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$\alpha \rightarrow \gamma$ TRANSFORMATION IN Fe-Ni AGGLOMERATED NANOPARTICLES

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Abstract. $\alpha \rightarrow \gamma$ transformation in two and three-particle agglomerates of $Fe_{80}Ni_{20}$ alloy clusters upon heating and subsequent cooling is studied by the molecular dynamic method. It is shown that the temperature of the transformation beginning is distinguished for all particles. The type of domain structure and its dependence on the number of particles in the configuration was investigated.

1. INTRODUCTION

One of the interesting scientific problems of nanocrystal physics is a study of factors that change martensite transformation, in particular its complete suppressions with the decrease of grain size to ten and hundred nanometers. At present, a possible reason for the influence of dimensional factor on the phase transformations is considered as complexity of nucleation of a new phase in small grains and suppression of the stage of their subsequent growth. It is also discussed the influence of a change in the chemical composition of a material and its stressed state. In nanoparticles, there is no influence of grain boundaries on the process of propagation of new phase crystals. In many respects, the problem of formation of a new phase is facilitated, since the surface of a particle can be the place of its origin. Comparison of the results of studying microcrystallites of the same size with the free surface atoms (clusters) and under different stress conditions (nanocrystals, nanopowders, nanoclusters in an amorphous matrix) will make it possible to divide the influence of its own structural transformations of small particles from special feature of the structure of grain boundaries and their influence on the resultant martensite crystals in the volume of a nanomaterial.

In [1] we investigated the influence of size on the kinetics of structural transformations in the clusters of alloy Fe –20 at.% Ni with a change of their diameter within the limits d ~ 1.0 – 3.7 nm. The sequence of changing mechanism and structural characteristics of martensite transformation in the dependence on temperature and concentration of the components of alloy was determined. It was found that in the clusters of alloy Fe- Ni with the size of $d \leq 1.5$ nm $\alpha \rightarrow \gamma$ transformation did not take place. During heating the initial configuration with BCC lattice was transformed into the icosahedron through the polytetrahedral or amorphous like configurations (Fig. 1a).

In the nanoparticles with size of $1.5 < d < 3.0$ nm, the transformation realized through an intermediate amorphous like configuration, which exists in the wide range of temperatures $T_s < T < T_f$. For the nanoparticles with size $3.0 < d < 3.5$ nm $\alpha \rightarrow \gamma$ transformation was accompanied by the correlated motion of atoms, close to Bain scheme. This resulted in the formation of monodomain state of FCC phase (Fig. 1b). For the nanoparticles with

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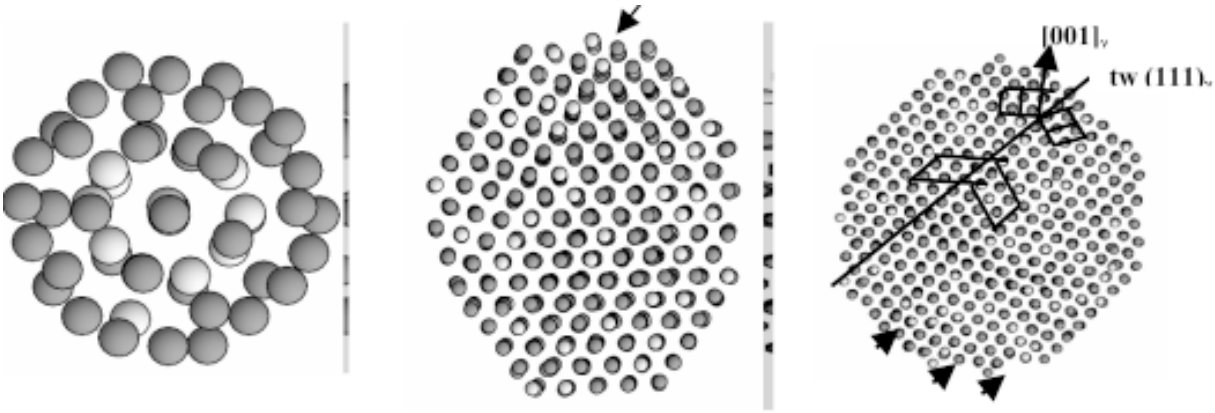

(a) (b) (c)

Fig. 1. $\alpha \rightarrow \gamma$ transformation in nanparticles of Fe-20 at.%Ni with size d=1.2 nm (a), d=2.3 nm (b), and d=3.7 nm (N=2869).

the size d > 3.5 nm, the $\alpha \rightarrow \gamma$ transformation proceeded by the mechanism of nucleation at the cluster boundaries and propagation of FCC phase plates. As a result, the transformation formed a twin lamellar domain structure (Fig. 1c) at temperature T=380K. During the subsequent cooling, the state of mono-domain with the BCC structure was restored at considerably lower temperature, T=40K.

