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Core Structure and Motion of Metadislocations in the Orthorhombic Structurally Complex Alloy $Al_{13}Co_4$

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The atomic structure of metadislocation cores in the phase o-$Al_{13}Co_4$ is investigated using aberration corrected scanning transmission electron microscopy. Metadislocations with Burgers vectors of -b/τ^4 [0 1 0] and b/τ^3 [0 1 0] having six and four stacking faults, respectively, are found. They are associated with separate phason defects, which escort the movement of the metadislocations through the material. A first partial atomic model for metadislocation glide motion, taking Cobalt atom jumps into account, is developed. Atom jumps take place in pairs along various crystallographic directions. Typical jumps occur between atomic columns separated by 1.5 Å.

Keywords: Complex Metallic Alloy, Metadislocation, Dislocation Core, Scanning Transmission Electron Microscopy

Metadislocations are large and structurally highly complex defects mediating plasticity in various complex metallic alloys (CMAs).[1,2] Likewise, their atomic mechanisms of motion are highly complex as they involve a large number of atomic jumps for an elementary step. As yet, there is no comprehensive model for metadislocation motion on the atomic scale for any CMA. Recently, a first atomic model for motion was developed considering merely the Pd atoms in ε_6-Al–Pd–Mn, a CMA phase with 318 atoms per unit cell. Repetitive jump patterns along various crystallographic directions were found, which involve about 100 atomic positions per individual step of metadislocation motion.[3] The case of metadislocation motion in ε_6-Al–Pd–Mn, however, is particularly complex due to an extraordinary high number of atoms involved and due to the fact that metadislocation motion in this material takes place by pure climb. For this reason, a detailed microstructural investigation of less complex metadislocations involved in a simpler glide mode and the development of an atomic model for these dislocations may support the comprehension of structurally related but more complex metadislocations.

A CMA phase, promising in these terms is o-$Al_{13}Co_4$, which possesses an orthorhombic structure with space group $Pmn2_1$, lattice parameters $a = 8.2$ Å, $b = 12.3$ Å and $c = 14.5$ Å, and 102 atoms per unit cell.[4,5] The main structural features of o-$Al_{13}Co_4$ are pair-connected pentagonal prismatic channels extending along the [1 0 0] direction.[5] Figure 1(a and b) show a structure model of o-$Al_{13}Co_4$. Yellow and green spheres represent cobalt and aluminium atomic positions, respectively. Figure 1(b) shows a projection along the [1 0 0] direction. The orthorhombic unit cell is shown in blue. The projected structure can be described by a tiling consisting of regular pentagons and rhombs.[6] Figure 1(b) shows an experimental micrograph taken by high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) of o-$Al_{13}Co_4$ along [1 0 0]. Due to the 'Z-contrast' conditions, columns containing heavy atoms are emphasized. White dots represent columns containing heavy cobalt atoms. Contrast of the aluminium positions is below the noise level of the micrograph. The pentagon rhomb tiling is superimposed. Rhombs are arranged in characteristic rows along the [0 1 0] direction with alternate orientation (yellow and blue in Figure 1(c)). The structure of monoclinic $Al_{13}Co_4$ (denoted m-$Al_{13}Co_4$) is homeotypic to that of monoclinic $Al_{13}Fe_4$, and structurally closely related to o-$Al_{13}Co_4$.[5–8] The tiling description of m-$Al_{13}Co_4$ is characterized by a parallel arrangement of the pentagon and rhomb elements using just a single type of rhombs.

The existence of metadislocations in the phase o-$Al_{13}Co_4$ was first postulated due to geometric considerations [9] and later verified experimentally.[10,11] First macroscopic uniaxial plastic deformation experiments

