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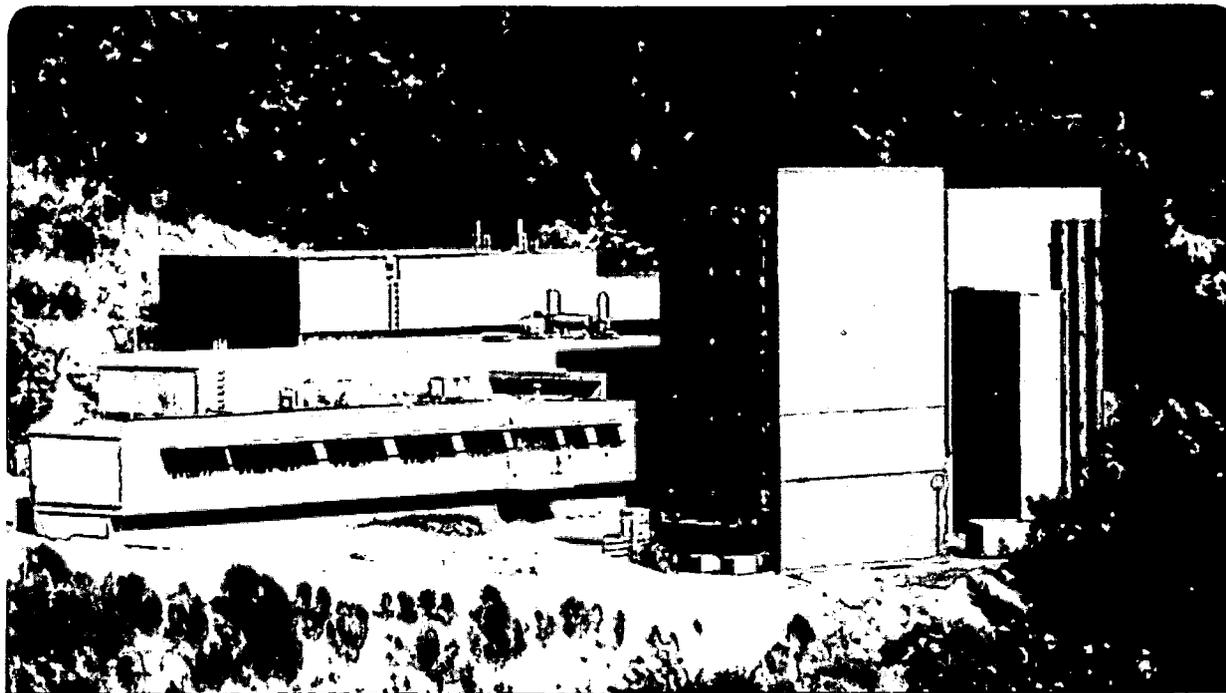
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**Misfit Dislocations Associated with Ultrathin Twins  
Along a Ni<sub>3</sub>Al / Ni<sub>3</sub>Nb Interface**

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# MISFIT DISLOCATIONS ASSOCIATED WITH ULTRATHIN TWINS ALONG A Ni<sub>3</sub>Al / Ni<sub>3</sub>Nb INTERFACE

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## Abstract

Typical defects of a Ni<sub>3</sub>Al (L<sub>12</sub>) / Ni<sub>3</sub>Nb (DO<sub>a</sub>) faceted interface associated with the orientation relationships  $(1\ 1\ \bar{1})\text{Ni}_3\text{Al} // (0\ 1\ 0)\text{Ni}_3\text{Nb}$  and  $[1\ \bar{1}\ 0]\text{Ni}_3\text{Al} // [1\ 0\ 0]\text{Ni}_3\text{Nb}$  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 Ni<sub>3</sub>Al crystal. The observed ledges are associated with a misfit dislocation (MD) with  $\mathbf{b} = (-1/6)[112]\text{Ni}_3\text{Al}$ . 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.

