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Research Protocol

Atomic and Electronic Structure in Thin Foils $Ni_{51}Ti_{49}$

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Introduction

Relevance

One of the most famous and widely researched materials with shape memory is titanium nickelide. Materials with shape memory are characterized by the presence of thermoelastic martensite in their structure. Such martensite arises as a result of deformation, leading to mechanochemical reactions in the localization zones of plastic deformation of the nanoscale level [1].

The result of mechanochemical reactions are phases with new structural states, and accordingly, with new properties. In the study of massive samples and thinned foils of titanium nickelide, it was not known about the possibility of the appearance of magnetization in them. For the first time, the authors of [2] indicated this possibility. The authors associated the appearance of magnetization with the appearance of deformation martensite with the tetrahedrally packed Frank – Casper structure. A feature of this structure is the displacement of atoms from the positions associated with the cubic symmetry of the crystal lattice. A decrease in symmetry can lead to the appearance of magnetization [3].

Thin-film samples subjected to cryomechanical processing exhibit magnetic properties. It was shown in [4,5] that powdered samples of titanium nickelide obtained by laser ablation have magnetization. It was shown that, during laser ablation, a reaction is possible with the formation of a nonmagnetic Ti2Ni phase and a ferromagnetic Ni4Ti3 phase.

Purpose of the work

The purpose of the work is to explain the nature of magnetization in thin Ni51Ti49 foils containing the Ni_4Ti_3 phase from the point of view of a change in the electronic structure in the localized zones of plastic deformation.

Samples and Research Methods

Samples are presented in two groups: before and after cryomechanical processing. Thin foils were obtained by electro polishing Ni51Ti49 samples. After electropolishing, thin foils were examined in a transmission electron microscope, then subjected to cryomechanical treatment 5-6 times and again examined in an electron microscope.

Results and Discussion

Figure 1 shows the image and microdiffraction patterns obtained from the Ni51Ti49 sample after cryomechanical processing. From the interpretation of the diffraction patterns, the atomically ordered phase Ni4Ti3 was revealed. Using electron microscopy in Figure 1 (a), finely dispersed needle-like discharge was revealed, in addition, significantly curved groups of needle-like discharge were visible. The nature of the diffraction reflections shown in the built-in field of Figure 1 (a) corresponds to this type of precipitates. The diffraction patterns 1 (b) and 1 (c) show the individual sections obtained by microdiffraction. In Figure 1 (b), the reflexes of the corresponding single-crystal precipitation should have fractional indices relative to those indices that are shown in Figure 1 (c). The interpretation of the electron diffraction pattern 1 (c) can correspond to the Ni4Ti3 phase [4]. Cryomechanical processing is the equivalent of high-speed plastic deformation, which led to the formation of an atomically ordered Ni4Ti3 phase. According to work [6], the Ni_4Ti_3 phase can be ferromagnetic, although according to the phase diagram shown in Figure 3, at room temperature, the phase should not be ferromagnetic. The effect of the appearance of magnetization is possible if the atoms of nickel and titanium mix from their positions in the correct crystalline structure into the interstices of such a structure, thus forming new structural states. Structural transformations in titanium nickelide-based alloys are the subject of quite a lot of papers and reviews [7]. However, the results obtained in them are controversial. According to the well-established notions in the $Ni_{51}Ti_{49}$ alloy, the martensitic transformation occurs in two stages. Austenite with a cubic structure of type B2 goes into phase with a trigonal rhombohedral structure of R. Then the R-structure goes into phase with a monoclinic B19` structure [8].

