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"Geometrical properties of interfaces."

presented by:

G. RADNÓCZI
Research Institute for Technical Physics
Hungarian Academy of Sciences
P.O. Box 76
Foti Ut. 56
H-1325 Budapest
Hungary

LECTURE 2

Geometrical properties of interfaces

György Radnóczi
Research Institute for Technical Physics of the
Hungarian Academy of Sciences
H-1325 Budapest, P. O. Box 76, Hungary
radnoczi@mufi.hu

1. Introduction

Materials properties are strongly influenced or governed by the presence of interfaces in metals (mechanical properties), semiconductors (electronic properties), composites (mechanical properties), metal/semiconductor systems (electronic properties: ohmic, Schottky contacts).
The basis for desired physical properties lays in the change of the crystal structure close to the interface. The simplest way of describing this change is in the terms of lattice parameter changes (compared to the bulk values) in the vicinity of the interface. Stresses and elastic properties play important role in surface reconstruction and thin film multilayer relaxation processes, so their role in the formation of the atomic geometry of internal interfaces can also be accepted. The spatial extension or relaxation of these interfacial stresses, their chemical consequences are dependent on the macroscopic structure of the system considered. According to this, interfaces can be classified as follows (fig. 1.):

a. Internal (bulk) interfaces:	grain boundaries (GB) phase boundaries (PB)
b. Semibulk interfaces	thin film/substrate interfaces surfaces
c. Thin film interfaces	self-supporting thin films multilayers nanograin structure boundaries (about 1 nm grain size)

2. Bulk interfaces

Other names of these interfaces are buried or internal interfaces. A bulk interface is schematically shown in fig 1a. The interface is situated between two bulk material volumes. The strains occurring at the interface can relax in the direction of both interface normal and the lattice parameter can reach its bulk value in both directions. The fraction of atoms belonging to the interface is small. The interface is considered to be atomically flat, ideal, without any defects.

2.1. The macroscopic geometry of GB

Degrees of freedom (DOF) of a grain boundary

A grain boundary (GB) possesses 8 degrees of freedom (DOF). From these 3 are *microscopic*, closely connected with the atomic structure of the GB, and describing the rigid body displacement $\mathbf{T}(T_x,T_y,T_z)$ of the two grains relative to each other. The 5 other DOF are describing the *macroscopic* geometry, the relative position of the two adjacent crystals. Three from the five macroscopic DOF are characterised by a unit length vector $\mathbf{n}_R$ fixing the rotation axis in the co-ordinates of one of the crystals and an angle, ϕ, the angle of relative rotation around $\mathbf{n}_R$, the remaining two defines the GB plane by its unit length normal, $\mathbf{n}_1$ in the same co-ordinate system. The five macroscopic degrees of freedom are very suitable to describe and classify different types of boundaries according to their common geometrical properties.
Three different ways or schemes of descriptions are used, these are equivalent, though explicitly expressing different geometrical parameters of the five macroscopic DOF.

a) Interface plane scheme
b) Misorientation (CSL) scheme
c) Tilt-inclination scheme

Interface plane scheme

This description focuses on the planes of the two crystals, parallel to the GB plane. In this scheme the GB is described according to fig. 2. Two unit length vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ are chosen in the two halves of the crystal (in the same co-ordinate system), and these will determine the normal of the (atomically flat) lattice planes forming the GB in both of the grains. The crystal is cut and the two GB normals $\mathbf{n}_1$ and $\mathbf{n}_2$ are turned parallel (this is a tilt operation). The two crystals are joined again in a plane, the GB, normal to the co-linear vectors $\mathbf{n}_1$ and $\mathbf{n}_2$. An additional rotation to an

angle (θ) around $\mathbf{n}_1$ of the first crystal will describe the twist of grain2 relative to grain1. In this way both tilt and twist GBs can be described by the same formalism (fig. 3.). The five macroscopic DOF (a *general or asymmetrical twist* GB) can be specified in the form (fig. 4.):

$$\mathrm{DOF}=(\mathbf{n}_1,\mathbf{n}_2,\theta) = 5 \qquad (1)$$

The corresponding rotation operation can be denoted as $\mathbf{R}(\mathbf{n}_1, \theta)$, the corresponding tilt operation can be denoted by the operation $\mathbf{R}(\mathbf{n}_T,\Psi)$, where:

$$\vec{n}_T = \frac{\vec{n}_1 \times \vec{n}_2}{\sin\psi}, \quad \sin\psi = \left|\left[\vec{n}_1 x \vec{n}_2\right]\right| \qquad (2)$$

If $\theta = 0$ or 180° , the GB is a pure *asymmetric tilt* GB (fig. 4b.), and the remaining number of DOF will be 4.

$$\mathrm{DOF}=((\mathbf{n}_1,\mathbf{n}_2,0) = 4 \qquad (3)$$

An interface is called symmetrical, when the vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ linearly related, i.e.

$$\mathbf{n}_2 = C\mathbf{n}_1 \qquad (4)$$

where C is constant.
In addition, in cubic crystals the linear relation between two vectors can be written in a more generalised form because of symmetry reasons for a set of h,k,l coordinates:

$$[h_1,k_1,l_1]=C<\pm h_2,\pm k_2,\pm l_2> \qquad (4a)$$

for example: $\mathbf{n}_1$=[3,2,1] and $\mathbf{n}_2$=[-1,2,3] denote crystallographically equivalent planes.
So, a symmetrical twist boundary (fig. 4c.) is a pure twist boundary since has obviously no tilt component since $[\mathbf{n}_1 x \mathbf{n}_2]=0$. The number of DOF:

$$\mathrm{DOF}=(\mathbf{n}_1,C\mathbf{n}_1,\theta)=3 \qquad (5)$$

Correspondingly for a symmetrical tilt boundary (fig. 4d.):

$$\mathrm{DOF}=(\mathbf{n}_1,C\mathbf{n}_1,0)=2 \qquad (6)$$

This description defines the symmetrical tilt boundary as a special twist boundary without tilt component since $\mathbf{n}_2 = C\mathbf{n}_1$, but with a twist component of 0 or 180° rotation. This seems to be some kind of contradiction, however, from atomic geometry it is understandable, that symmetrical tilt boundaries separate crystals with identical lattice planes on each side of the boundary, but with a reversed stacking (C=1, θ=180°, C=-1, θ=0°).

For the case of a centrosymmetric crystal this can be easily shown:

$$DOF=(\mathbf{n}_1,-\mathbf{n}_1,0)=(\mathbf{n}_1,\mathbf{n}_1,180°) \qquad (7)$$

Besides of the symmetrical tilt boundary (STGB), the same description (eq. 6.) applies to the stacking fault (SF) and the free surface (FS), which is included here only for generalisation of the description and terminology.
In special cases like symmetrical twin and STGBs the macroscopic operations can be equivalent to microscopic translation of one part of the crystal relative to the other.
The interface plane scheme supposes, that a GB contains atomically flat crystal planes. This is not a general case. If the GB plane differs slightly from an atomic plane, then the GB becomes vicinal (fig. 5). This concept has been known for surfaces already for decades, for GBs it was introduced not very long ago. This will result in the formation of steps and plateaux on the GB plane.

The CSL misorientation scheme

Focuses on the misorientation between the two grains, rather than on the plane of the defect. The CSL scheme requires that a superlattice existed between the two grains (fig. 6). This involves, that this description is applied only to GBs and rarely to other (heterophase) interfaces.
The relative orientation of the two crystals is characterised by the rotation matrix $\mathbf{R}(\mathbf{n}_{CSL},\phi_{CSL})$, and the GB plane is defined by the normal of the lattice planes, parallel to the GB in one of the adjacent crystals $\mathbf{n}_1$. Thus, the DOF can be given as:

$$DOF_{CSL}=(\mathbf{n}_{CSL},\phi_{CSL}, \mathbf{n}_1) = 5 \qquad (8)$$

consequently,

$$\mathbf{n}_2 = \mathbf{R}(\mathbf{n}_{CSL},\phi_{CSL})\, \mathbf{n}_1 \qquad (9)$$

In this scheme a pure tilt boundary is defined by the condition $(\mathbf{n}_{CSL},\mathbf{n}_1) = 0$ and a pure twist GB is defined by $[\mathbf{n}_{CSL} \times \mathbf{n}_1]=0$. The tilt and twist components can also be separated in the rotation matrix, and we can write:

$$\mathbf{R}(\mathbf{n}_{CSL},\phi_{CSL})= \mathbf{R}(\mathbf{n}_1,\theta)\mathbf{R}(\mathbf{n}_T,\psi) \qquad (10)$$

where $\mathbf{R}(\mathbf{n}_1,\theta)$ is the twist component and $\mathbf{R}(\mathbf{n}_T,\psi)$ the tilt component. The order of the operations is not interchangeable. As we saw in the interface plane scheme, the twist component does not change the interface plane, so eq. 10. becomes:

$$\mathbf{n}_2= \mathbf{R}(\mathbf{n}_{CSL},\phi_{CSL})\mathbf{n}_1=\mathbf{R}(\mathbf{n}_T,\psi)\mathbf{n}_1 \qquad (11)$$

From here we can see, that that the planes parallel to a GB are fully determined by its tilt component and vice versa, the tilt component of a GB is completely determined by the planes, parallel to it.
The CSL concept also allows deviations from the exact CSL orientations. Analogously to the small angle GB and vicinal interfaces, deviations by small tilt or twist misorientations can be compensated by edge or screw dislocation networks, respectively, located in the interface. Deviations of the GB plane from its atomic plane can be compensated by steps of the GB plane. The angle of deviation (δ) from a CSL misorientation (tilt or twist) can be written in the form:

$$\delta=b/D$$

where: b is the length of Burgers vectors in the GB,
D is the distance between dislocations

D can not be shorter then the periodicity in the GB, which defines a maximum deviation for each CSL orientation separately. This can be approximated by the formula $\delta(max)= \delta_0/(\Sigma)^{1/2}$, where $\delta_0=15^\circ$ is limiting angle of small angle GB(fig. 6.).