In the present work, the martensite transformation in two and three-particle agglomerates of the clusters of alloy $Fe_{80}Ni_{20}$ is investigated by the molecular dynamics method, with the use of N-body potentials of interatomic interaction [2]. The number of atoms in each cluster is N=2869.

2. COMPUTER SIMULATON RESULTS

In the initial configuration, the atoms of all clusters completely filled coordination spheres near a certain fixed atom in accordance with the positions of BCC lattice with random disordered atomic arrangement of two atom types. In the agglomerate of two particles, one of the clusters was disoriented relative to another to create a twin symmetrical boundary in the place of their contact on the plane $(111)_a$. In the agglomerate of three particles, two particles were not disoriented, whereas for two others there formed a twin symmetrical boundary (on the plane $(111)_a$) and an asymmetrical boundary. Prolonged annealing before the formation of the sintering state of two or three clusters was done. Further the clusters were subjected to heating by a stepped variation of the temperature with the rate of $4 \cdot 10^{12}$ K/s up to T=800K and to subsequent cooling for studying the $\alpha \leftrightarrow \gamma$ transformation.

2.1. Structural transformations in the sintering two particle cluster

The initial configuration of two clusters is shown in Fig. 2a. Process of sintering (Fig. 2b) was accomplished at T=300K during ~1 ns. After that, the heating was conducted and we studied structural changes as a result of $\alpha \rightarrow \gamma$ transformation. It is found that the phase transformation occurs not at one and the same temperature in each of the particles. First transformation occurs in one of the particles (lower particle in Fig. 2c) at temperature T=340K, which is somewhat lower than obtained for one particle with the same size. In this particle, the lamellar plate-like domain structure is formed; similar to that we obtained for one particle (compare Figs. 1c and 2c, 2d). For the second particle, the transformation does not occur; there is only motion of separate atoms. Only at T=400K, the transformation begins in the second particle, where twin domain structure is also formed.

During cooling $\gamma \rightarrow \alpha$ transformation occurs at a temperature of T=80K simultaneously for both particles. In Fig. 3 the resultant configuration after transformation is shown. This configuration differs substantially from the initial configuration (compare Figs. 2b and 3a). Disoriented domains are formed in the upper particle. At the plane $\{110\}_\alpha$ the domain boundary is not visible (Fig. 3b), i.e., the shift of one part of the particle relative to another oc-

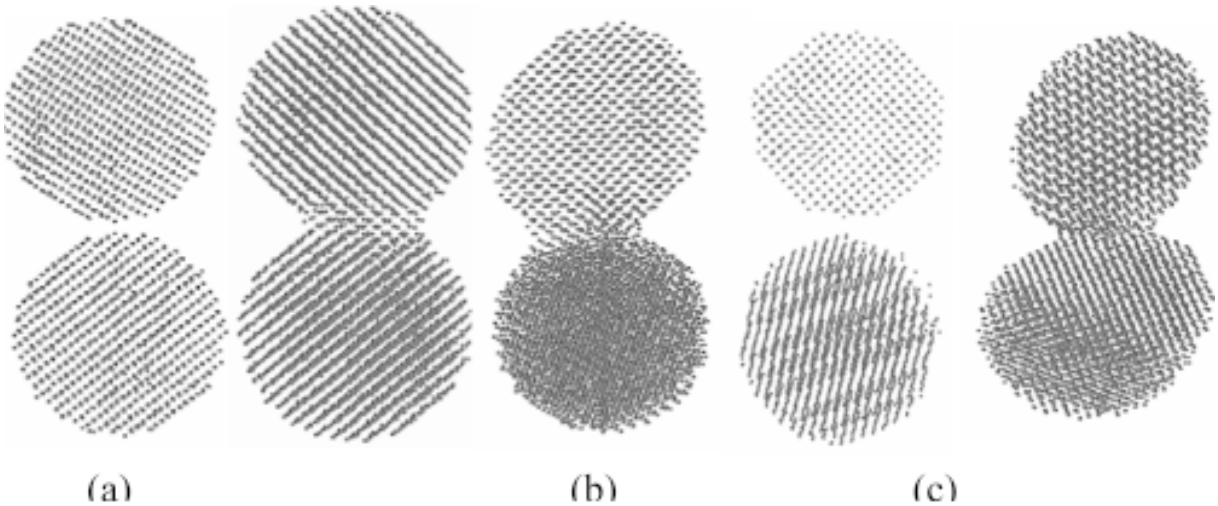

Fig. 2. Sequential stages of sintering (a, b); $\alpha \rightarrow \gamma$ transformation at T=340K (c) at lower particle and at T=400K for two agglomerated particles with heating.