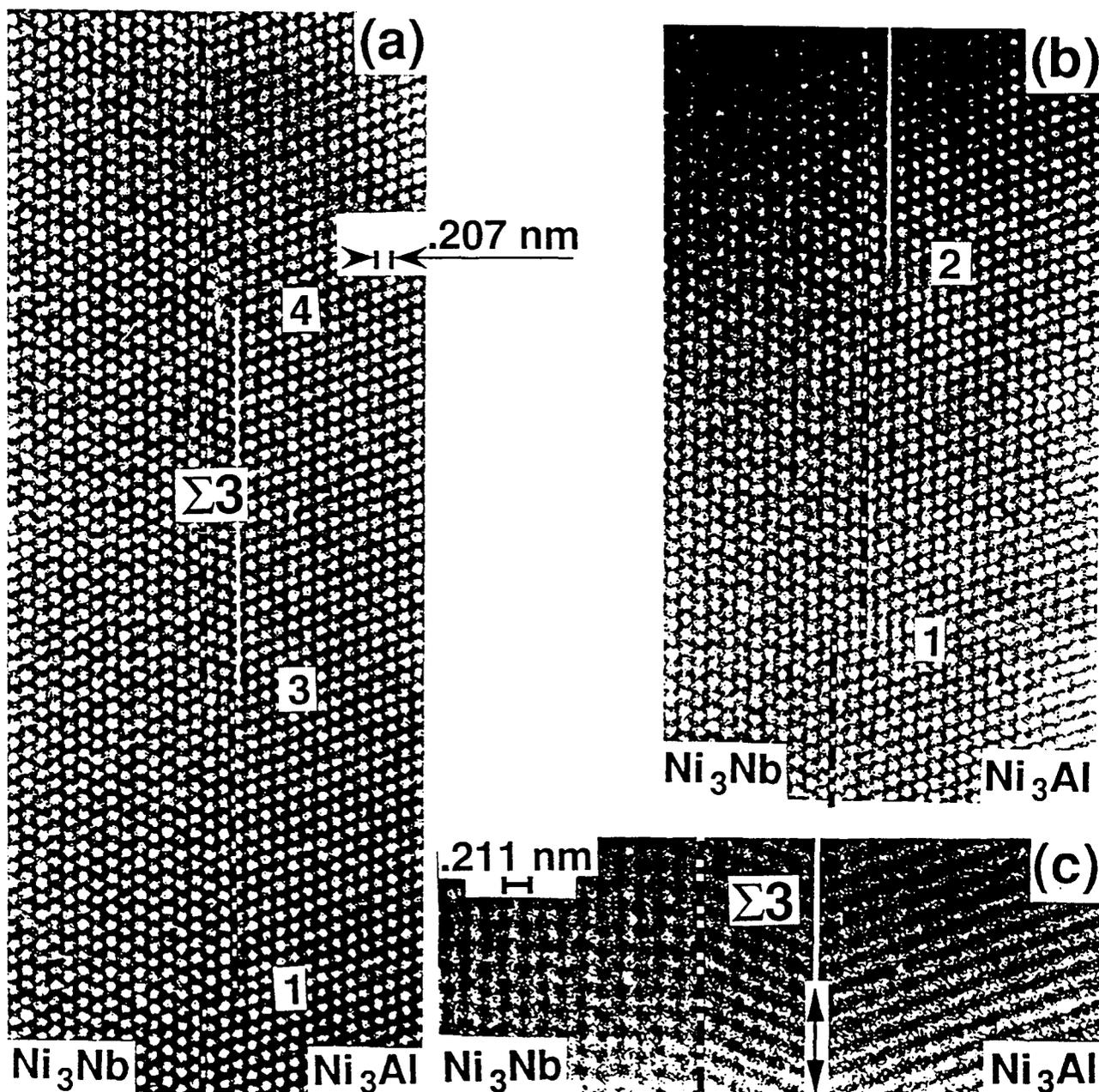
## Introduction

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.  $(111)\text{cfc} // (0001)\text{hex}$  [1,5],  $(111)\text{L}_{10} // (0001)\text{hex}$  [6-10] and  $(111)\text{cfc} // (010)\text{ortho}$ . [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  $\mathbf{b} = 1/6\langle 112 \rangle\text{Ni}_3\text{Al}$ , 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 Ni<sub>3</sub>Al-Ni<sub>3</sub>Nb quasi-binary eutectic obtained by directional solidification, observations are reported of intermediate interfacial defects extended on the Ni<sub>3</sub>Al side, parallel to the heterointerface facets. The L<sub>12</sub>/DO<sub>a</sub> heterointerface is such that the following relationships are verified:  $(1\ 1\ \bar{1})\text{Ni}_3\text{Al} // (0\ 1\ 0)\text{Ni}_3\text{Nb}$  and  $[1\ \bar{1}\ 0]\text{Ni}_3\text{Al} // [1\ 0\ 0]\text{Ni}_3\text{Nb} // \text{electron beam}$ . 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.