The tilt-inclination scheme

This scheme uses the concept of the inclination of the GB plane. This results in a selection of the macroscopic DOF that resembles an experimental situation, in which the tilt misorientation between the two crystals is fixed, while the GB plane can chose an inclination, leading to a low energy GB (e.g. in growing bicrystals from two seeds). Since in this scheme we want to determine the GB plane, we can start from the interface plane scheme, where the two vectors $\mathbf{n}_1$ and $\mathbf{n}_2$ completely define

the tilt component of a GB and the GB plane (this required 4 DOF). So, defining the parameters $\mathbf{n}_T$ and ϕ, which means 3 DOF, one more DOF is needed to fix the GB plane. For this purpose in this scheme an additional angle α is used. This parameter is called the inclination angle. As a consequence, the five DOF in the tilt inclination scheme is given by:

$$DOF=(\mathbf{n}_T,\phi,\alpha,\theta) = 5 \qquad (12)$$

The geometrical meaning of this scheme and the inclination angle α is illustrated in fig. 7.
According to the DOF in this scheme, a symmetrical tilt GB (STGB) is represented by $\mathbf{n}_T,\psi$ (eq. 2.), $\alpha=0$ or 90° (for a cubic crystal), and $\theta=0$. For an asymmetric tilt GB α can be any angle and $\theta=0$. For a general GB also $\theta\neq0$. A symmetrical twist GB is characterised by $\mathbf{n}_T,\psi$, $\alpha=0$ or 90° (for a cubic crystal), and $\theta\neq0$.

2.2 The atomic geometry of GB.

Both sides of a crystalline interface contains stacks of well defined lattice planes (by $\mathbf{n}_1$,$\mathbf{n}_2$). The crystal lattice can be considered to be built from primitive (one atom) unit cells (Bravais lattice) In this case each atom position can be written in the form of linear combination of the basic vectors of the Bravais unit cell.
According to the interface plane scheme a crystallographic plane is parallel to the interface, and the Bravais cell can be selected in such a way, that two of its vectors were co-planar with this plane. Then the third vector will point to the closest atom of the next plane parallel to the GB, defining by this the staggering of the atomic planes, parallel to the interface.
The projection of this third Bravais vector onto the GB normal $\mathbf{n}_1$, will define the interplanar spacing parallel to the interface. Since all such cells are primitive, for all possible selections of the Bravais cell, the volume of the cell will be the same, and identical to the atomic volume of the crystal. As the parallel planes are staggered, the stacking period P(hkl) (like ABCABC for FCC crystals, P(111)=3) can be defined according to the eq.:

$$c_{GB}P(hkl)=xa+yb, \quad \textbf{or} \quad P(hkl)=\delta(h^2+k^2+l^2)$$

where: c_{GB} is the projection of the third (out of the GB plane vector of the Bravais cell on the plane of the GB,
a and b are the lengths of the in-GB plane Bravais vectors,
x and y are integers.
δ = 1 or 2

From the above considerations for the Bravais lattices follows, that

$$A(hkl)d(hkl)=\Omega=\text{const},$$

A(hkl) being the size of the planar unit cell in the GB plane

GBs with macroscopic DOF=$(\boldsymbol{n}_1, C\boldsymbol{n}_1, 0)=2$

These GB are the symmetrical tilt GBs (STGB), the stacking faults (SF) and free surfaces (FS).
An important feature is, that all these interfaces have identical planar unit cells (dimension and area) and this unit cell is identical to the projection of the unit cell of the perfect crystal on the same plane. The difference between the SF and STGB on the same plane is only in their stacking sequence, the STGB has an inverted sequence relative to the SF. For SF C=1, for STGB C= -1, i.e. the atomic planes making up the interface have the same atomic arrangement and (h,k,l) (Fig. 8). On this basis one can expect their physical properties to be also similar. Nevertheless, STGB are treated as large angle grain boundaries between two crystals, and SF are treated as planar defects in a single crystal. According to their classification on the basis of the DOFs, and their atomic geometry this notation is not quite correct, and it would be more natural to refer to STGB as inverted SF which would just mean the broadening of the definition of the SF (not only rigid body translations but also inversion of the stacking sequence). On the other hand, STGB are very sensitive to the translations in their plane in terms of their energy. This is the reason of the deep energy cusp of the symmetrical GBs, when the STGB orientation ($\theta=180^\circ$) is approached (fig. 9.).
The similarity between STGB and free surfaces (FS) is not so straightforward. Besides of the identical number of DOF, cleaving along a STGB can reveal some of the geometrical consequences in the atomic arrangement. Since the planar unit cells are the same, upon cleaving two identical surfaces are created. Edge dislocations in the STGB will be converted to steps in the surfaces. Revealing closer relationships in these transformations can bring us closer to the understanding of the mechanism of cleavage for example.
The atomic geometry of a STGB can not be understood without considering the atomic arrangements obtained after inversion. The inversion of the two halves of the crystal can be carried out in different ways, resulting in structures of different atomic arrangements and stability. Fig. 10. shows the possible inversion geometry in a system consisting of five fold stacking. When the GB plane is a mirror plane but not an atomic plane the STGB is

called unstable, because atomic positions are located on the top of each other, resulting in an increase of the interplanar spacing between the two adjacent planes. This instability can be removed by a translation, bringing the GB into the position of an atomic plane, either simultaneously being the mirror plane as well, or not (Fig. 10b and c). The configuration fig. 10b. is called special twin, in the threefold stacking system (e.g. FCC, its common name is coherent twin), the one showed in fig. 10c. is called general twin, while all three configurations are coherent.
From the atomic arrangements of fig. 10. it is also clear, that at least threefold stacking is necessary to create a STGB configuration. STGB operation on onefold or twofold stacking will lead to a single crystal, no interface.
As far as an STGB has DOF=2, in the tilt inclination scheme it is determined (eq.12) by three, but not independent, parameters:

$$DOF=(\mathbf{n}_T,\psi)=2 \qquad (13)$$

The apparent contradiction is even more emphasised, when on the basis of eq. 6, in the interface plane scheme description we see, that no tilt axis can be really prescribed to this boundary, since the surface normals are parallel vectors. This apparent contradiction can be resolved, when the symmetry of the crystal is also considered, and the really parallel planes are replaced by their equivalent. In a cubic crystal e.g. 90^0 rotations around <100> type directions bring the crystal into coincidence with itself, so a change from $\mathbf{n}_1(h,k,l)$ to $\mathbf{n}_1(h,k,-l)$ will not change the GB geometry, but removes the apparent lack of the tilt axis. This also shows, that the three parameters in eq. 13. are not uniquely defined and a finite number of tilt axes and angles exist describing the same $\mathbf{R}(\mathbf{n}_T,\psi)$ operation.

Relation between miller indices of the crystallographic planes of the STGB and geometrical parameters

The parameters in eq. 13. can be written through and are determined by the Miller indices h, k, l of the STGB plane:

$$\vec{n}_T=(h^2+k^2)^{-1/2}\begin{pmatrix}-k\\ h\\ 0\end{pmatrix}$$

$$\sin\psi=\frac{2l(h^2+k^2)}{h^2+k^2+l^2} \qquad (14)$$

Other geometrical features can be expressed through the Miller indices of the GB plane in the following manner:

$$\Sigma = \beta P(hkl), \quad (15)$$

where β=0.5 or 1 for odd and even P(hkl), respectively.

$$\Sigma = \beta'' a^2 [d(hkl)]^{-2}$$

where β''= 1, 0.5, 0.25 or 0.125 (Σ must be odd)

Where a is the size of the unit cell of the crystal, d is the spacing of (hkl) lattice planes.