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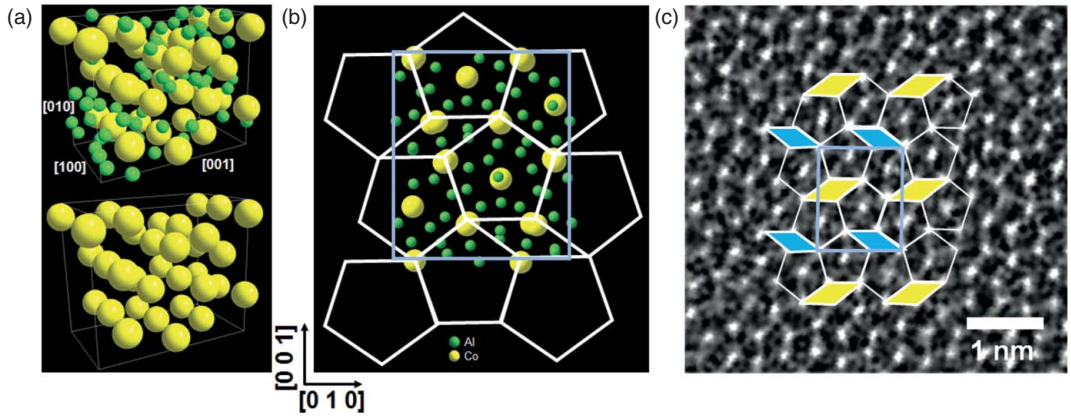

Figure 1. (a) Structure model of o-$Al_{13}Co_4$ showing the Cobalt (yellow) and Aluminium (green) atomic positions (upper image) and just the Cobalt position (lower image) within one unit cell (white lines). (b) Structure model of o-$Al_{13}Co_4$ along [1 0 0] showing Cobalt (yellow) and Aluminium (green) atomic positions within the unit cell (blue rectangle). The structure is described by a pentagon/rhomb tiling. (c) HAADF-STEM micrograph of o-$Al_{13}Co_4$ with pentagon/rhomb tiling showing rhombs with alternate orientation (yellow and blue).

and microstructural investigations using transmission electron microscopy (TEM) were performed on single crystalline o-$Al_{13}Co_4$. Deformed samples exhibited localized zones of inhomogeneous deformation on their surfaces which correspond to slip traces along (0 0 1) planes. TEM investigations revealed a high density of [1 0 0] dislocations attached to (0 0 1) planar defects.[10]

A subsequent microstructural investigation [11] identified the dislocations as metadislocations. In contrast to metadislocations in ε-phases, however, metadislocation motion in o-$Al_{13}Co_4$ takes place by [0 1 0] glide on (0 0 1) planes. This finding was confirmed by recent microstructural investigation on o-$Al_{13}Co_4$ deformed below the ductile–brittle transition temperature using microcompression.[12] Closer inspection of the glide planes by aberration-corrected electron microscopy revealed (0 0 1) slabs of a monoclinic phase in the orthorhombic $Al_{13}Co_4$ matrix [11] partially compensating the strain of the metadislocation core. The Burgers vector of the metadislocation investigated in [11] was determined as b/τ^3 [0 1 0], where $\tau \approx 1.618$ is the irrational number of the golden mean.

Although different tiling models for metadislocations in orthorhombic $Al_{13}Co_4$ were proposed, e.g. with and without the presence of escort defects,[1,11,13] the atomic structure of a metadislocation core and its surrounding are unknown as yet. However, detailed knowledge on the atomic core structure is a prerequisite for the development of an atomic scale model for metadislocation motion. Such a model would be of large interest, as it would represent the first atomic model for metadislocation glide in complex materials. In the present work, the atomic core structure of a metadislocation in the o-$Al_{13}Co_4$ phase is analysed using probe-corrected STEM. Using this information, a first atomic model for metadislocation motion is developed.

We investigated plastically deformed single crystalline o-$Al_{13}Co_4$ samples, which have been uniaxially deformed to about 6% strain. Detailed information on the plastic deformation tests and sample preparation can be found in [10,11]. Atomic-resolution STEM was performed in a probe-corrected FEI TITAN 80-300 employed with a HAADF detector. 'Z-Contrast' conditions were achieved for sufficiently thin specimen areas using a probe semi-angle of 25 mrad and a detector inner collection angle of 70 mrad. Under these conditions, the image intensity associated with an atom column is approximately proportional to the square of the mean atomic number of the atoms in the column for sufficiently thin samples.[14]

