1. INTRODUCTION

A number of transmission electron microscopy observations of interphase boundaries and X-ray experiments in metals and semiconductors have demonstrated the presence of the network of dislocations known as linear singularities. Cherns et al. observed two relations for the Si substrate and NiSi2 epilayer; one of these relations is called A and the other B. The cubic cells are parallel to each other in A type and have a three-fold axis in B type. These authors stated that the tetrahedral coordination of silicon remains unchanged in passing completely from the silicon to silicide structures. Hereinafter, geometry of the hexagonal network will be used in the calculations corresponding to B type.

A number of metals such as copper, aluminium, gold, silver, nickel and their alloys have a face-centred cubic structure. Low angle twist boundaries along the (111) planes of the f.c.c. crystals give rise to regular networks of pure intrinsic screw dislocations aligned with <110> directions. Several authors have investigated the relationship between the geometries of the networks and the Burgers vectors.

In this study, the displacement and stress fields are determined by a classical Fourier series analysis. The two phases are supposed to obey classical Hooke’s law and assumed to be elastically isotropic. The stress fields are derived from the displacement fields via Hooke’s law.

2.1. Notation and Conventions

Figure 1 is a schematic representation of hexagonal network of misfit dislocations at an interface separating a thin layer deposited on a planar semi-infinite medium. The axis Ox2 is perpendicular to the interface, parallel to the plane x1Ox3. Ox′,x′2x′3 is an oblique frame of which axis parallel to and Ox3 axis parallel to period vectors. θ is the angle between the and Ox1 and Ox3 axis. For a regular hexagonal network the period vectors have the same length (a=c) and θ equal to 60 degrees. The orthonormal frame used for the
calculation is $\text{Ox}_1x_2x_3$. h is the thickness of the thin layer. The symbol + and - indicate the medium $x_2 > 0$ and $x_2 < 0$, respectively. These symbols are used in some formulae to represent the medium under consideration.

An vector, referring to a point on the interface plane, is expressed as

$$\vec{R} = \frac{x_1}{a \sin \theta} - \vec{a} + \frac{1}{c} \left( x_3 - \frac{x_1}{\tan \theta} \right) \vec{c}$$

in the orthonormal frame.

The reciprocal lattice which represent the interface, is described by vectors

$$\vec{G} = n\vec{a}^* + m\vec{c}^*$$

where $\vec{a}^*$ and $\vec{c}^*$ are basis vectors of the two-dimensional lattice of the interface plane; n and m take all the integer values.

Since the network of dislocations at interface has a periodic structure, the displacement $u_k$ can be developed in double Fourier series at any point of the two media outside the discontinuity regions:

$$u_k = \sum_{G} U_k(G) \exp(2\pi iG \cdot \vec{R})$$

where the products $\vec{G}, \vec{R}$ are

$$\vec{G}, \vec{R} = G_1x_1 + G_3x_3$$

with

and

Let us denote by $D$, the set of vectors $\vec{G}$ such that for $M > 1; n > 0$ and for $m < 0; n > 1$ and by Re the real part of the displacement expressions:
463
\[\sigma_{22} = 8\mu \Re \left\{ \sum_D [i(GR_1 + GR_3) - 2GR_1(1 - v - \pi G x_2)] \right\} \exp(2\pi Gx_2) \exp(2\pi iG\vec{R})\]

\[\sigma_{33} = 8\mu \Re \left\{ \sum_D [i(GR_3 + 2vGR_2) + iGR_2 x_2 - \pi G x_2 \sum D GR_2] \right\} \exp(2\pi Gx_2) \exp(2\pi iG\vec{R})\]

\[\sigma_{21} = 4\mu \Re \left\{ \sum_D [j(GR_1 + GR_3)] + 2GR_1(1 + 2v + 2\pi G x_2) + GR_1 \right\} \exp(2\pi Gx_2) \exp(2\pi iG\vec{R})\]

\[\sigma_{23} = 4\mu \Re \left\{ \sum_D [j(GR_1 + GR_3)] + 2GR_1(1 + 2v + 2\pi G x_2) + GR_3 \right\} \exp(2\pi Gx_2) \exp(2\pi iG\vec{R})\]

\[\sigma_{13} = 4\mu \Re \left\{ \sum_D [iGR_1 + iGR_3 + 4\pi G_i GR_3 x_2] \exp(2\pi Gx_2) \exp(2\pi iG\vec{R}) \right\}\]

These stress fields are also calculated by Bonnet (1996). The equations (39) and consequently (40) of Ref. 13 have to be replaced by the correct equations (23) and (24) above respectively.

