ATOMISTIC SIMULATION OF MARTENSITIC TRANSFORMATION IN $Fe_{80}Ni_{20}$ NANOPARTICLES INITIATED THEIR AGGLOMERATION

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Abstract – The mechanisms governing the formation of structural state and kinetics of transformations in the metallic clusters $Fe_{80}Ni_{20}$ during martensitic transformation are investigated by molecular dynamics (MD) method.

I. INTRODUCTION

Martensitic $\gamma \rightarrow \alpha$ transformation in a defect-free crystal is not happening during MD study. Analysis of the free energy of the alloy Fe80Ni20 depending on the lattice along the path at Bain deformation at $\alpha \leftrightarrow \gamma$ transformation shows that there is a high energy barrier between the fcc and bcc states, so the transformation is not obtained in the MD simulations at cooling the fcc phase. By lattice defects, locally, the barrier is lowered, so there may be a nucleation of a new phase. For example, in the crystallites with periodic boundary conditions, simulating an infinite crystal, the martensitic transformation could be observed in the presence of ~ 2at% vacancies. Martensitic $\gamma \rightarrow \alpha$ transformation has been studied by the MD method in cubic nanocrystalline particle size of 24 nm with free surfaces [1]. The transformation started from the top of the cube, where the atomic coordination number is reduced and lowered the $\gamma \rightarrow \alpha$ transformation barrier. During the time interval t ~Δ 30 ps at T = 50K the transformation is completed, the typical twinned martensite crystals are emerging on the edges of the surface of the cube and are distributed inside the crystallite.

In [2] studied the martensitic transformation in polycrystalline alloy Fe80Ni20 fine-grained (~ 3 nm in diameter), which were obtained by compacting under pressure at a temperature T = 800K. Analysis of the radial distribution function showed that in the regions near the grain boundaries formed bcc - like structure. Upon cooling of the polycrystalline $\gamma \rightarrow \alpha$ transformation begins from the grain boundaries. Number bcc phase continuously increases and reaches at T = 25K of ~ 52%. Thus, martensitic transformation could be observed only in lattice with defects, where the barrier is lowered locally, for example nearby the grain boundaries.

In this work, the martensitic transformation was studied near the boundaries, formed by agglomeration of the two nanoparticles. It was studied the effect of particle disorientation on the coalescence processes and on disorientation of the particles after the martensitic transformation.

II. RESULTS OF MD SIMULATION

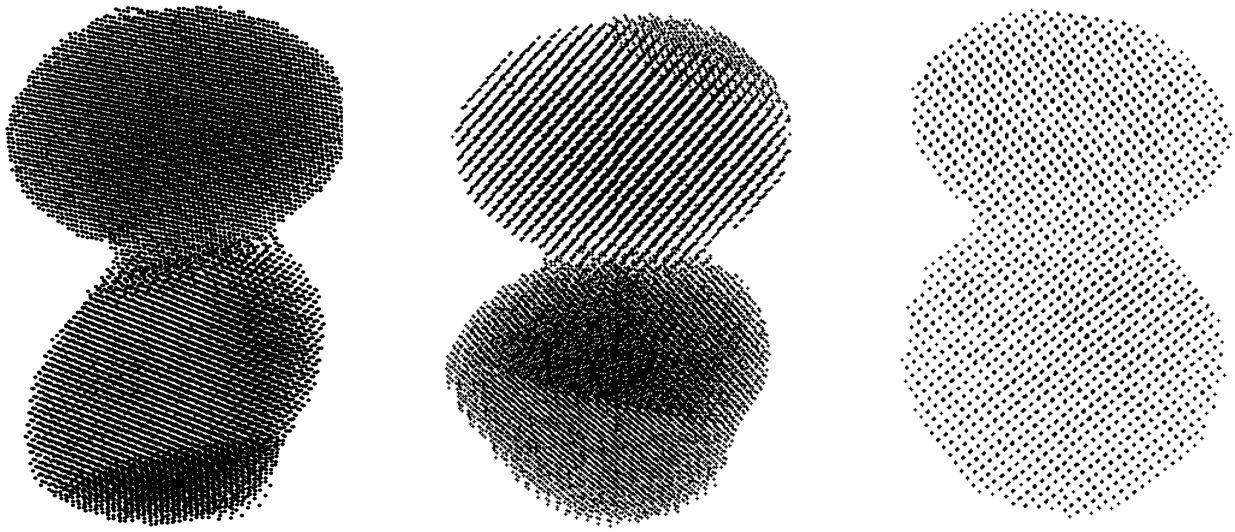
The kinetics of structural transformations was performed by the molecular dynamic method using N-body Meyer-Entel [3, 4] potentials of interatomic interactions constructed by embedded-atom method. These potentials permit one to calculate the values of the lattice parameters, elastic modules, cohesive energy, and vacancy-formation energy for Fe and Ni. They also give the magnitudes of the energy differences between fcc and bcc phases for Fe-Ni alloys close to the experimental ones and correctly reproduce the concentration dependences of the temperatures of martensitic and austenitic transformations in bulk materials.

