Novel Type of Metadislocation in the Complex Metallic Alloy Al-Pd-Fe

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IFF-8: Microstructure Research

We report on the observation of new variants of metadislocations in the orthorhombic complex metallic alloy phase Al-Pd-Fe. At Fe contents above about 3 at.% we find a novel type of metadislocation in the ξ-structure, which has a complementary counterpart hosted in all ε-type phases possessing phason lines as structural elements.

Among the group of complex metallic alloys (CMAs), materials which feature a few hundreds of even thousands of atoms per unit cell, the so-called ε-type phases are one of the most fascinating. Several structurally related orthorhombic phases have been identified and are denoted ε_l (l = 6, 16, 22, 28, 34) according to the index of the strong (0 0 l) reflection. They are ternary extensions of the binary Al_3Pd phase in the Al-Pd-(Mn, Fe) alloy systems [e.g. 1]. ε-type phases are also found in the alloy systems Al-Pd-(Rh, Re, Ru, Co, Ir) and Al-Rh-(Ru, Cu, Ni) [2].

In the CMA phase ε_6-Al-Pd-Mn, which features about 350 atoms per unit cell, Metadislocations (MDs) were firstly observed [3]. The concept of metadislocations addresses an inherent problem in the plasticity of large-unit-cell crystals: if the lattice parameters of a structure are large, conventional dislocation mechanisms tend to fail. Perfect dislocations are unfavourable as they involve very high elastic line energies (the elastic line energy of a dislocation increases with b_2, where b is the length of the dislocations Burgers vector) and partial dislocations are connected to high stacking fault energies. The concept of MDs provides a solution to this problem. A MD consists of a core dislocation with a short Burgers vector, typically of the order of 1 or 2 Å. Its elastic line energy is therefore comparable to that of simple metals as Al or Cu. The core dislocation, which is a partial in the large-unit-cell structure, is associated with a local phase transformation to a related structure. The latter has lattice parameters related to those of the host structure in such a way that the partial dislocation is accommodated into the lattice.

MDs were up to now found only in the orthorhombic phase ε_6-Al-Pd-Mn and the related phase ?28-Al-Pd-Mn [3, 4]. They are associated to a distinct number of so-called phason planes, the number of which follow a series of double Fibonacci numbers, i.e. 2,4,6,10,16... [4].

Here, we report on the observation of a novel type of MD in the Al-Pd-Fe alloy system. The defects observed possess the essential structural features of a MD, i.e. they consist of small partials in a large-unit-cell crystal, accommodated into the lattice by a local phase transformation. On the other hand, they display characteristic features distinguishing them from the formerly observed MDs, which allows us to classify them as a novel type of MDs.
The investigations described were performed on samples with a composition of $Al_{72.0}Pd_{22.8}Fe_{5.2}$. The samples were annealed at 750°C for 981 h in a closed quartz ampoule with Ar atmosphere and subsequently quenched in water. Transmission electron microscopy (TEM) investigations were performed using a JEOL 4000FX electron microscope.

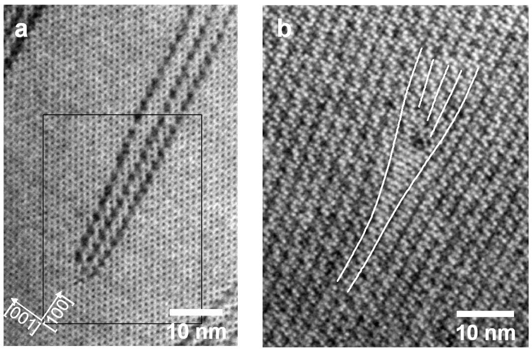

FIG. 1: TEM micrographs of metadislocations with three associated phason half-planes in the ξ-structure (a) and in the monoclinic variant (-1,1) of the ε_{22}-structure (b).

Fig. 1a is a transmission electron micrograph of a dislocation in this phase. The dislocation core is located in the lower left part of the image. It is associated with three phason planes extending to the upper right (dark contrast). The surrounding host structure is formed by a parallel arrangement of flattened hexagons and can be identified as ξ-phase. Fig. 1b is a micrograph of a dislocation in a sample region with a high density of phason planes. The host structure can be identified as the monoclinic (1,-1) variant of the ε_{22} structure with additional local modulations [5]. The dislocation core terminates three phason planes extending to the upper right part of the image. Below the core, a small region showing parallel flattened hexagons, i.e. of ξ-structure, is observed.