The number of planes in the repeat stacking sequence P(hkl) for FCC and BCC lattices are shown in table 1.
The geometrical consequences, which may be drawn from the above considerations can be summarised as follows:

1) All symmetrical boundaries can be characterised by DOF=($\mathbf{n}_1$,$\mathbf{n}_2$,θ), with linearly related $\mathbf{n}_1$, and $\mathbf{n}_2$, where the tilt boundaries belong to the value of θ=180°. In cubic Bravais lattices $\mathbf{n}_1$, and $\mathbf{n}_2$ can be written in the form to formally display a tilt axis in the case of θ=180° by using symmetrically equivalent but not linearly related h,k,l indices for $\mathbf{n}_1$, and $\mathbf{n}_2$.

2) The properties of the STGB are the following:

-They represent a special subset of twist boundaries

-they represent GBs with the smallest planar unit cell dimension, equal to those of a perfect crystal. This gives rise to the deep energy cusp and special properties of these boundaries.

-The geometry of the tilt boundaries can be expressed through the Miller indices of the GB plane (eq. 14.).

- The value of Σ is governed by the number of planes in the repeat stacking sequence of the planes parallel to the GB, therefore by their Miller indices.

- For a nontrivial (not equivalent to the single crystal) STGB at least three planes are required in the repeat stacking sequence of the GB plane.

Atomic geometry of asymmetrical GBs

Asymmetrical GBs are those, for which $\mathbf{n}_1$ and $\mathbf{n}_2$ are not linearly related i.e. the lattice planes parallel to the GB on the two sides of the GB are

different (fig. 4). The asymmetrical tilt GB (ATGB) are a subset of general (asymmetrical twist GB) boundaries, and to each tilt axis belongs two ATGB, at 0^0 and 180^0 of twist angle. Generally, an asymmetrical GB must be formed by two sets of lattice planes, each with more than two planes in the stacking period for the two configurations to be different, according to the removal of the difference by an in plane translation for P(hkl)=1 or 2 stacking periods as discussed for STGBs above (fig. 10).

Coherency, incoherence

An interface is called coherent, when atom by atom matching is perfect (fig. 11) in the interface. This also means, that no dislocations are allowed, and atom planes and lines are continuos across the boundary. If this condition is not fulfilled even locally, the interface is called incoherent. Coherent interfaces usually form in heterophase interfaces, when the misfit, $\varepsilon=(a_B-a_A)/a_A$ is small, and can be compensated by the elastic strain of the lattices. This strain can result in the relative tilt of the two lattices (fig. 12.). An incoherent interface is called semicoherent, when coherent areas are separated by defects like misfit dislocations. These dislocations in contrast to the regular lattice dislocations are an inherent part of the atomic geometry of the GB.

Commensurability

In a *commensurate* interface the atoms are arranged on both sides of the interface in a long range order parallel to the interface, and a *common planar unit cell* exists, which describes this long range ordered (crystalline) structure. If the structure is nonperiodic, the interface is usually referred to as incommensurate (fig.13.). The mathematical formulation of the condition of commensurability can be given on the basis of the Bravais lattices of the two crystals, forming the interface, and their projection onto the interface. Let us characterise these projections by unit cell vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ as well as $\mathbf{b}_1$ and $\mathbf{b}_2$ respectively for the two adjacent crystals. The unit cell vectors of the common superlattice $\mathbf{c}_1$ and $\mathbf{c}_2$ must exist and be defined.
The condition of existence of such a superlattice is, that infinitely many points exist, for which:

$$n_1 \vec{a}_1 + n_2 \vec{a}_2 = m_1 \vec{b}_1 + m_2 \vec{b}_2 \qquad (16)$$

with n_i and m_i integers.

A commensurate interface is coherent only, when all the points of the two Bravais lattices, **a** and **b** belong to the superlattice **c.** Otherwise the interface is incoherent.
An interface can also be commensurate if n_i and m_i are irrational, but a rotation of one unit cell relative to the other is allowed.
This can be written in the form:

$$nA=mB=|[\mathbf{c}_1 x\, \mathbf{c}_2]|, \qquad (17)$$

where: $A=|[\mathbf{a}_1 x\, \mathbf{a}_2]|$ and $B=|[\mathbf{b}_1 x\, \mathbf{b}_2]|$,
n and m are positive integers.

From this also follows, that $\mathbf{c}_1$ and $\mathbf{c}_2$ are not parallel.

Vicinal and spatial interfaces.

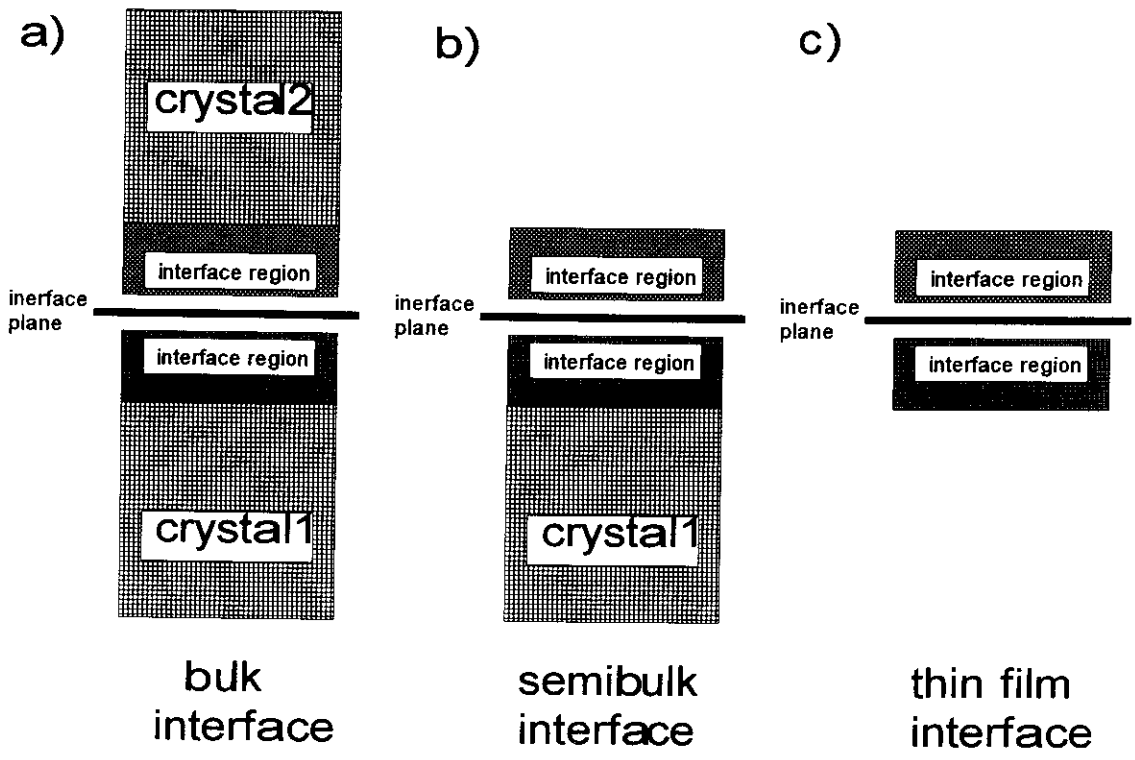
For surfaces the terminology is used for almost a century, and a surface is called spatial when it is atomically smooth, and its surface normal **n** is a low index crystallographic direction. The surface energy has a cusp at this orientation, and any deviation from this special surface will result in a stepped surface, consisting from spatial terraces and steps of usually monoatomic height.
The same terminology can be extended to the interfaces in a little more generalised form.
An interface will be called spatial, when the orientation of its plane corresponds to a (low index) crystallographic plane. Mistilting relative to this low index GB plane one or both of the crystals will lead to inserting steps into the interface. In addition, the symmetrical and asymmetrical low angle twist GBs can be considered as vicinal to the corresponding tilt boundaries.
The symmetrical low angle twist boundary can be considered as a vicinal to the perfect crystal. The disorientation is taken by inserting screw dislocations into the interface, which similarly to the steps on vicinal surfaces preserve areas of perfect interface between themselves. The planar unit cell area increases by inserting the dislocations. According to Frank's formula the spacing between these dislocations D is:

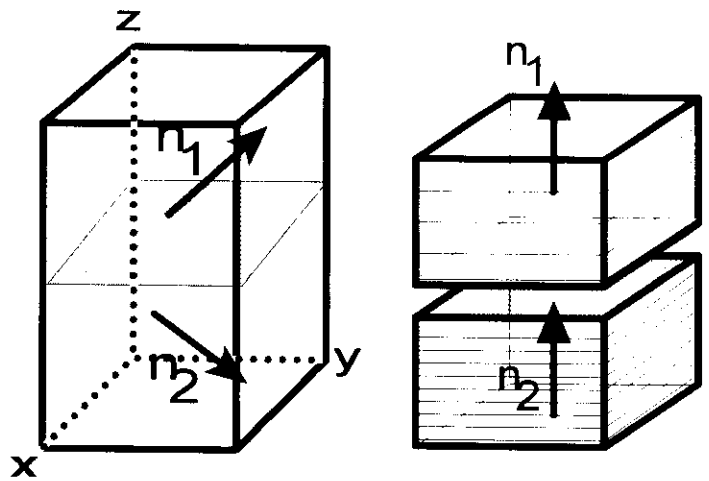
$$D = \frac{b}{2\sin(\theta/2)} \approx \frac{b}{\theta} \qquad (17)$$

where b is the length of the Burgers vector.