Figure 2(a) shows a high-resolution HAADF-STEM micrograph of a metadislocation in the phase o-$Al_{13}Co_4$. A tiling of the surrounding area is superimposed and a full tiling of the electron microscope image is given in Figure 2(b). The core is outlined as green polygon. At the right-hand side of the core, a slab of the monoclinic $Al_{13}Co_4$ phase is located, which is characterized by a parallel arrangement of rhombs (yellow) within the pentagon/rhomb tiling. This observation is in accordance with earlier observations, reporting (0 0 1) planar defects in as-cast and deformed $Al_{13}Co_4$, which were identified by means of X-ray diffraction and high-resolution TEM as monoclinic slabs in an orthorhombic matrix.[6,11] Since the ideal orthorhombic $Al_{13}Co_4$ phase contains alternating rows of rhombs along the [0 0 1] direction (Figure 1(c)), two subsequent rows of rhombs oriented in parallel constitute a (0 0 1) stacking fault. In this sense, the metadislocation in Figure 2 is associated with six stacking faults (dashed red lines). The stacking faults extend to the right-hand side, which indicates the direction of motion: the metadislocation shown moves from right to left, and the stacking faults are located in its wake.

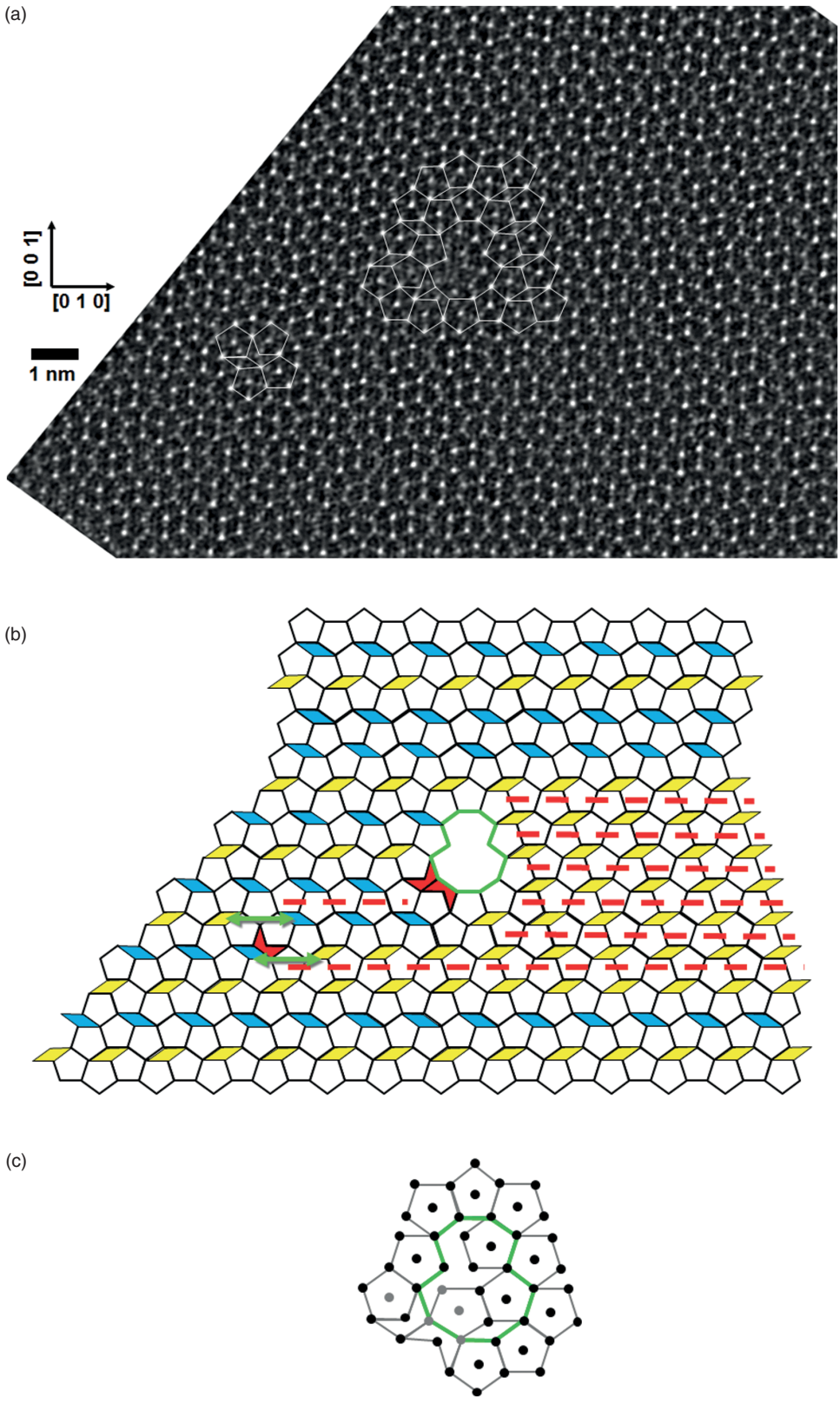

Figure 2. (a) HAADF-STEM micrograph of a metadislocation core and tiling description (white). The image shows slight contrast variation, possibly due to thickness variation, local straining or covering of the specimen surface. The image was subjected to rotation, which exhibits the initial scanning frame as inclined edges at the left, and to slight fast Fourier transform (FFT) filtering to reduce high-frequency noise. (b) Full tiling of the micrograph in (a). Metadislocation core (green polygon), phason defects (red polygons) and stacking faults (red dashed lines) are indicated. (c) Observed and derived Cobalt positions (black and grey circles) within and around the metadislocation core (green) extracted from the micrograph in (a).

A Burgers circuit around the core yields a Burgers vector of $\vec{b} = -b/\tau^4$ [0 1 0] which is an irrational fraction of the lattice constant. The observed Burgers vector is smaller by a factor of τ than the metadislocations observed in the o-$Al_{13}Co_4$ phase before.[11] Figure 2(b) furthermore shows three red tiles, two of which are located directly at the left-hand side of the core and a third one at a distance of about 5 nm left from the core. The red tiles are identified as phason defects [9] (also referred to as phasons).