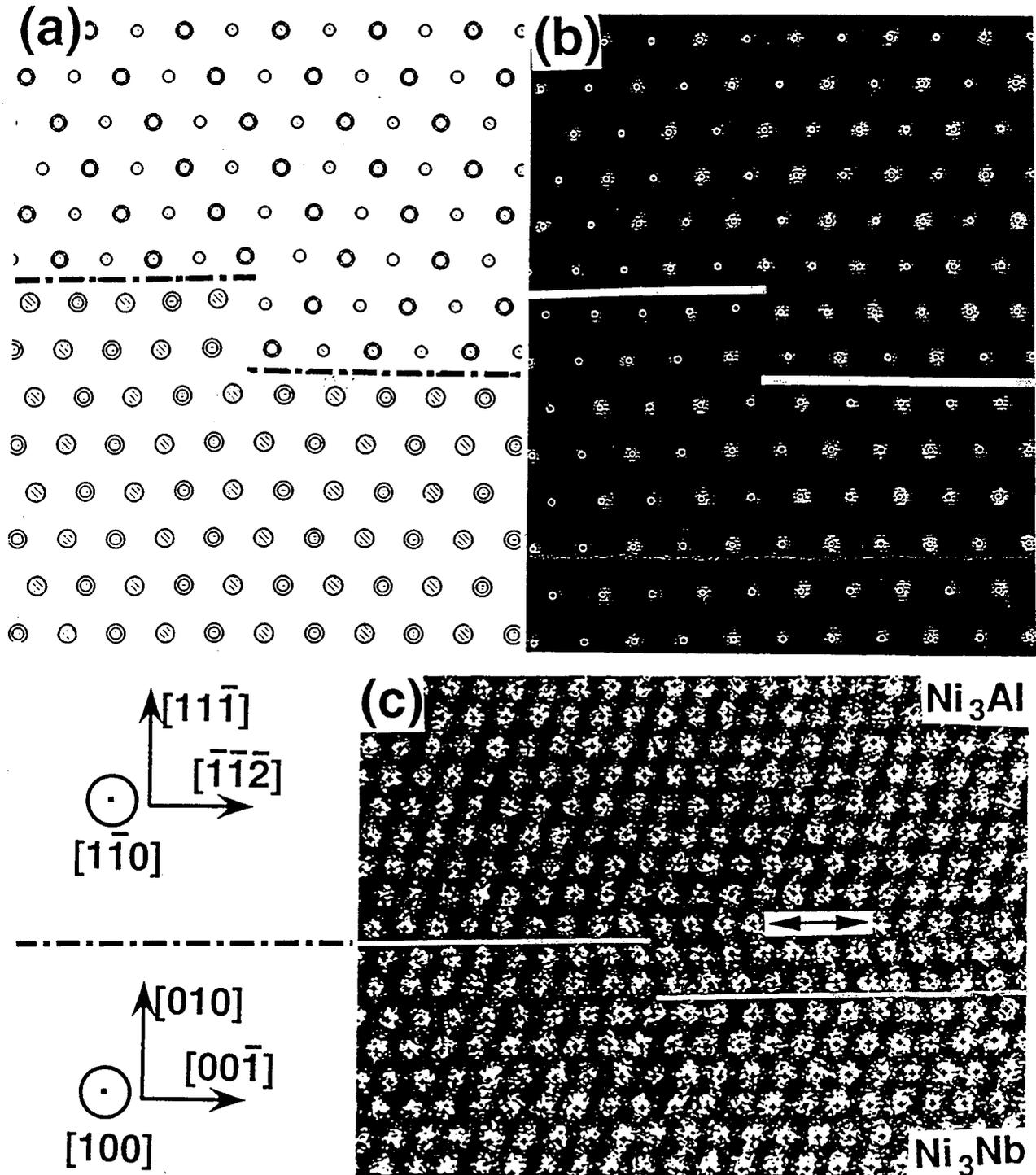
## Results and interpretation

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  $\text{Ni}_3\text{Nb}$  crystal, each atomic row has a known position. It is not the case for the  $\text{Ni}_3\text{Al}$  crystal because its ordered structure is not revealed



**Fig. 1:** Aspects of the facets of the  $\text{Ni}_3\text{Al}/\text{Ni}_3\text{Nb}$  interface. They are separated by  $90^\circ$  MD's denoted 1, 2, 3, 4, all associated with a Burgers vector  $b = (-1/6) [112]_{\text{Ni}_3\text{Al}}$ . The MD-ledges 1 in (a) and (b) are similar to the  $90^\circ$  MD's observed in a  $\text{cfc}/\text{DO}_{19}$  interface [5]. The MD-ledge 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  $\text{Ni}_3\text{Al}$  crystal in a  $\Sigma 3$  orientation. The close-packed symmetry plane is indicated by a white line. In (c), the ultrathin  $\text{Ni}_3\text{Al}$  crystal has 5 or 6 atomic planes in height.

on the image, so that the atomic rows in Figs. 1(a,b) are known only within a  $1/2\langle 110 \rangle \text{Ni}_3\text{Al}$  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



*Fig. 2 : Identification of a MD-ledge. The heterointerface is in black dotted line in (a), horizontal white line in (b,c). The MD also limits an ultrathin  $\text{Ni}_3\text{Al}$  crystal. (a) theoretical atom box, (b) simulated image, (c) Excellent agreement between the experimental (white dots) and the theoretical (small black points) positions of the atomic columns. The twin plane is along the double arrow.*

Burgers vector content  $\mathbf{b} = -1/6[112]$ . 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  $\text{Ni}_3\text{Al}$  side with a shift equal to  $\mathbf{b}$ . 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  $\text{Ni}_3\text{Al}$  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  $\text{Ni}_3\text{Al}$  side). When the average direction of the heterointerface deviates substantially from the plane  $(1\ 1\ \bar{1})\text{Ni}_3\text{Al}$ ,  $\Sigma 3$  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  $\mathbf{b}$  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  $\text{Ni}_3\text{Al}/\text{Ni}_3\text{Nb}$  heterointerface can accommodate the 1% length misfit with MD-ledges of various structures, still keeping the same Burgers vector  $\mathbf{b} = -1/6[112]\text{Ni}_3\text{Al}$ . Some MD-ledges limit faults and  $\Sigma 3$  ultrathin twins participate to the interfacial structures.

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