Investigation of Growth Ordered Phases in the Alloy Nial Equiatomic Composition During Stepwise Cooling

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Monte Carlo method was used to study the process of disorder-order phase transformation with stepwise cooling of the alloy NiAl equiatomic composition. The estimated alloy cell is 32×32×32 (65536 atoms), and for the boundaries, we used periodic boundary conditions. In the completely disordered crystal unit bcc lattice introduced one vacancy. The study was performed using the Metropolis algorithm; at each temperature $5 \cdot 10^6$ iterations were performed [1-3]. The step was 100K. Interactions between distincnt pairs were presented in the form of interatomic Morse potentials in three coordination spheres. The parameters for the potentials in the NiAl alloy were taken from [4].

Microblocks first ordered by type B2 superstructure were found at 1700K. With decreasing temperature, the germs were transformed into ordered phases. At 1400K, the material was completely streamlined into a superstructure with two antiphase domains. Within the boundaries of the domain, the layer of disordered phase contained 3 atomic rows.

Figures 1 and 2 show the atomic structure of NiAl alloy after cooling at various temeratures. The temperature of 1800K in the alloy is characterized by the appearance of isolated germs of domains of different orientations. Lowering the temperature to 1700K causes grows and unification in one orientation domains. At 1500K, the domains begin to form the structure corresponding to the two-domain crystal with disordering elements on the boundaries. There are elements corresponding to the partial dislocation in the <100> directions.

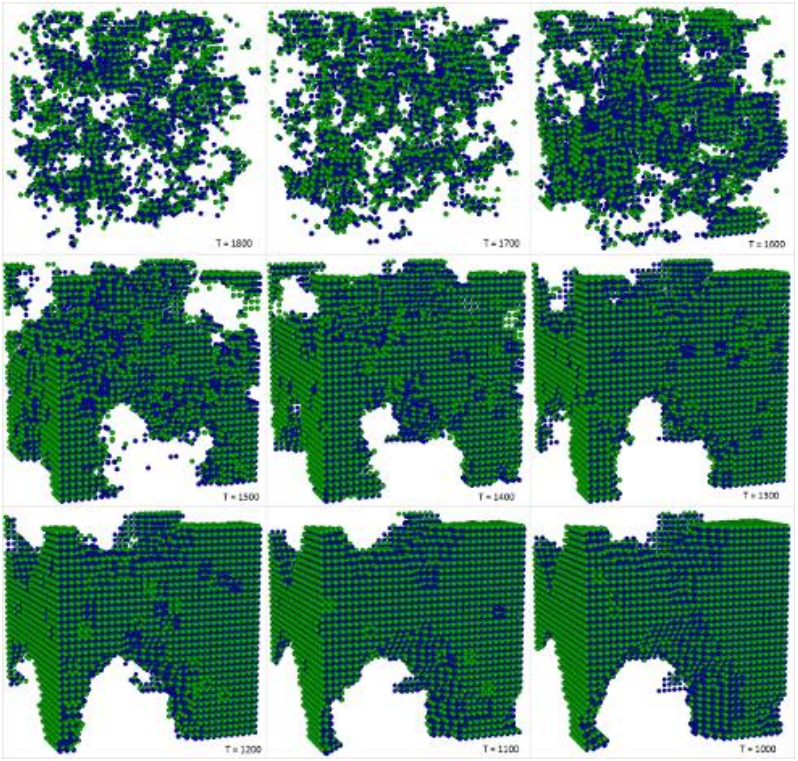

Figure 1: First antiphase domain after cooling at different temperatures.

The ordering process develops as temperature is lowered to 1400K and fills the area corresponding to the partial dislocations and antiphase boundaries. Cooling to 1300K retains elements of superdislocation and superdislocations loops; the boundaries are smoothed. Lowering the temperature to 1200K leads to an increase in the proportion of the ordered phase; the volume of the domain is increased by the addition of the border ordered regions. At 1100K, the process develops, the structure becomes more perfect, and partial dislocations disappear. The boundaries are predominantly at <110> direction. At 1000K, antiphase boundaries oriented along the <110> and <100> directions appear between domains. The continued drop in temperature does not lead to visible changes of the domain

structure of the alloy.

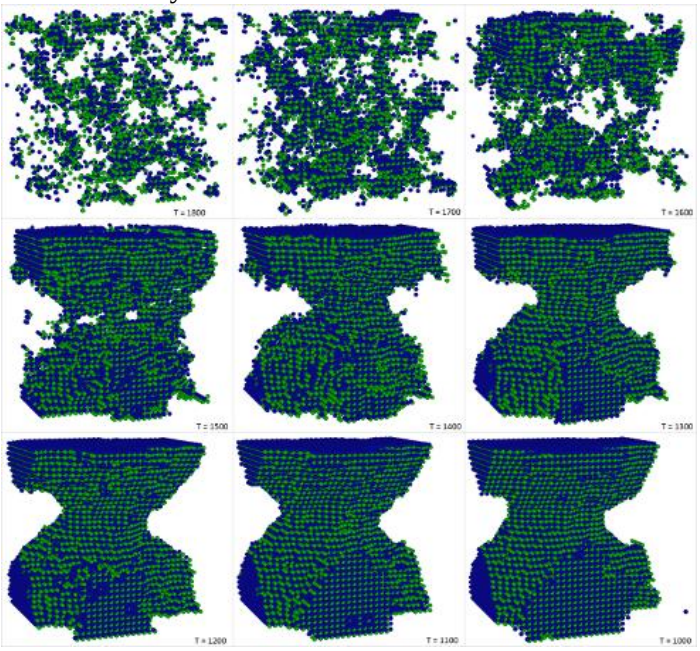

Figure 2: Second antiphase domain after cooling at different temperatures.

References

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