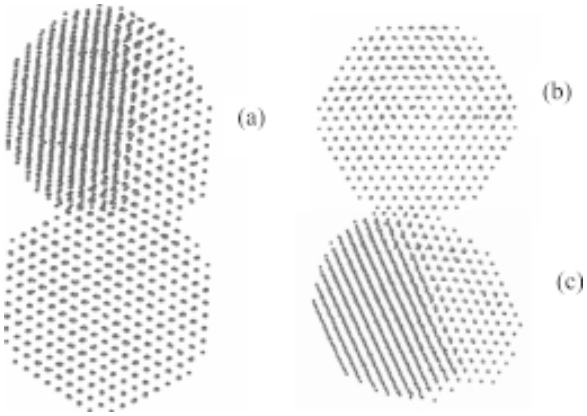

Fig. 3. Atomic transformations of two-particle agglomerate $\alpha \rightarrow \gamma$ transformation (a); (b, c)- two projects of a particle with domain boundary.

curs in the direction, perpendicular to this plane. Resultant boundary is not a twin symmetrical boundary (Fig. 3c).

2.2. Structural transformations in the sintering three particles cluster

The initial configuration of the agglomerate of three particles being investigated is shown in Fig. 4a. Calculation showed that the processes of sintering and phase transformation occur simultaneously at T=300K. For this reason, to obtain the sintering state, we selected the temperature T=100K. The orientation relations between the particles are concerved after sintering. There is a pore in the center of the three- particle configuration. In this configuration between the particles of I and II, the symmetrical twin boundary in plane (111) is formed, and there is no disorientation between the particles I and III, the asymmetrical twin is formed between the particles II and III.

The transformation occurs not simultaneously in all particles with heating this configuration. First, at T=320K the transformation occurs at two particles II and III (Fig. 4c). In these particles, plate-like domain structure is formed. Only at T=360K $\alpha \rightarrow \gamma$ transformation completes (Fig. 4d).

During cooling, first the $\gamma \rightarrow \alpha$ transformation occurs only in one particle at T=140K (Fig. 5a). During the subsequent cooling at T=100K the phase transformation completes (Fig. 5b). Particles with the numbers I and III, and the region in the center of the sintering particles have one orientation. Particle II, which in the initial configuration had twin disorientation, has more complex structure. This particle has an ellipsoidal form and an internal boundary, which testifies about the disorientation of its one part relative to another.

3. CONCLUSIONS

We have studied $\alpha \rightarrow \gamma$ and $\gamma \rightarrow \alpha$ transformation in agglomerated disorientated two and three-particle clusters of $Fe_{80}Ni_{20}$ alloy by the method of molecular dynamics. We found the sequence of the martensite transformation passage and the type of domain structure in the dependence on temperature and number of particles, which form an agglomerate.

