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Comprehensive model of metadislocation movement in $Al_{13}Co_4$

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Metadislocations are highly complex defects mediating plasticity in several complex metallic alloys. Available models characterizing the atomic rearrangements during the movement of these defects are limited to two dimensions and heavy atomic species. Combining high-resolution scanning transmission electron microscopy, density functional theory and simulated annealing we develop a three-dimensional model of a metadislocation glide step of 12.3 Å in the complex metallic alloy $Al_{13}Co_4$ including all atomic species. The rearrangements within the core are shown to involve maximum atomic jump distances of 3.4 Å.

Keywords: Microscopy and microanalysis techniques; High-angle annular dark-field (HAADF); scanning transmission electron microscopy (STEM); Aluminium alloys; dislocation dynamics

Complex metallic alloys (CMAs) are intermetallic phases characterized by a considerable amount of structural complexity, involving unit cells larger than simple alloys and containing a large number of atoms, typically from tens to thousands of atoms. Since the elastic line energy of a dislocation is proportional to the square of the Burgers vector [1], the formation of perfect dislocations is energetically unfavourable and conventional plastic deformation mechanisms are prone to failure. Rather, plastic deformation is often mediated by metadislocations [2,3]. Metadislocations are line defects with a Burgers vector corresponding to a τ^{-n}-fraction ($\tau = \frac{1}{2}\cdot(1+\sqrt{5})$, i.e. the golden ratio) of a lattice constant. By this means the dislocation energy is reduced to tolerable values. Metadislocations are always associated with a region of transformed phase, by which the irrational Burgers vector is accommodated in the crystal lattice. The transformed region can be realized by a slab of different but structurally closely related phase, or by so-called phason defects [4]. Although remarkable progress has been achieved in the analysis of various metadislocations in different CMAs [5,6], model descriptions of metadislocation motion are so far limited to heavy atomic species and two dimensions. For example, Ref. [7] reports the first model for metadislocation motion in ϵ_6-Al–Pd–Mn, taking into account atomic jump patterns in different crystallographic directions for the Pd–Mn columns only. Since ϵ_6-Al–Pd–Mn includes more than 70 at.% Al, this restriction to heavy elements poses a severe limitation.

In this work we report on the first development of a fully three-dimensional model of a moving metadislocation including all atomic species. The CMA chosen for our study is the moderately complex o-$Al_{13}Co_4$, an orthorhombic phase with space group $Pmn2_1$, lattice parameters $a = 8.2$ Å, $b = 12.3$ Å, $c = 14.5$ Å and 102 atoms per unit cell [8,9]. For this CMA phase it was first postulated [10], and later shown experimentally [11], that its deformation involves metadislocations. These were demonstrated to move by glide [11,12], and very recently an analysis of the metadislocation core structure and movement mechanism, solely covering the Co atoms, was published [5]. It can be shown that a metadislocation in o-$Al_{13}Co_4$ is associated with a slab of a structurally closely related monoclinic phase, m-$Al_{13}Co_4$, as well as to phason defects necessary to accommodate the metadislocation core. Monoclinic m-$Al_{13}Co_4$ has been reported in Ref. [13] to belong to the space group $C2/m$, the lattice parameters are $a = 8.109$ Å, $b = 12.349$ Å, $c = 15.173$ Å and $\beta = 107.84°$.

A single-crystalline o-$Al_{13}Co_4$ sample, grown by the Bridgman technique, was uniaxially deformed to about 6% strain and subsequently prepared for scanning transmission electron microscopy (STEM) investigation by wire-saw cutting, mechanical grinding and argon ion milling [11,12]. STEM measurements were carried out using a FEI Titan 80–300 kV transmission electron microscope equipped with a Fishione high-angle annular dark-field (HAADF) detector.

Figure 1 is an experimental HAADF STEM image showing a metadislocation (core region marked in green) in o-$Al_{13}Co_4$. In this imaging mode the contrast is

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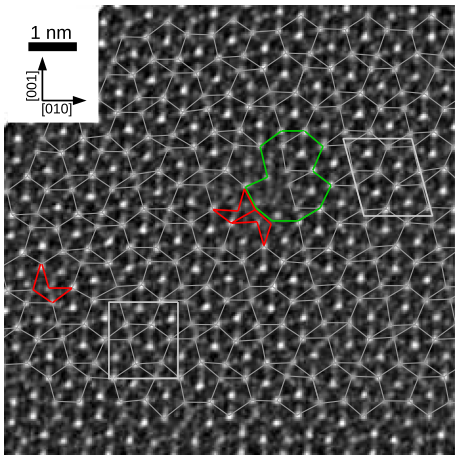

Figure 1. HAADF STEM micrograph of a metadislocation in orthorhombic $Al_{13}Co_4$. Bright dots correspond to Co columns. A pentagon-rhomb tiling is overlaid. Unit cells of the orthorhombic (lower left) and the monoclinic phase (right) are indicated by white boxes. The metadislocation core is marked by a green polygon, while crown-shaped phason elements are marked in red. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