### 2.3 The Relative Interfacial Displacements

To preserve the same atomic structural units along the interface, these units have to be elastically deformed. As a consequence, the relative interfacial displacement \((u^+ - u^-)x_2=0\) varies linearly versus \(x_1\) and \(x_3\) inside each hexagonal pattern. These functions can be expressed as

\[\left[ u^+ - u^- \right]_{x_2=0} = b_k^{(zu)} \frac{x_1}{a} + b_k^{(uv)} \frac{x_3}{c}\]

in the oblique frame and

\[\left[ u^+ - u^- \right]_{x_2=0} = b_k^{(zu)} \frac{x_1}{a} + b_k^{(uv)} \frac{x_3}{c} + \frac{1}{c} (x_3 - x_1 \tan \theta)\]

in the orthonormal frame. \(\vec{b}^{(uv)}\) and \(\vec{b}^{(zu)}\) are the Burgers vectors of the dislocation segments UV and ZU respectively (Fig. 1).

With the chosen origin O, the relative interfacial displacement \((u^+ - u^-)x_2=0\) is an odd function of \(R\). As a result, it can be written in Fourier series form as

\[\left[ u^+ - u^- \right]_{x_2=0} = \sum_D [iT_k^G] \exp(2\pi iG\vec{R})\]

The \(T^G\) components are presented in Ref. 15.

### 3. THE BOUNDARY CONDITIONS AND EXPLICIT SOLUTIONS

The nine unknown complex constants \(P_1, P_2, P_3, Q_1, Q_2, Q_3, R_1, R_2, R_3\) are found from boundary conditions:

I) Along the interface, normal forces are transmitted. Consequently for \(x_2=0\)

\[\sigma_{2j} (j = 1, 2, 3) \text{ are continuous} \]

I.e.

II) Along the free surface there are no applied stresses \(\sigma_{2j}\). Therefore, for \(x_2=h\) \(\sigma_{2j}(j=1,2,3)\) are zero i.e.

\[\left[ \sigma_{2j} \right]_{x_2=h} = 0\]

III) Along the interface, the relative displacement of both crystals is a biperiodic function (periods \(a\) and \(c\)) which varies linearly with \(x_1\) and \(x_3\) inside each hexagonal pattern\(17\) (equation (26)).

### 4. APPLICATIONS

The validity of the analytical formulae have been verified numerically with a Fortran program for pure screw and edge dislocations. The convergencies of
equations (14), (15), (20) and (21) have been studied in copper with pure screw intrinsic dislocations \( (b_s = \frac{1}{2} < 110 >) \); lattice parameter, 0.360 nm), and in NiSi \(_2\)/Si with pure edge intrinsic dislocations \( b_e = \frac{1}{6} < 112 > \); lattice parameter, 0.540 nm), using four different \( h \) thickness.

Figures 2 (a) and (b) illustrate the change in \( U_{11} \) with \( x_2 \) for Cu(111) / Cu and NiSi \(_2\)(111) / Si systems. For both systems (i.e. pure screw and edge dislocations) in the substrate the \( U_{11} \) takes the same values for different \( h \) thickness. But in the epilayer \( U_{11} \) takes various values for different thickness. Although in the substrate these stresses are compressive, in the epilayer they are both compressive and tensile.

Figures 3 (a) and (b) illustrate the change in \( \sigma_{22} \) with the \( x_2 \) for Cu(111) / Cu and NiSi \(_2\)(111) / Si systems. Of course, the values reach zero at the free surface and continuous across the interface for both systems (Cu(111) / Cu and NiSi \(_2\)(111) / Si). For both systems (i.e. pure screw and edge dislocations) in the substrate the \( \sigma_{22} \) are compressive stresses, whereas it is tensile for Cu(111) / Cu system (i.e. pure screw dislocations) in the epilayer. It is also obtained that for \( h < 10 \text{nm} \) it is small compressive for NiSi \(_2\)(111) / Si system (i.e. pure edge dislocations) in the epilayer.
5. CONCLUSIONS

This study considers displacement and stress fields of an epitaxial system which involves hexagonal network of misfit dislocations at the interface. For a two-dimensional periodic network formal solutions the coefficients depend on the boundary conditions have been given. This study also gives explicit solutions for the displacement and stress fields and allows us to take into account the different thickness of the epilayer. The normal stresses along the normal axis Ox_2 strongly depend on the thickness if h is smaller than the period. This is of special interest for imaging techniques in electron microscopy investigations of epitaxial systems.

REFERENCES