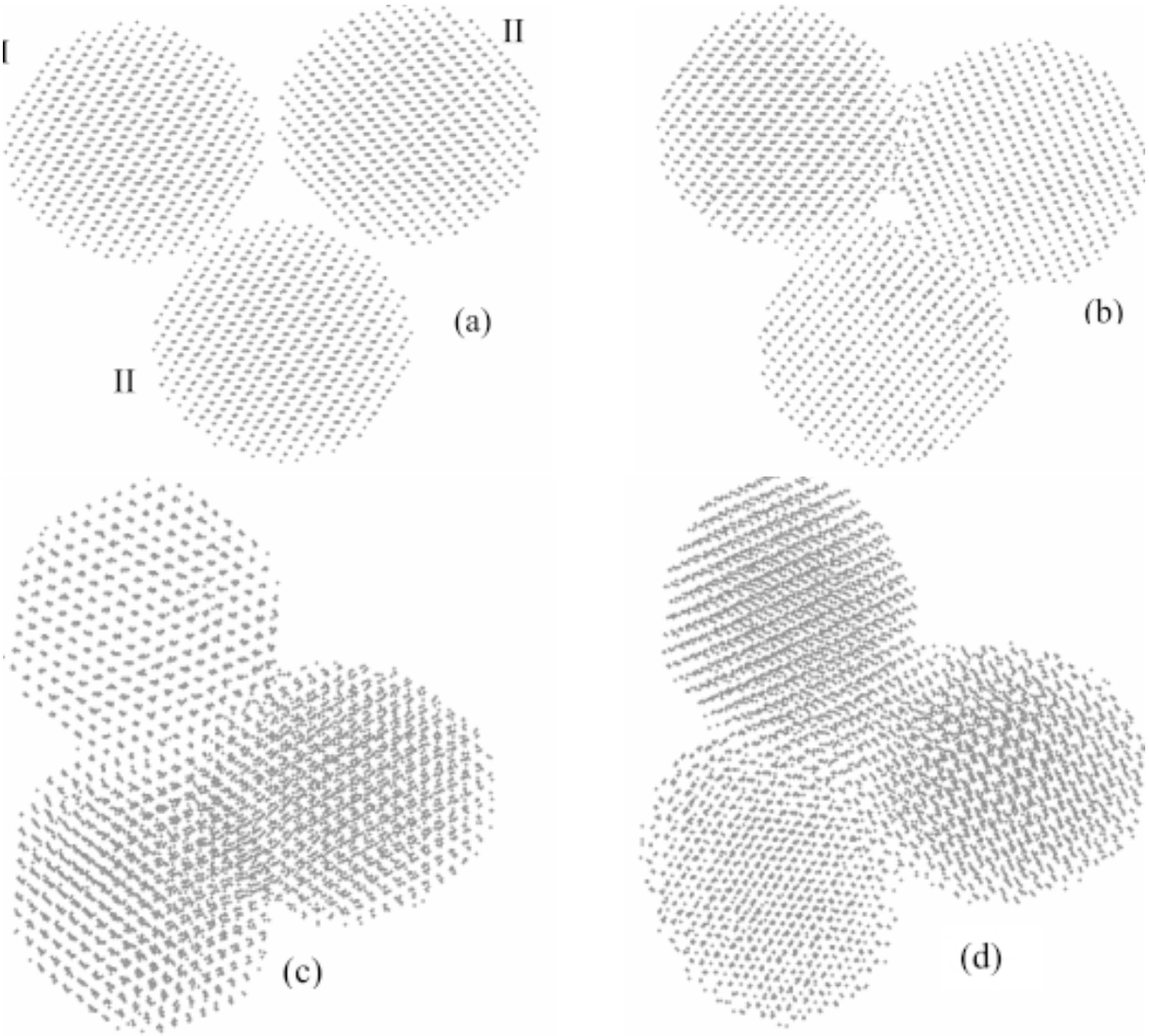

Fig. 4. Structure changes of three particles sintering cluster: (a) –initial configuration. (b) – annealing at T=100K, $\alpha \rightarrow \gamma$ transformation at T=320K (c), and T=360K (d).

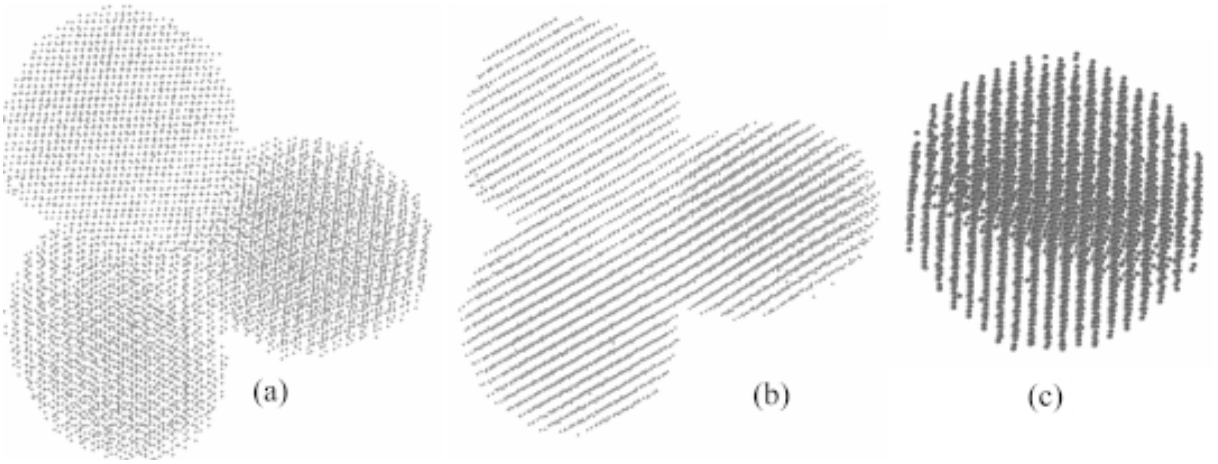

Fig. 5. Successive stages of $\gamma \rightarrow \alpha$ transformation during cooling of three particles configuration. (a) – T=140K, (b) – T=100K, (d) – the peculiarities of particle II configuration.

ACKNOWLEGEMENT

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