Recently, a new type of metadislocation was observed in the complex T-Al–Mn–Pd phase.[15,16] This metadislocation consists of a complex core and three separated phason defects, which were referred to as escort defects. Upon deformation, the escort defects move ahead and locally transform the T-phase structure for accommodation of the dislocation core. Metadislocation core and phason defects leave a slab of R-phase in their wake, which can be interpreted as six stacking faults. It is obvious that the $Al_{13}Co_4$ observations in the present work are very similar to the T-Al–Mn–Pd case. In both cases, metadislocations are escorted by phason defects and cause a structural transformation from an orthorhombic to a monoclinic phase in a slab of several nanometre thickness in their wake. Furthermore, in both cases, the transformed slab can be interpreted as the introduction of six stacking faults.

In contrast to the case of the T-phase, two phason defects in o-$Al_{13}Co_4$ (Figure 2(a) and 2(b)) are directly connected to the core. Accordingly, it can be argued that they are not separated defects but part of the core, which is then larger and non-symmetric. In this sense, the shape of the polygon describing the metadislocation core is not strictly unique. We, however, decided for the symmetric representation since there is no strict requirement for the associated phasons to be connected to the core. From a geometrical point of view, the phasons can be separated from the core and are still able to fulfil their function in the arrangement.

The function of the phason defects can best be seen at the example of the left phason, which is separated from the metadislocation core. It inverts the stacking sequence of two neighboured (0 0 1) planes of rhomb tiles such that the orientation of the rhombs changes from the left to the right-hand side of the phason (arrows in Figure 2(b)). Interpreted in terms of stacking faults (dashed lines), the function of the phason is to provide a redirection: stacking faults, which are extending ahead of the core, are redirected by phason defects, so that all structural changes induced by the movement of the dislocation are in its wake. The same mechanism of phason defects redirecting stacking faults and escorting a metadislocation core upon movement was observed in the T-Al–Mn–Pd phase.[15,16]