As long as the linearization in this equation is valid we can talk about low angle GBs (up to 15°), otherwise the GB is called a high angle one.

Fig.1.


a)
b)
c)
crystal2
interface region
inerface plane
interface region
crystal1
interface region
inerface plane
interface region
crystal1
interface region
inerface plane
interface region
bulk interface
semibulk interface
thin film interface


z
n_1
n_2
y
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n_1
n_2

Fig. 2

Fig. 2

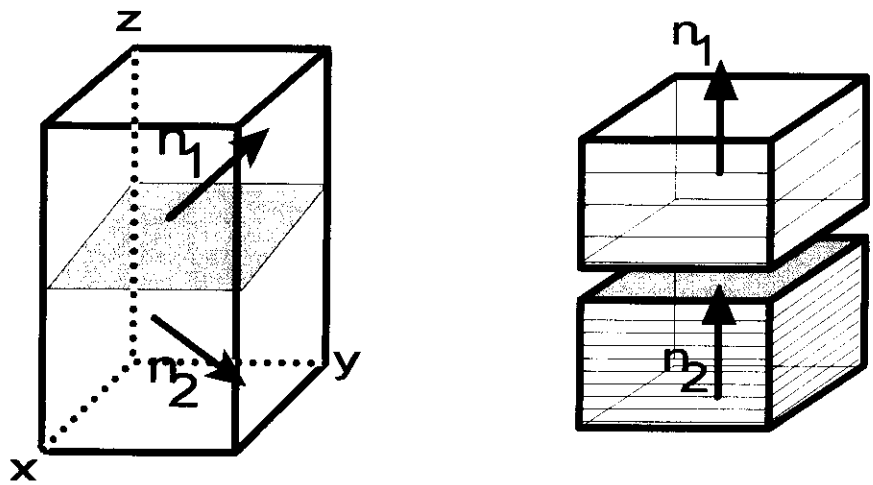


Fig. 3

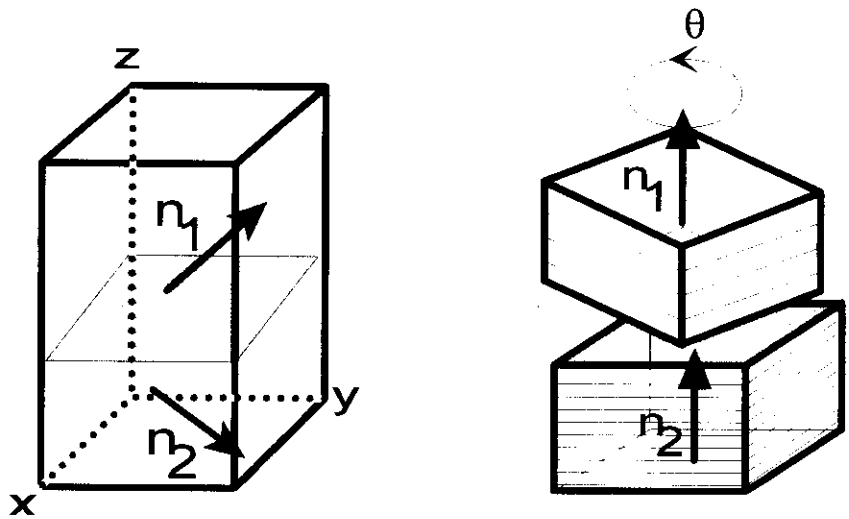
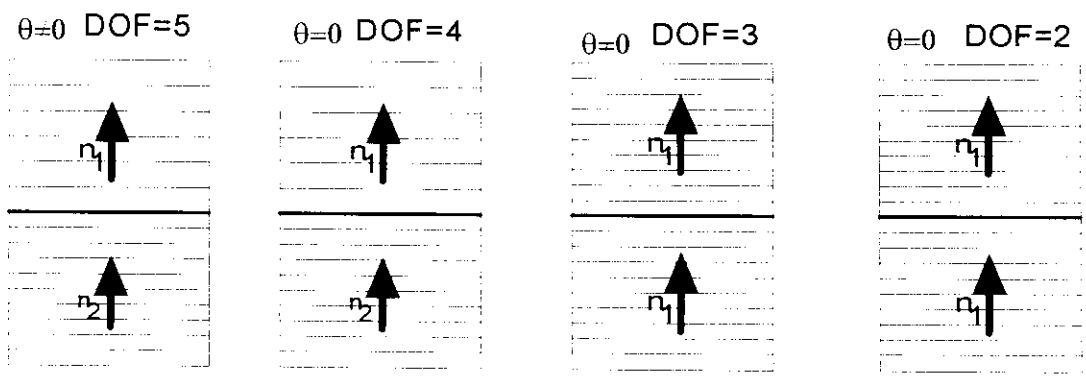


Fig. 4.



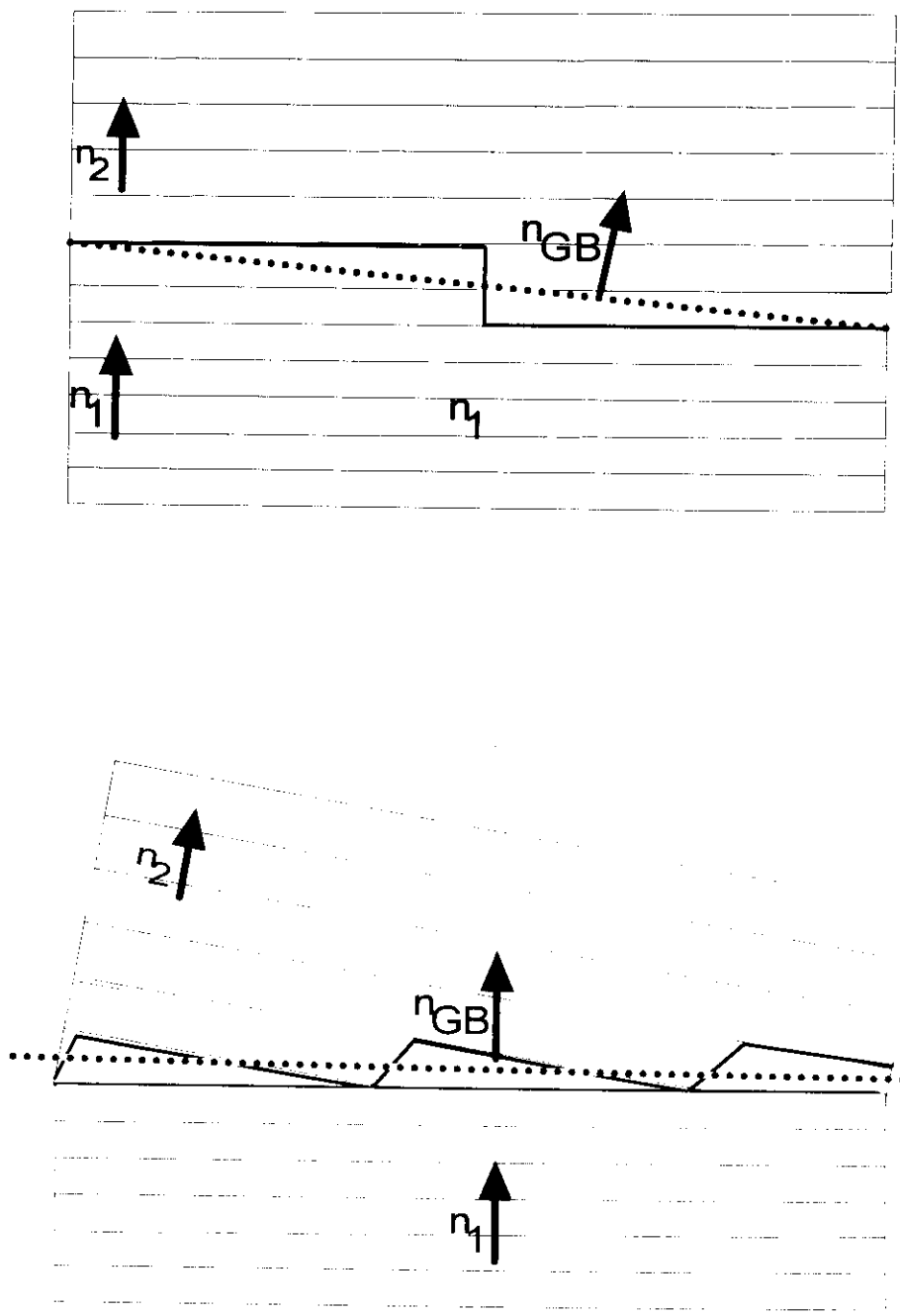
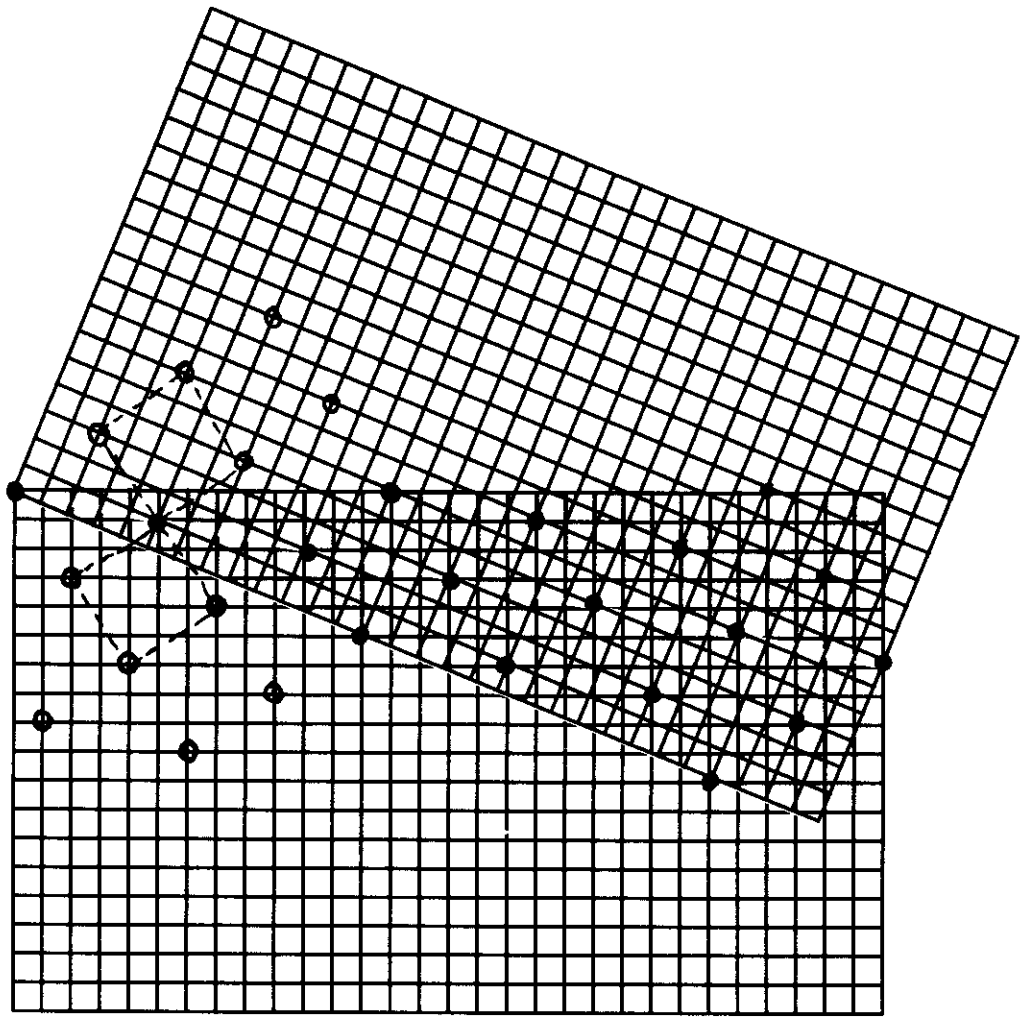