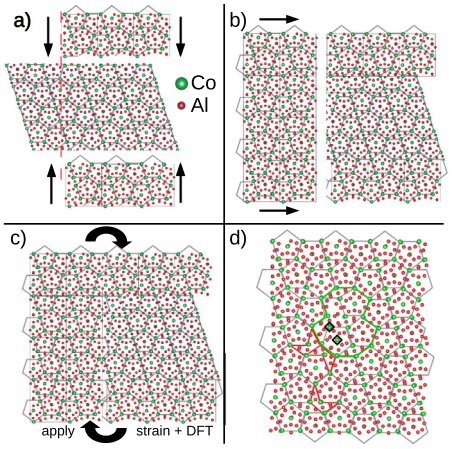

Figure 2. Construction of a metadislocation in orthorhombic $Al_{13}Co_4$ based on orthorhombic and monoclinic unit cells as building blocks (see text). Diamonds in (d) represent Co positions, which are not observed experimentally.

proportional to Z^p (with Z the atomic number Z and p in the range of 1.2–1.7) and therefore the bright dots correspond to atomic columns rich in Co. A pentagon-rhomb tiling is overlaid. In the left part of Figure 1 the orientation of the rhombs alternates along the [0 0 1] direction, which is characteristic of the orthorhombic phase. The white box in the lower left part of Figure 1 indicates the orthorhombic unit cell. A different structure characterized by a parallel arrangement of rhomb elements, which is characteristic for the monoclinic phase m-$Al_{13}Co_4$ (unit cell marked by a white box), extends from the core region (green polygon) to the right-hand side, i.e. the wake of the metadislocation. This slab of monoclinic m-$Al_{13}Co_4$ with a thickness of two unit cells accommodates the metadislocation in the orthorhombic crystal. The crown-shaped phason elements (red in Figure 1) serve as escort defects [6], which are required to adjust the orthorhombic structure in front of the dislocation so that it can connect to the symmetric metadislocation core. The experimental HAADF image in Figure 1 clearly displays the position of the Co columns but does not provide any information about the Al positions. For the construction of our metadislocation model we used the unit cells of established structure models for the orthorhombic and monoclinic phase [9,13] as building blocks. Figure 2 shows a sketch [14] of the approach used to construct the model, with Al and Co positions in red and green, respectively. A slab of monoclinic phase with a height of two unit cells is created and two slabs of orthorhombic phase are congruently attached to its top and bottom (Fig. 2a). This leads to a horizontal offset between the upper and lower orthorhombic slab (red dashed line), which corresponds to the Burgers vector of b = 1.79 Å [7]. The upper left orthorhombic unit cell is taken as a boundary, the monoclinic part left of which is removed. The remaining crystal is connected to a block of orthorhombic phase slab of 2 × 4 unit cells (Fig. 2b). This leads to coinciding atomic positions for the upper part of the interface but leaves a gap, corresponding to the Burgers vector, in the lower part (Fig. 2c). We then displaced the atom positions according to the strain field of an edge dislocation [1], which leads to a first-order model of the metadislocation. The most prominent apparent disagreement between the experimental image and the model concerns the position of the isolated escort defect at the lower left-hand side of Figure 2d. This defect, according to the construction of our model, appears at the boundary of the set of orthorhombic and monoclinic slabs and the left block of the orthorhombic phase. In the experimental image, on the other hand, this defect occurs farther in front of the metadislocation core. It was demonstrated [5], however, that escort defects can move freely along the [0 1 0] direction. Therefore, the configurations in Figures. 1 and 2d can be taken as equivalent.

Geometric optimization of the first-order model was performed using density functional theory (DFT) employing the Vienna Ab initio Simulation Package plane-wave pseudo-potential code [15]. Calculations were performed under the generalized gradient approximation, and used the projector augmented wave potentials for Al and Co supplied with the code [16]. The structural relaxations were performed to within 0.05 eV/Åper atom, using an energy cut-off of 270 eV, and a k-point sampling of 1 × 1 × 5. The size of the metadislocation model makes it difficult to construct a supercell containing a tractable number of atoms that is periodic in all three dimensions. We therefore resorted to a 34 × 34 × 8.16 $Å^3$ supercell for the core region containing 269 atoms. It is periodic only along the *a* direction, i.e. parallel to the metadislocation line. In the perpendicular directions, the core was surrounded by 2–3 atom thick structural motif layers, which were in turn surrounded by an about 10 Åthick vacuum region. The outermost atoms of the surrounding motif layers were held at fixed positions during the relaxation (corresponding to the experimentally observed atom positions in the surrounding lattice in Figure 1), while all internal atoms were allowed to relax. This relaxation led to displacements smaller than 0.8 Å for most atoms, with the exception of a small number of Al atoms that were displaced up to 1.5 Å. A two-dimensional projection of the resulting relaxed model is seen in Figure 2d, together with an overlaid tiling. The DFT relaxation led mainly to displacements of Al atoms, which cannot be directly compared to the experimental image. A