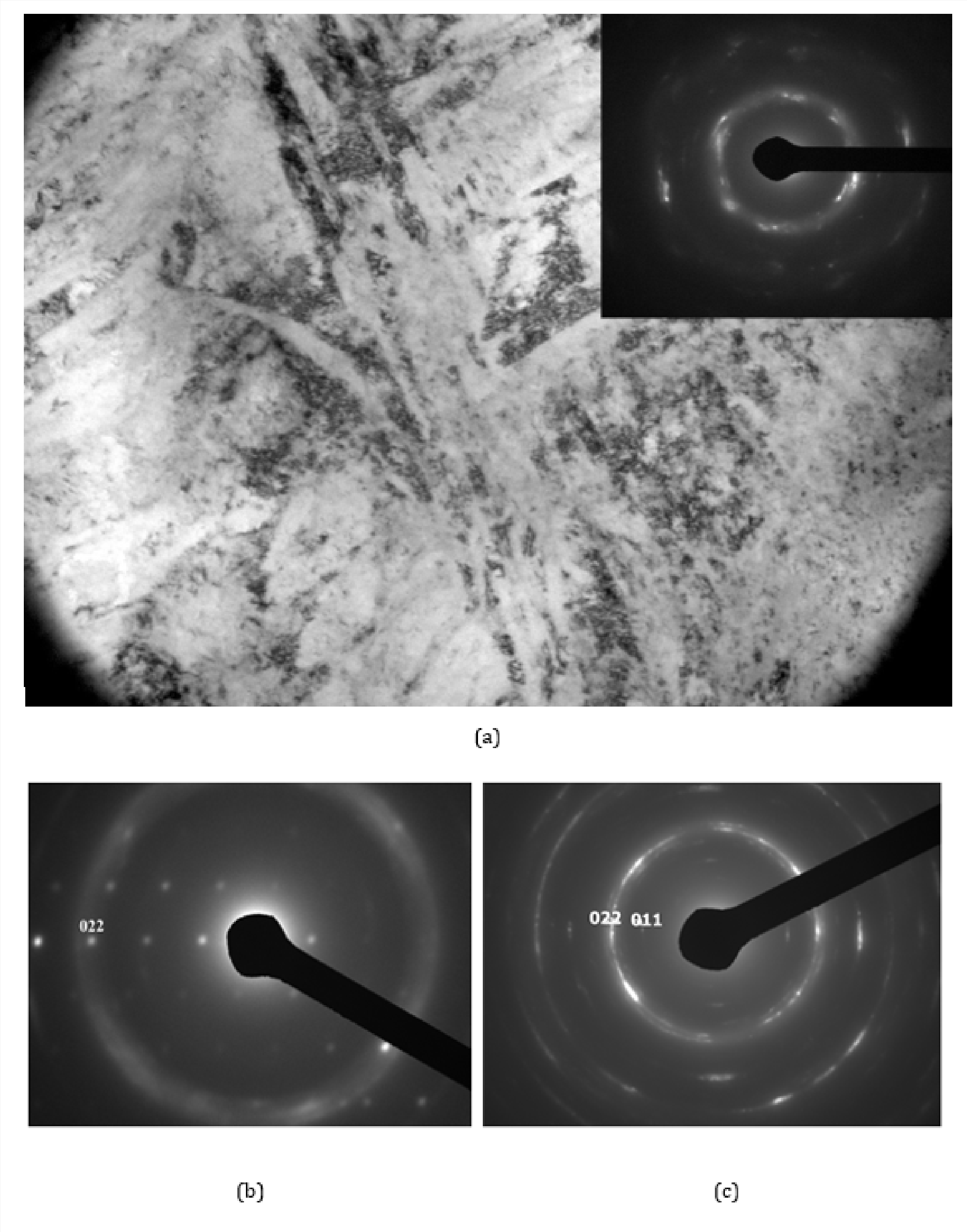

Figure 1: Image (a) and pictures (b, c) of microdiffraction obtained from a thinned Ni-Ti sample after cryomechanical processing.

The temperature range of the martensitic transformation for this alloy lies in the region of negative temperatures [9] and can vary significantly depending on the degree of decomposition of the solid solution and the precipitation of the Ni_4Ti_3 phase enriched with nickel [10].