Fig. 5.



$$\Sigma = \frac{\text{number of all atoms}}{\text{number of coincident atoms}} = 13$$

$$\vec{n}_{CSL} = [001] \qquad \phi_{CSL} = 22{,}62^\circ$$

Fig. 6

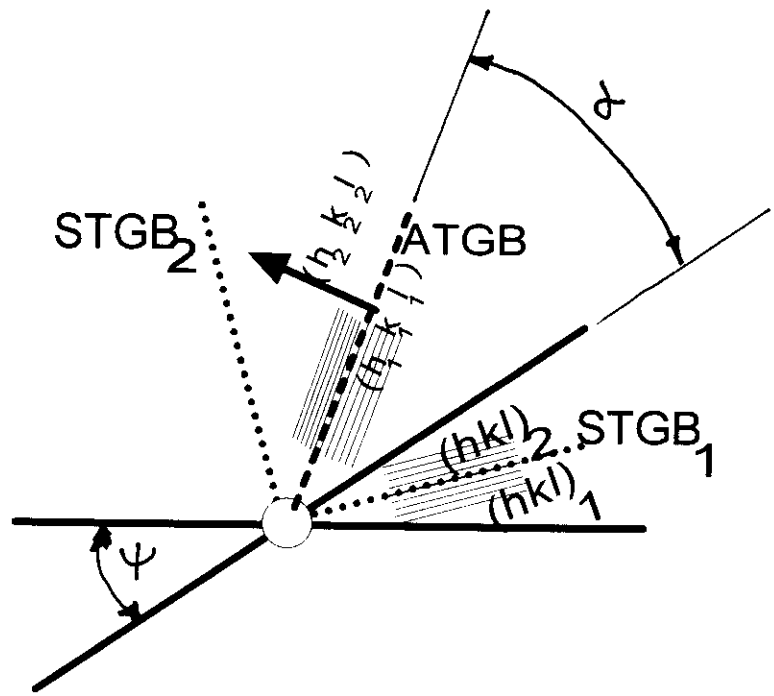
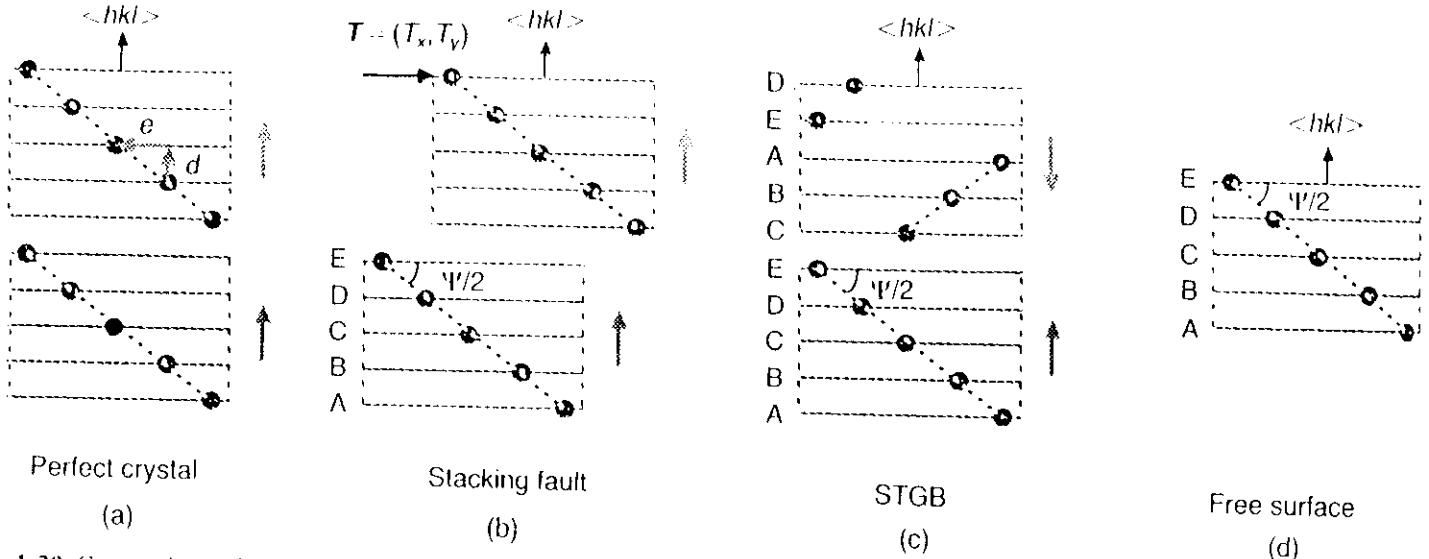
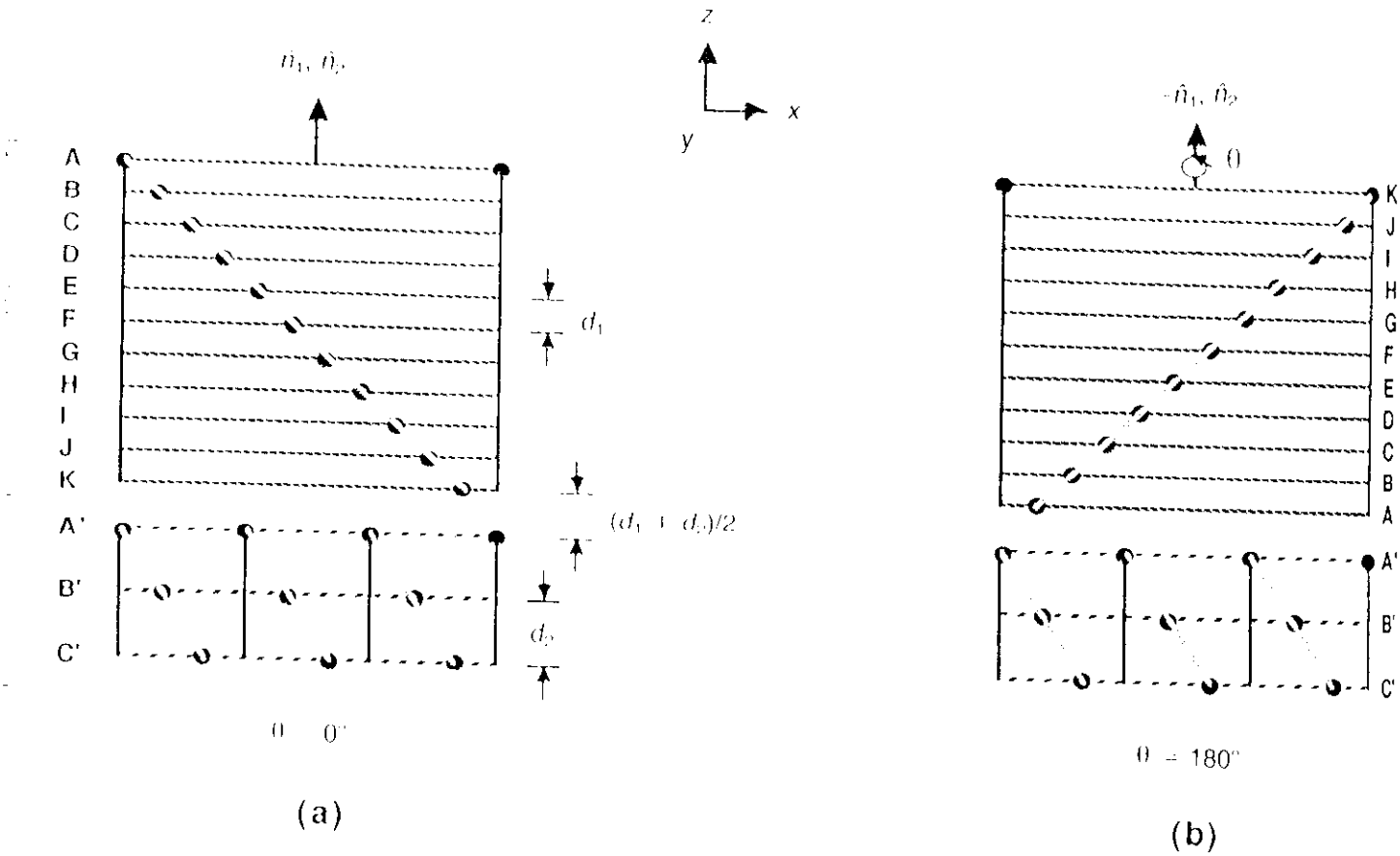


