RQ11 Rapidly Quenched & Metastable Materials

25-30th August 2002 Oxford University, U.K.

MICROSCOPIC MECHANISMS OF NUCLEATION AND DIFFUSION IN QUENCHED Al-Si ALLOYS

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Si precipitates formation in Al-Si alloys is a subject of many investigations. Al alloys are widely used as structural materials in nuclear reactors and have many other important applications. Quenching and reactor experiments show that to understand precipitation mechanisms in these materials we have to decide problems linked to first stages of nucleation and low-temperature diffusion.

In this study we found by computer simulation of the Al-Si solid solution that in quenched state at the first stages of Si precipitation small Si_3 clusters are formed in distorted tetrahedral configurations. They are characterized by stressed S-Si chemical bonds. Si_3 clusters aspire to change the angles between chemical bonds and to bring nearer them to ~109^0. This process is accompanied by the effect of Al atom forcing out from the lattice site by one of the Si atoms of nuclei.

The model and simulations are based on the classic Molecular Dynamics scheme. The program allowed to investigate a behavior of about five thousands atoms. The model consisted of Al cluster with small Si_3 nuclei and allowed to have a high degree of calculation precision.

As a result of computer simulation we observed a transition of Si atom to a node occupied by Al. A forcing out of Al atom by Si is caused by aspiration of stressed chemical bonds to restore the tetrahedral angles. It was obtained that the energy, which corresponds to transition of Si atom to Al node, is equal to 0.75 eV. This is a value of energy for the vacancy formation in Al.

Experiments on quenching metal alloys lead to necessity to decide a problem linked to too high mobility of solute atoms that reveals in precipitation processes. Such situation arises in investigations of Si precipitation in Al.

To decide this problem we turned to the basic mechanisms of diffusion processes in metals. In a lot of works it was found that elementary defects in metal lattices form complexes. In particular, in the state of thermodynamic equilibrium in metals together with monovacancies there is a significant part of divacancies.

We found that polyvacancies (and first of al, divacancies) play a significant role in low-temperature diffusion accompanying quenching processes. A physical background of this result based on experimental relations between physical parameters of vacancy diffusion:

For divacancies, as a rule $\varepsilon_f > U$, but for monovacancies, on the contrary, $\varepsilon_f \le U$. Besides that in all cases $U_{2v} < U_v$.

Here ε_f and U are corresponding enegies of formation and migration of vacancy defects.

The situation observing in Al-Si alloys is typical for many alloys with small solubility of components.

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