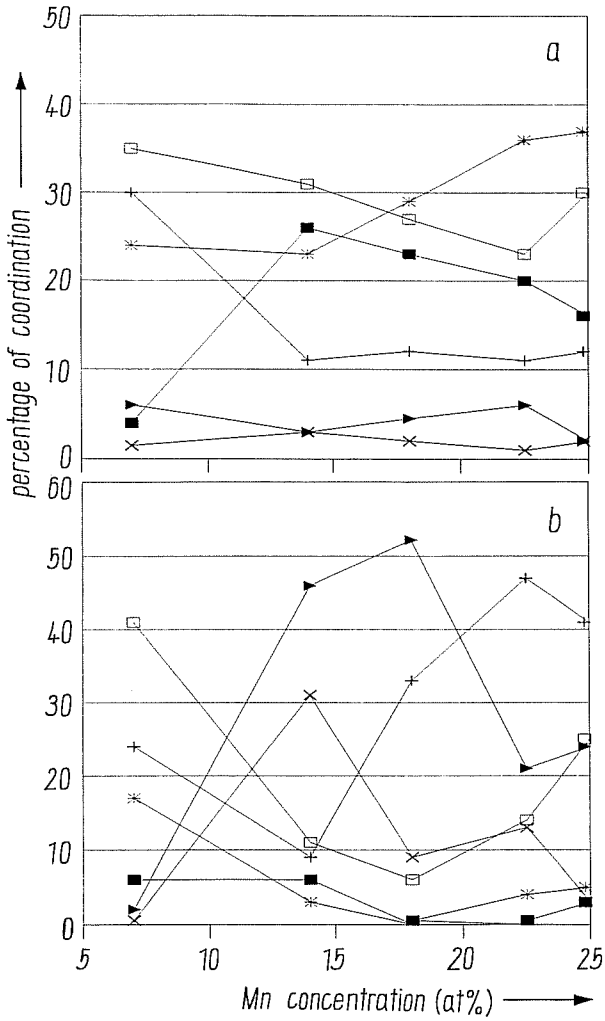

Fig. 4. Coordination statistics of a) Al and b) Mn for different compositions: (coordination numbers) (■) 12, (*) 13, (□) 14, (+) 15, (►) 16, and (×) 17

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(Received December 7, 1992; in revised form March 24, 1993)