Fig. 7.



. 1.30 Comparison of the atomic-level geometry of the simplest three interface systems in (b)–(d) with a perfect crystal in (a) (see Fig. 1.1). Most importantly, the four systems sketched here have identical planar unit-cell dimensions and areas; this unit cell is the llest possible for any atom arrangement involving this particular lattice plane, with a $\langle hkl \rangle$ normal. The shaded arrows indicate the ction of planar stacking. We note that Figs. 1.17 and 1.30 may be directly superimposed, illustrating the considerable similarity ong these three systems and with the perfect crystal.



1.33 Two **asymmetrical-tilt** configurations, with identical unit-cell dimensions but inverted stacking sequences in one with respect ie other, are obtained for $\theta = 0°$ and 180°, respectively. In the case shown, the upper crystal was inverted (i.e. turned upside down) he twist rotation. Since only a **relative** rotation of the two halves is involved, the same ATGB configuration in (b) would have been ined had the lower semicrystal been inverted (provided the crystal lattices have inversion symmetry). $d_\alpha = d(\hat{n}_\alpha)$ and $P\alpha = P(\hat{n}_\alpha)$ 1, 2) denote, respectively, the interplanar lattice spacings and stacking periods in the two halves. To preserve the perfect-crystal sity, the effective interplanar spacing at the interface is given by the arithmetic average, $d_{eff} = (d_1 + d_2)/2$.

Fig. 8. from [2]

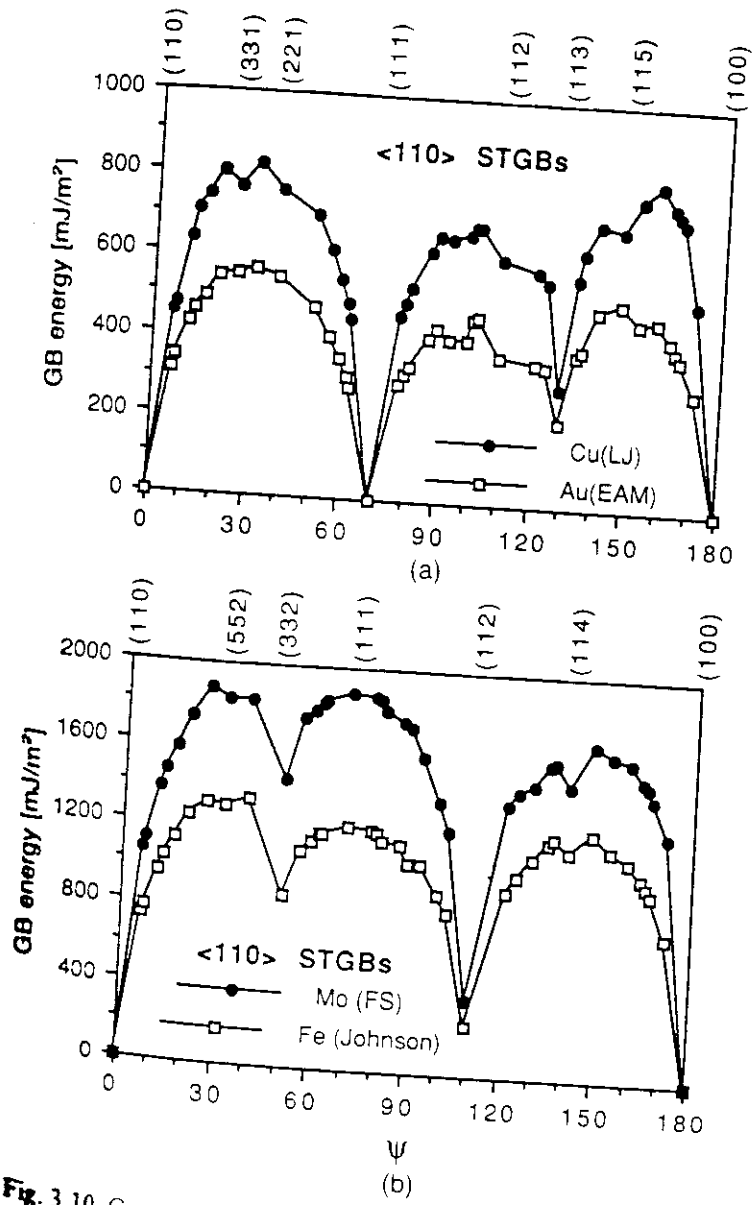


Fig. 3.10 Comparison of the energies (in mJ/m^2) of symmetrical $\langle 011 \rangle$ tilt boundaries in the fcc lattice [81] (a) with those in the bcc lattice [82] (b) obtained by means of both potentials ~~in each~~

Fig. 9

from [2]

Fig. 10
from [2]