The phason planes surrounding the dislocation core are marked by white lines as a guide to the eye.

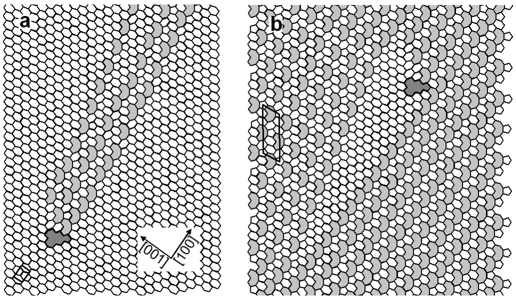

FIG. 2: Tiling representations of metadislocations with three associated phason half-planes in different host structures (see text).

Fig. 2 shows structural models of these dislocations using a tiling approach [cf 3, 5]. The host structure in Fig. 2 a is given by parallel hexagons, representing the ξ-phase. The corresponding unit-cell projection is depicted by a thick rectangle in the lower left corner. The dislocation core is represented by the dark-grey tile and the three associated phason half-planes by the light-grey tiles. A closed circuit in terms of edges of the hexagon tiles around the dislocation core reveals a closure failure, which corresponds to the dislocations Burgers vector. We obtain 1/2τ^4 [1 0 1] in terms of the ξ-lattice, corresponding to a Burgers vector length of 1.79 Å. Fig. 2b can be understood as an ideal hexagon-tiling representation of the MD in Fig. 1b. The experimental image shows, however, that structural relaxation of the phason planes takes place which are not accounted for in the structural model. The host structure is still mainly given by the monoclinic (1,-1)-phase, but now on the left hand side of the schematic, an area containing the monoclinic (3,-1) phase [5] is drawn.

Comparing the tiles representing the dislocation cores in the ξ- and the ε_6-structure (Fig. 2 and Ref. [3]) it is obvious that the same polygon is used. The differences in Burgers-vector length for ε-Al-Pd-Fe and ε_6-Al-Pd-Mn (the latter amounts to 1.83 Å[3]]) is only due to the slightly different lattice parameters of these phases. Accordingly, it is expected that the dislocation core structures in these phases are very similar. However, detailed information cannot be resolved from the present TEM images. For this dedicated work using high-resolution electron microscopy is currently performed.

Fig. 3 shows a TEM micrograph of MDs with five and eight associated phason half-planes in the monoclinic variant (-1,1) of the ε_{22}-structure. A structural model for these MDs can be set up in the same way like for the MDs shown in Fig. 1. It is shown that the cores of those MDs and their Burgers-vectors correspond to those of MDs associated to 10 and 16 phason planes in the ε_6- and ε_{28}-structure [cf. 4, 6]. It can be generalized that the number of phason planes of MDs in ξ- and ε_6-structures [4] and in the material investigated in the present study correspond to Fibonacci and a double Fibonacci sequence.

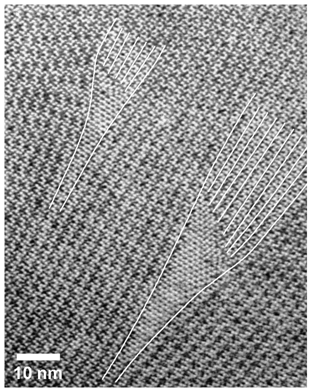

FIG. 3: TEM micrograph of metadislocations with five and eight associated phason half-planes in the monoclinic variant (-1,1) of the ε_{22}-structure.

The present study shows that the concept of MDs can be applied to various ε-type complex metallic alloys. The construction principle can be generalized: on the one hand, the MD in the ε_6-structure can have associated phason half-planes forming a slab of any variant of ε-phase that possesses phason lines as structural elements. On the other hand, the complementary MDs can be embedded in host structures of any type of ε-phase possessing phason lines as structural elements. The decisive difference between the two types of MD, the previously known and the novel one, is the local structure in which the dislocation core is embedded: that of the previously observed MDs is embedded into the ε_6-structure, while that of the novel type is embedded into the ξ-structure. The different host structures directly result in different numbers of associated phason half-planes required for accommodation of the metadislocation core, i.e. a Fibonacci and a double Fibonacci sequence for MDs in ξ- and ε_6-structures, respectively.

Acknowledgements

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