Reflexes with fractional indices shown in Figure 1 (b), appear when close-packed Frank – Casper structures are formed [11]. By combining several tetrahedra, as shown in Figure 2, it is possible to obtain a spiral packing of tetrahedra corresponding to the structure of Ni4Ti3. Here, dark circles show nickel atoms, and light circles show titanium atoms. Packing can be continued in both directions to infinity, while being non-periodic: not one of the atoms along the axis of the spiral will occupy a position exactly above the first atom. Such a tetra spiral serves as an example of noncrystallographic long-range order, which is realized in only one direction [13,14].

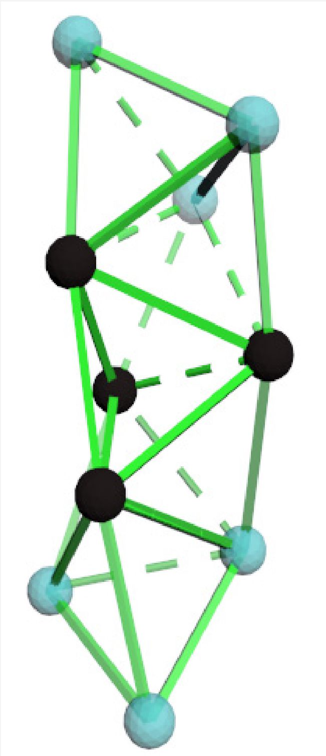

Figure 2: Cluster model Ni_4Ti_3.

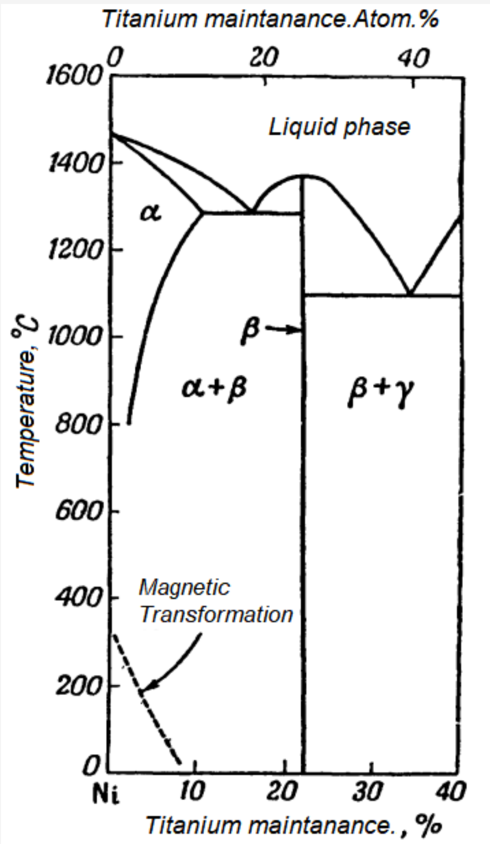

Figure 3: The phase balance diagram of Ni-Ti [12].

According to Panin [15], new structural states in metals and alloys appear in zones of localization of plastic deformation when atoms are displaced from the correct crystallographic positions into interstices. The atoms trapped in the internode create new electronic configurations, the result of which are new structural states of materials, and, therefore, new physical properties.

The calculations of the electronic structure are carried out in the framework of the theory of the functional density of electronic states. The magnetic properties of cluster formations in the Ni4Ti3 structure shown in Figure 2 are studied. The parameters for calculating the electronic structure are based on determining the coordinates of the atoms detected using X-ray diffraction and electron diffraction data, as well as by modeling the cluster structure in the 3D max program.

The structure of thin foils was studied by the authors of work [16], where the Ni_4Ti_3 phase was detected in the form of needle-shaped precipitates. X-ray diffraction and electron microscopic methods of investigation revealed structural multiphase of wrought alloys, which confirms the correctness of the model of V.E. Panin.

The calculations of the density of electronic states performed by the scattered wave method for clusters explain the appearance of magnetization in titanium nickelide containing finely divided neoplasms of the Ni_4Ti_3 phase.

Acknowledgement

None.

Conflict of Interest

No conflict of interest.

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