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Misfit Dislocations Associated with Ultrathin Twins Along a Ni₃Al / Ni₃Nb Interface

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Abstract
Typical defects of a Ni₃Al (L₁₂) / Ni₃Nb (DO₆) faceted interface associated with the orientation relationships (1 1 1)Ni₃Al // (0 1 0)Ni₃Nb and [1 1 0]Ni₃Al // [1 0 0]Ni₃Nb are reported. High resolution electron microscopy reveals the presence, along the same interface, of ledges separating facets with different atomic structures. Some facets are associated with certain interfacial thicknesses since their structures involve one planar fault or an intermediate ultrathin Ni₃Al crystal. The observed ledges are associated with a misfit dislocation (MD) with \( b = (-1/6)[112] \)Ni₃Al. This vector is determined from the comparison of the experimental images and simulated images. The multislice method has been applied with atom boxes which account for the elastic field surrounding each misfit dislocation core.

Introduction
The atomic structures of heterointerfaces parallel to close-packed planes of a (pseudo-)cubic crystal and a hexagonal or orthorhombic crystal have been intensively studied by high resolution electron microscopy (HREM) in the past years, e.g. (111)cfc // (0001)hex [1,5], (111)L₁₀ // (0001)hex. [6-10] and (111)cfc // (010)ortho. [11]. In all these references, well developed facets are reported, limited by misfit dislocations (MD's). To date, the identified MD's have Burgers vectors \( b = 1/6<112> \)Ni₃Al, inclined at 90° or 30° with respect to the electron beam direction and are parallel to the facet plane. Similar heterointerfaces have been observed in [1-5].

In the present HREM investigation, performed on a foil prepared from the same material than in [11], namely the Ni₃Al-Ni₃Nb quasi-binary eutectic obtained by directional solidification, observations are reported of intermediate interfacial defects extended on the Ni₃Al side, parallel to the heterointerface facets. The L₁₂/DO₆ heterointerface is such that the following relationships are verified: (1 1 1)Ni₃Al // (0 1 0)Ni₃Nb and [1 1 0]Ni₃Al // [1 0 0]Ni₃Nb // electron beam. The experiments are performed with the ARM of NCEM at Berkeley, with the following specifications: voltage=800 kV, spherical aberration Cs= 2 mm, spread of focus=16 nm, beam semi-angle=0.6 mrad, radius of the objective aperture (large)=0.0886 nm.
Results and interpretation

Figs. 1(a,b,c) represent three HREM images of the same heterointerface, taken for different interfacial regions. To locate the atomic columns on the images of Figs. 1(a,b), multislice calculations have been undertaken using the EMS software [12]. They show that the defocus was close to -76 nm and the thickness not far from 4 nm. As a result, the white dots in Figs. 1(a,b) represent the atomic columns for the two crystals. For the Ni$_3$Nb crystal, each atomic row has a known position. It is not the case for the Ni$_3$Al crystal because its ordered structure is not revealed.

![Fig. 1: Aspects of the facets of the Ni$_3$Al/Ni$_3$Nb interface. They are separated by 90° MD's denoted 1, 2, 3, 4, all associated with a Burgers vector $b = (-1/6) [112]$Ni$_3$Al. The MD-ledges 1 in (a) and (b) are similar to the 90° MD’s observed in a cfc/DO$_{19}$ interface [5]. The MD-edge 2 in (b) limits a planar fault with a symmetry plane indicated by a white line. The MD-ledges 3 and 4 in (a) limit the two ends of an ultrathin Ni$_3$Al crystal in a $\Sigma 3$ orientation. The close-packed symmetry plane is indicated by a white line. In (c), the ultrathin Ni$_3$Al crystal has 5 or 6 atomic planes in height.](image-url)
on the image, so that the atomic rows in Figs. 1(a,b) are known only within a \(1/2<110>\text{Ni}_3\text{Al}\) translation. Facets are in black dotted lines. They are separated by four kinds of linear defects denoted by the numbers 1, 2, 3 and 4. These defects, which accommodate a length misfit of 1\%, have been studied using the method developed in [5,11,13,14]. It uses the elasticity properties of the MD's and multislice calculations. The calculations confirm that these defects have all the same...
Burgers vector content $b = -1/6[112]$. The following assumptions are used: (i) a chemically abrupt heterointerface and (ii), on each side of a theoretical facet, the nearest atomic neighbours are the same. Defect 1 has a structure similar to that already studied in [5]. Defect 2 limits a fault on the Ni$_3$Al side with a shift equal to $b$. At the upper part of Fig. 1b, the symmetry plane for the white dots is indicated by a straight white line. Defects 3 and 4 limit the two ends of an ultrathin Ni$_3$Al crystal. Defect 3 is linked to an interfacial MD-ledge, while defect 4 is a MD slightly away from the heterointerface (two atomic planes on the Ni$_3$Al side). When the average direction of the heterointerface deviates substantially from the plane $(\text{11}\overline{1})\text{Ni}_3\text{Al}$, $\Sigma 3$ ultrathin twins are thicker as shown in Fig. 1(c).

Figs. 2(a,b,c) illustrates an example of the determination of the Burgers vector $b$ associated to defect 3. Fig. 2a is an atom box constructed according to the method proposed in [11,13]. The elastic data are the same than in [11]. Fig. 2b is a simulated image of the atom box attesting that the calculated white dots represent the positions of the theoretical atomic rows of the two crystals (in small black points), even in the highly deformed region of the MD-ledge. Fig. 2c permits a comparison to be made between the experimental positions of the atomic columns (white dots) and the theoretical positions (small black points). The excellent agreement emphasizes the safety of the method to describe the elastic fields of the MD's.

**Conclusion**

The Ni$_3$Al/Ni$_3$Nb heterointerface can accommodate the 1% length misfit with MD-ledges of various structures, still keeping the same Burgers vector $b = -1/6[112]$. Some MD-ledges limit faults and $\Sigma 3$ ultrathin twins participate to the interfacial structures.

**References**