Figure 2(c) represents the distribution of cobalt columns at the metadislocation core experimentally observed as bright dots in Figure 2(a). At the right-hand side inside the core, the cobalt positions can be clearly identified and matched by two pentagons. At the lower left-hand side, however, the distribution of bright dots is somewhat ambiguous, which may be due to the presence of the strain field or kinks along the dislocation line. Here, the location of cobalt atoms was interpreted in terms of a suitable location within the pentagon/rhomb tiling. They are indicated in grey in Figure 2(c). A clear difference between the metadislocations in o-$Al_{13}Co_4$ and T-Al–Mn–Pd is thus present in the atomic distributions within the cores. While the atomic structure within a metadislocation core in T-Al–Mn–Pd shows a distinct mirror symmetry with respect to the (0 0 1) plane, our observations reveal a non-symmetric intensity distribution within the metadislocation core in o-$Al_{13}Co_4$.

Figure 3(a) shows a HAADF-STEM micrograph of another type of metadislocation with superimposed tiling. Again, the core is associated with phason defects (red tiles) and stacking faults (red dashed lines). In this example, four stacking faults are observed on the left-hand side of the core and the dislocation moves to the right into the ideal o-$Al_{13}Co_4$ phase region. Further bypassing stacking faults (pink dashed lines) which are not associated with the metadislocation are observed at the bottom of the image. A Burgers circuit around the core yields a Burgers vector $\vec{b} = b/\tau^3$ [0 1 0], which coincides with that in [11]. On the left-hand side of the metadislocation core, the stacking faults are, however, not densely stacked as in Figure 2(b); a line of yellow rhombs intermits the parallel stack of blue rhombs. In this sense, this example does not correspond to the most compact and simple elementary arrangement, which may be due to the presence of external disturbances such as the bypassing stacking faults. Nevertheless, the characteristic features of the metadislocation, the number of associated stacking faults and the corresponding Burgers vector length are invariable.

Figure 3(b)–(d) illustrates tiling descriptions of simple, elementary metadislocations in o-$Al_{13}Co_4$ using a pentagon/rhomb tiling. Metadislocations with 4, 6 and 10 stacking faults are shown. For simplicity, just the metadislocation core and the stacking faults are shown (dashed red lines), phason elements redirecting stacking faults are not considered. They have Burgers vectors of b/τ^3 [0 1 0], $-b/\tau^4$ [0 1 0] and b/τ^5 [0 1 0]. Simultaneous existence of a sequence of Burgers vectors, scaled by factors of τ and the double-Fibonacci number of stacking faults or phason planes is characteristic of metadislocations in various materials.[2,15–19]

The investigation of the atomic metadislocation core structure in the present investigation offers a basis towards the development of an atomic model for metadislocation glide motion in the o-$Al_{13}Co_4$ phase. We use the tiling description (Figure 2(b)) and its decoration with cobalt atoms derived from the experimental images (Figure 2(c))