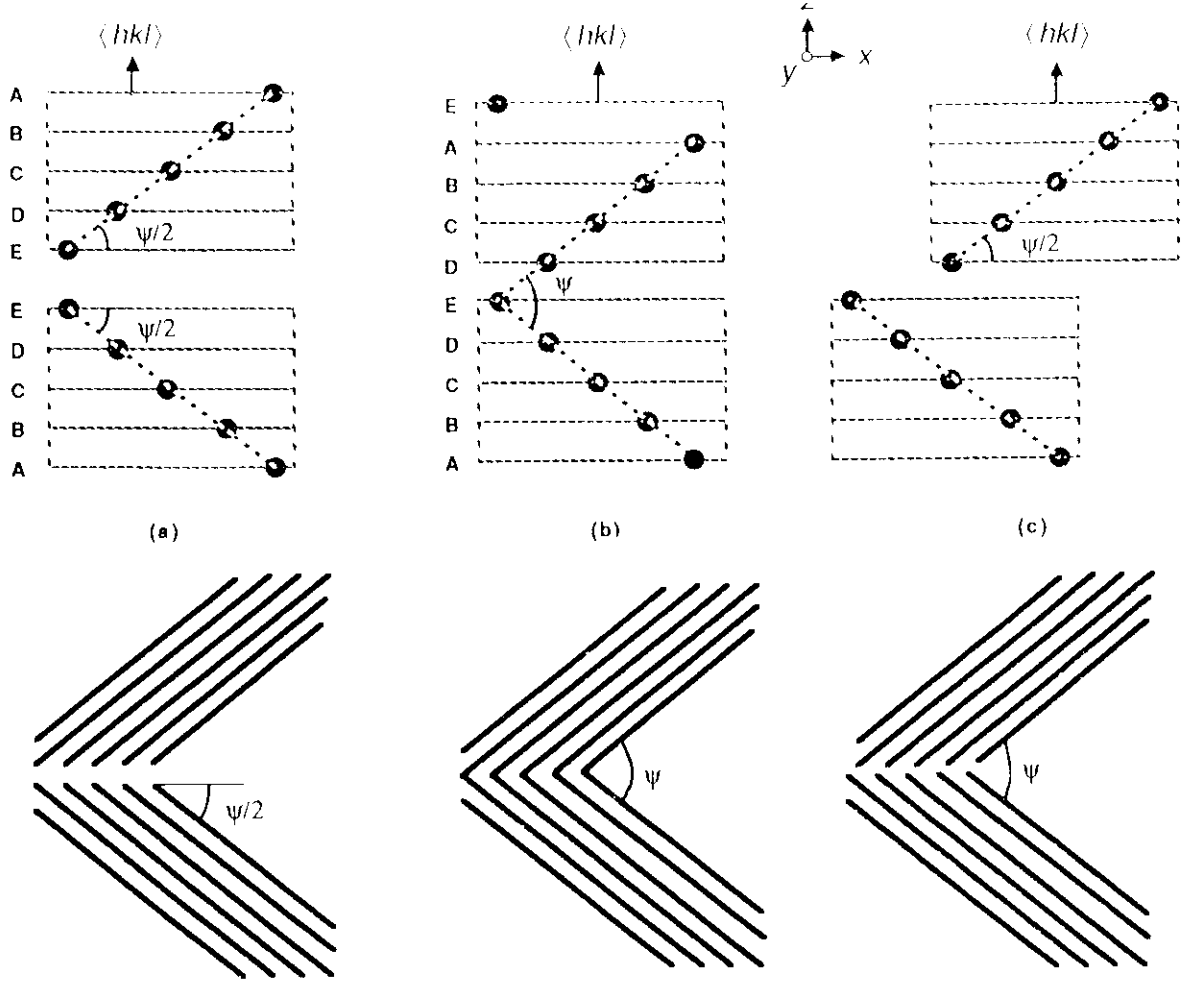


Fig. 1.38 Definition of three well-characterized translational states of an STGB. (a) Directly inverted (and usually unstable) configuration of Fig. 1.36(b) in which two identical (*hkl*) planes face each other across the interface. Notice that in this configuration the GB-plane is a twinning plane, but not an atom plane. (b) In the 'special' twin, the GB is both the twinning and an atom plane. (c) In most cases, an STGB exhibits some rather arbitrary rigid-body translation, referred to as a general twin, emphasizing the fact that its planar structure is still characterized by the inversion at the GB ('twin') but that no special rigid-body translation exists.

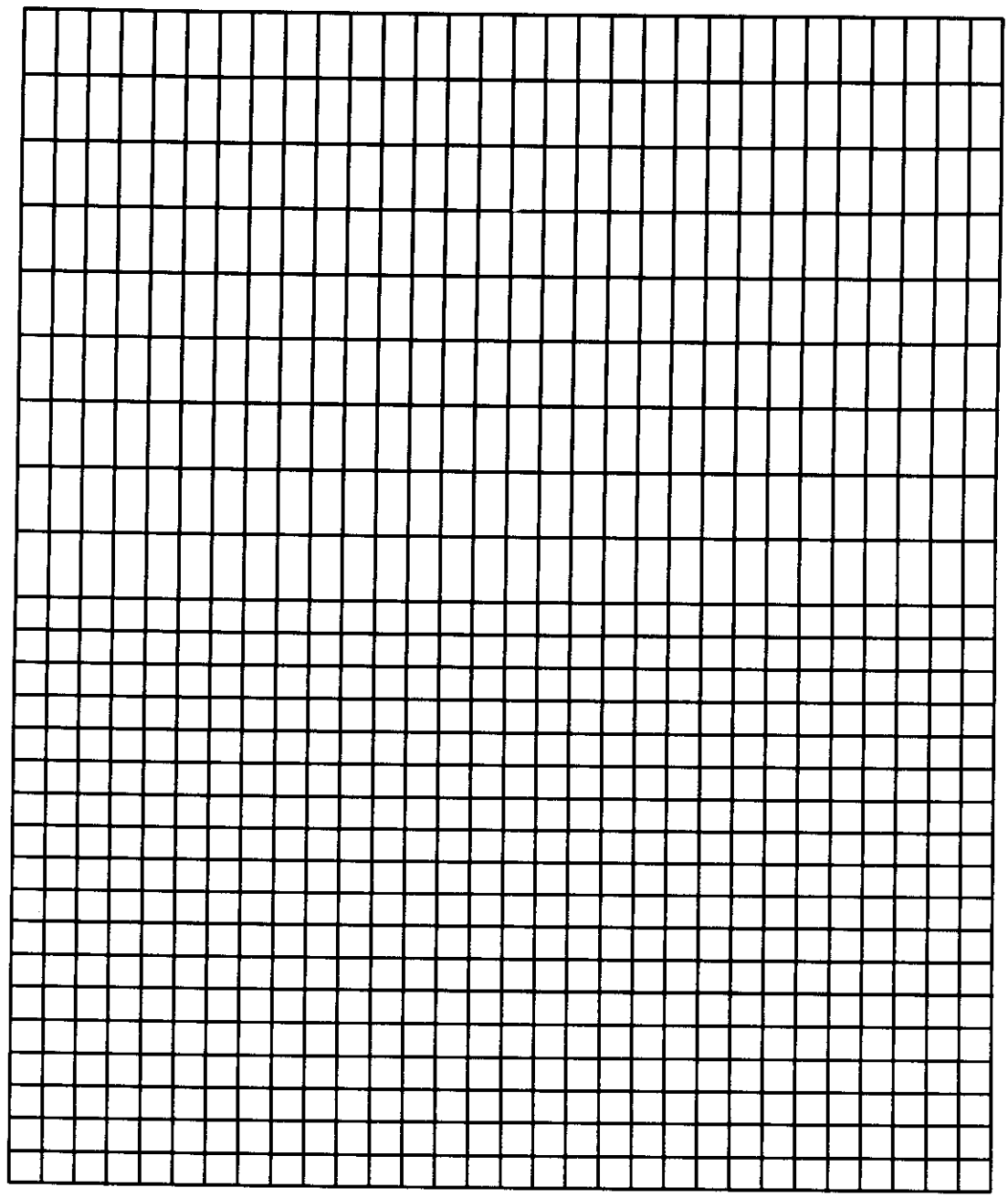


Fig. 11.

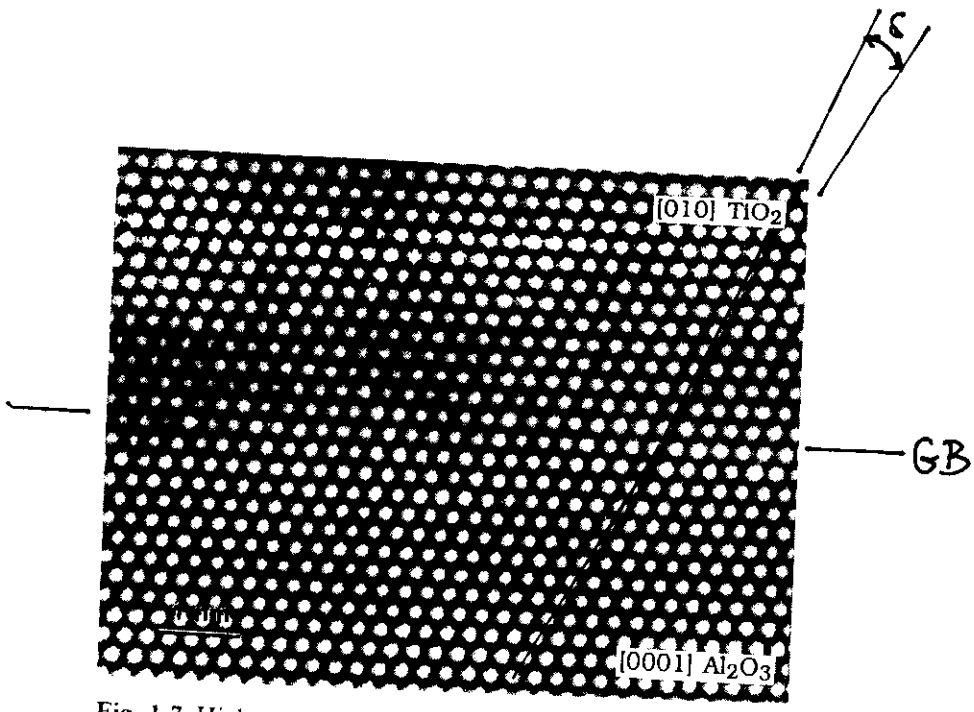


Fig. 1.7 High-resolution transmission-electron micrograph of a perfectly coherent epitaxial interface (dashed line) formed between a thin film of TiO_2 and an Al_2O_3 substrate. Notice the small change in the 'tilt' angle across the interface, resulting from a virtually sudden change at the interface of the lattice parameter in the direction of the interface normal [11] (Courtesy of K. L. Merkle).