Two agglomerated particles with fcc lattice and with the atoms number N=10185 (diameter d~6 nm) cooled from the temperature T=1400K to T=0K. The cooling of clusters was carried out by a discrete change of temperature with a step of 20K. The cooling rate equals to ~4×10^{12} K/s. In the initial configuration the two particles were rotated relative to each other to obtain desired disorientation. The disorientation of particles corresponded to the special large-angle asymmetrical tilt grain boundaries Σ11, Σ3 and Σ9. Disorientation axis was <110>, the disorientation angles were 70.53 degrees for the boundary Σ3, 50.47 degrees for the boundary Σ11 and 38.94 degrees for the boundary Σ9. The plane of contact was selected (010).

After cooling to T ~ 200-300K each particle undergoes martensitic transformation (Fig.1). The shift in the transformation process starts from the boundary between two particles near the surface and

further extends through the entire particle. Depending on the initial disorientation of the particles we obtained either single-domain state (Fig1,c), or there is an agglomerate of two disoriented particles with a bcc lattice (Fig1a,b). Each particle consists of 1-2 domains (Fig.1a,b).

Sintering in the fcc phase leads only to insignificant change in the disorientation of one particle with respect to the other particles of a given size [5]. Figure 2 shows the orientation relationship between one of the particles after sintering in fcc phase and after martensitic transformation for Σ11 boundary. The analysis shows that between fcc and bcc phases are realized Kurdjumov-Sachs orientation relations. The dotted line near the center of the pole figure marked parallel poles <110> fcc phase and <111> bcc phase. Center pole figure also coincides with the axis of disorientation FCC particles in the initial configuration. For the boundary Σ 11 disorientation angle between the particles in the initial configuration is 180-129.53 = 50.47 degrees. Axis of disorientation in the bcc phase is parallel to the <111> direction, so that the angle of disorientation is close to an element of the point group symmetry of the bcc phase (Fig.1c) after completion of the martensitic transformation.



a) b) c)

Figure 1 – $\gamma \rightarrow \alpha$ transformation of the two particles agglomerate with the grain boundaries Σ3 (a), Σ9 (b) and Σ11 (c), temperature T=0K.

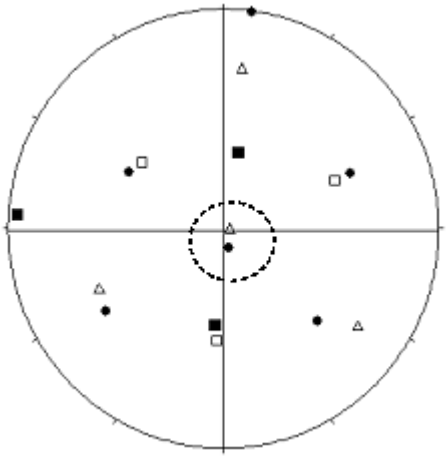


Figure 2 – Cooperative pole figure fcc and bcc phases. Shaded symbols refer to the fcc phase, not hatched - to the bcc phase. Circles denote the poles of the <110> squares - <100>, triangles - <111>

III. CONCLUSIONS

We have studied $\gamma \rightarrow \alpha$ transformation during cooling in agglomerated disorientated two particle clusters of Fe80Ni20 alloy by the method of molecular dynamics. It has been found that the shift in the transformation process starts from the boundary between two particles near the surface and

further extends through the entire particle. It is demonstrated that depending on the initial disorientation of the particles it was obtained either single-domain state or there was an agglomerate of two disoriented particles with a bcc lattice.

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