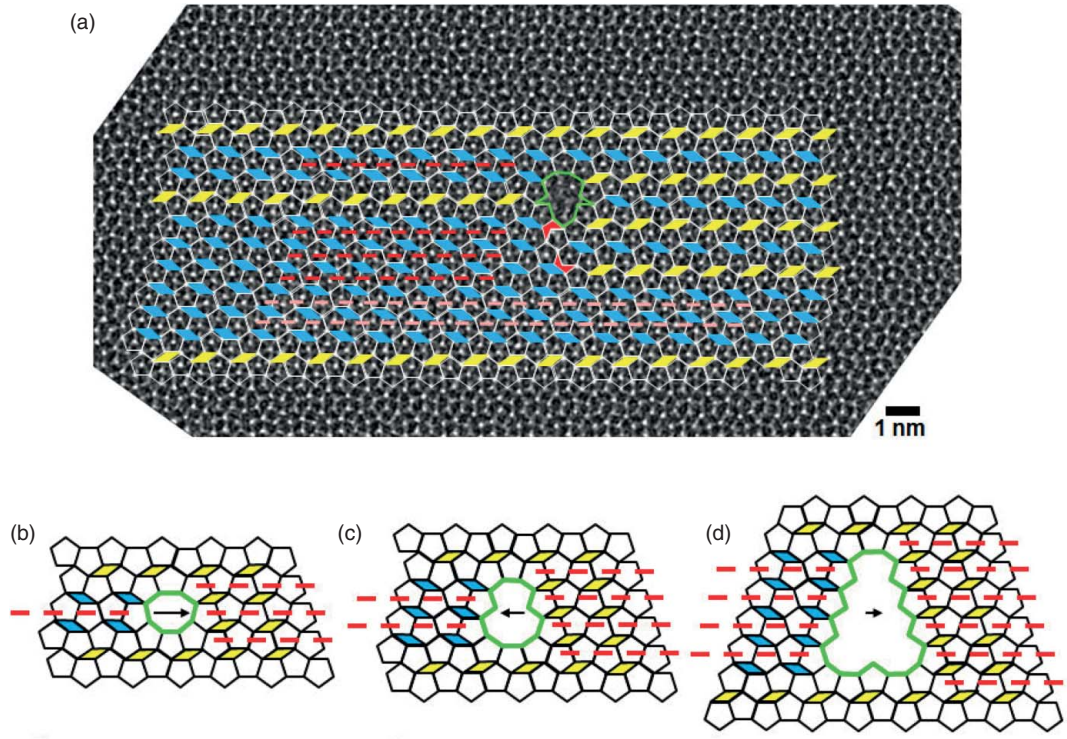

Figure 3. (a) HAADF-STEM micrograph of a metadislocation with superimposed tiling showing a complex core structure (green) phason defects (red) and stacking faults (red dashed lines) and stacking faults not associated to the metadislocation (pink dashed lines). (b–d) Tiling descriptions of elementary metadislocations with four, six and ten stacking faults. Burgers vectors are indicated as black arrows (not to scale).

and shift the location of the metadislocation by one unit along the direction of movement.

Figure 4 shows the initial (grey) and final (red) tiling and the respective cobalt positions. Initial and final positions of the cobalt columns correspond in most areas around the metadislocation core (small deviations are present due to the elastic strain field around the core). Within the core and at the location of the phason defects, atomic jumps between initial and final positions occur (black arrows). The atomic jumps take place along various crystallographic directions and are generally short—typical jump distances are 1.5 Å. Four jumps take place between cobalt columns at the phason element on the left and 14 jumps occur in and around the metadislocation core. It can be noticed that jumps often occur paired and in a symmetric way. At the location of the phason element, for instance, two jumps at the left occur in a $[0 \quad \tau - 3 \quad -\sqrt{2+\tau}]$ direction, whereas on the right two jumps occur inversely in a $[0 \quad \tau - 3 \quad \sqrt{2+\tau}]$ direction. It should be kept in mind that the presented model only takes into account the cobalt positions, since the involvement of the aluminium atoms is experimentally not accessible by our HAADF-STEM approach. Density functional theory or molecular dynamics simulations will be required for the further development towards a full model including the aluminium atoms as well.

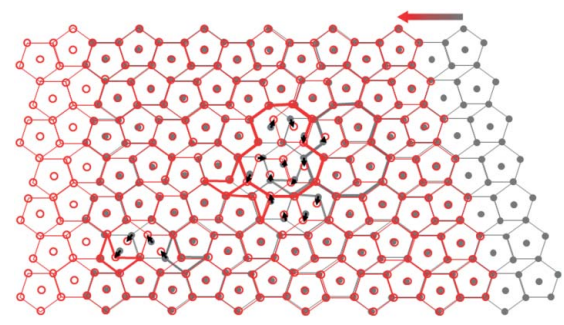

Figure 4. Atomic model for metadislocation motion considering Cobalt atomic positions (circles). Final (red) and initial (grey) positions are displaced by one unit cell along the direction of movement (red and grey arrow). Atomic jumps between initial and final positions are indicated by black arrows.

In summary, we have investigated the atomic structure of metadislocation cores in the phase o-$Al_{13}Co_4$. Two metadislocations with Burgers vectors of $-b/\tau^4$ [0 1 0] and b/τ^3 [0 1 0] are found. They are associated with six and four stacking faults, respectively. Like for metadislocations in other complex alloy phases, the sequence can be geometrically extended,[2,15–19] but only two instances of the series are experimentally observed here. The metadislocations are associated with separate phason defects, which escort the metadislocation

cores though the material as they move. This mechanism of metadislocation glide using escort defects is very closely related to the plastic deformation mechanism in the complex phase T-Al–Mn–Pd.[15,16] In both cases, metadislocations and escort defects create a structural transformation from an orthorhombic to a monoclinic phase in a slab of several nanometre thickness behind the metadislocation.