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Fig. 12

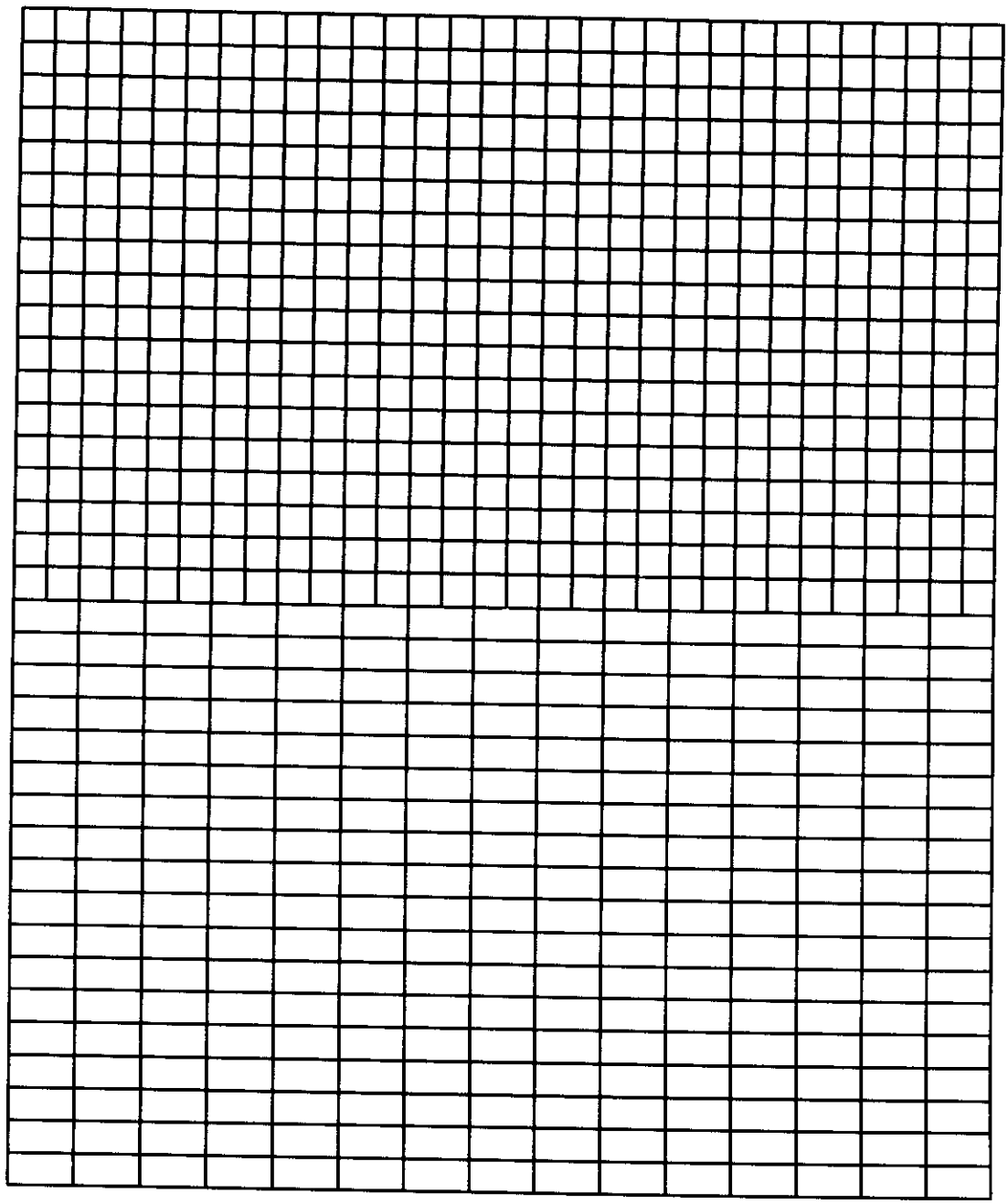

Fig 13a

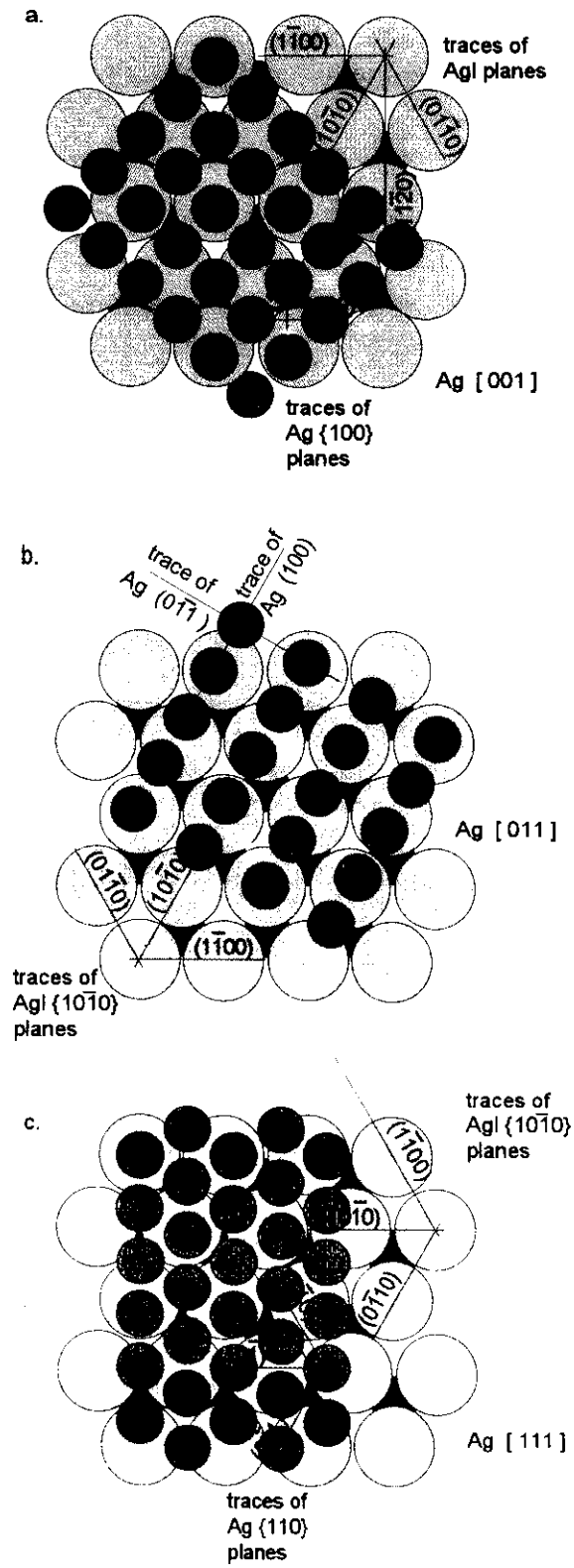

Fig. 13b incommensurate IF

Table 3.2 Interplanar spacing, $d(hkl)$ (in units of the lattice parameter a), for the 11 most widely spaced planes in the fcc and bcc lattices. These planes also correspond to the ones with the highest planar density of atoms, i.e. the smallest planar repeat unit cells. Also listed is the number of planes in the repeat planar stacking unit, referred to as the 'period', $P(hkl)$ (see also Chapter 1 of this volume)

	fcc			bcc		
No.	(hkl)	$d(hkl)/a$	$P(hkl)$	(hkl)	$d(hkl)/a$	$P(hkl)$
1.	(111)	0.5774	3	(110)	0.7071	2
2.	(100)	0.5000	2	(100)	0.5000	2
3.	(110)	0.3535	2	(112)	0.4082	6
4.	(113)	0.3015	11	(310)	0.3162	10
5.	(331)	0.2294	38	(111)	0.2887	3
6.	(210)	0.2236	10	(321)	0.2673	14
7.	(112)	0.2041	6	(114)	0.2357	18
8.	(115)	0.1925	27	(210)	0.2236	10
9.	(513)	0.1690	35	(332)	0.2132	22
10.	(221)	0.1667	18	(510)	0.1961	26
11.	(310)	0.1581	10	(341)	0.1961	26

Table 2.
from [2]

FIGURES

Tables

Reading Material:

1. V. Randle: The measurement of GB geometry, Ins. of Phys. Publ. Bristol, 1993.
2. D. Wolf, S. Yip: Materials Interfaces, Chapman& Hall, NY, 1992.