The atomic core structure extracted in the present investigation was furthermore used to create a first atomic model for metadislocation motion considering the cobalt atomic positions. Atomic jumps take place in pairs along various crystallographic directions and typical jump distances of 1.5 Å are found.

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References

[1] Klein H, Feuerbacher M. Structure of dislocations and stacking faults in the complex intermetallic ξ'-(Al–Pd–Mn) phase. Phil Mag. 2003;83:4103–4122.
[2] Feuerbacher M, Heggen M. Metadislocations. In: Hirth JP, Kubin L, editors. Dislocations in solids. Vol. 16. Amsterdam: Elsevier; 2010. p. 109–170.
[3] Heggen M, Feuerbacher M. Metadislocation core structure and atomic model for metadislocation motion. Acta Mater. 2013;61:3851–3857.
[4] Gödecke T, Ellner M. Phase equilibria in the aluminium-rich portion of the binary system Co–Al and in the cobalt/aluminium-rich portion of the ternary system Co–Ni–Al. Z Metallkd. 1996;87:854–864.
[5] Grin J, Burkhardt U, Ellner M, Peters K. Crystal structure of orthorhombic Co_4Al_{13}. J Alloys Comp. 1994;206:243–247.
[6] Saito K, Sugiyama K, Hiraga K. Al13M4-type structures and atomic models of their twins. Mat Sci Eng A. 2000;294–296:279–282.
[7] Hudd RC, Tailor WH. The structure of Co_4Al_{13}. Acta Crystallogr. 1962;15:441–442.
[8] Grushko B, Wittenberg R, Bickmann K, Freiburg C. The constitution of aluminum-cobalt alloys between Al_5Co_2 and Al_9Co_2. J Alloys Comp. 1996;233:279–287.
[9] Feuerbacher M, Heggen M. On the concept of metadislocations in complex metallic alloys. Phil Mag. 2006;86:985–990.
[10] Heggen M, Deng D, Feuerbacher M. Plastic deformation properties of the complex metallic alloy phase $Al_{13}Co_4$. Intermetallics. 2007;15:1425–1431.
[11] Heggen M, Houben L, Feuerbacher M. Metadislocations in the orthorhombic structurally complex alloy $Al_{13}Co_4$. Phil Mag. 2008;88:2333–2338.
[12] Walter C, Wheeler JM, Barnard JS, Raghavan R, Korte-Kerzel S, Gille P, Michler J, Clegg WJ. Anomalous yielding in the complex metallic alloy $Al_{13}Co_4$. Acta Mater. 2013;61:7189–7196.
[13] Heggen M, Feuerbacher M. Metadislocations: the case of pure glide. MRS Proc. 2013:1517:1-12. doi:10.1557/opl.2012.1754
[14] Nellist PD, Pennycook SJ. The principles and interpretation of annular dark-field Z-contrast imaging. Adv Imag Electron Phys. 2000;113:147–203.
[15] Heggen M, Houben L, Feuerbacher M. Plastic deformation mechanism in complex solids. Nat Mater. 2010;9:332–336.
[16] Heggen M, Houben L, Feuerbacher M. Metadislocations in the complex metallic alloys T-Al–Mn–(Pd, Fe). Acta Mater. 2011;59:4458–4466.
[17] Feuerbacher M, Heggen M. Elastic energy of metadislocations in complex metallic alloys. Acta Mater. 2012;60:1703–1711.
[18] Engel M, Trebin HR. A unified projection formalism for the Al–Pd–Mn quasi-crystal Xi-approximants and their metadislocations. Philos Mag Lett. 2005;85:2227–2247.
[19] Feuerbacher M, Balanetskyy S, Heggen M. Metadislocations in xi-AlMnPd. Acta Mater. 2008;56:1849–1856.