APPENDIX A

CRYSTALLOGRAPHY AND DESCRIPTION OF TEXTURE

Basic Crystallography

Crystallographic directions

A direction in a crystal lattice is represented by a vector $\boldsymbol{j}$ with co-ordinates [UVW] such that

$$\boldsymbol{j} = \mathrm{U}\boldsymbol{a} + \mathrm{V}\boldsymbol{b} + \mathrm{W}\boldsymbol{c} \tag{A1}$$

Where a set of directions in a crystal system are equivalent by symmetry, they may be denoted <UVW>. Hence <100> in the cubic system comprises the directions [100], [010], [001], $[\bar{1}00]$, $[0\bar{1}0]$, $[00\bar{1}]$.

Crystallographic planes

Crystallographic planes are represented by Miller indices (*hkl*), such that the plane intercepts the *x*, *y* and *z* axes at $h/\boldsymbol{a}$, $k/\boldsymbol{b}$ and $l/\boldsymbol{c}$ respectively. A set of planes equivalent by symmetry are denoted by $\{hkl\}$. Hence in the cubic system, the $\{111\}$ planes are (111), $(\bar{1}11)$, $(1\bar{1}1)$ and $(11\bar{1})$.

Epitaxial Relationships

The indices of the substrate interface are denoted by $(hkl)_s$ and those of the film by $(hkl)_f$. Directions in these planes are then represented by $[UVW]_s$ and $[UVW]_f$.

Hence parallel growth of Ni on MgO (shown in figure 4.6) would be represented by
(001) Ni // (001) MgO; [100] Ni // [100] MgO.

Descriptions of Crystallographic Texture

In order to describe the orientation of crystals in a polycrystalline sample, it is necessary first to define a set of co-ordinates. The standard choice in a rolled metallic sheet is that shown in figure A1, with the cartesian *X*, *Y* and *Z* axes coinciding with the tape rolling direction, transverse direction and normal direction respectively. Each crystal also has its own co-ordinate system, fixed with respect to the crystal axes – for cubic crystals, it is appropriate to select the axes (labelled *X*′, *Y*′ and *Z*′) parallel to the cube edge directions. The orientation of a given crystallite with respect to the sample axes may then be described by a rotation g, which transforms the sample co-ordinate system into the crystal co-ordinate system.

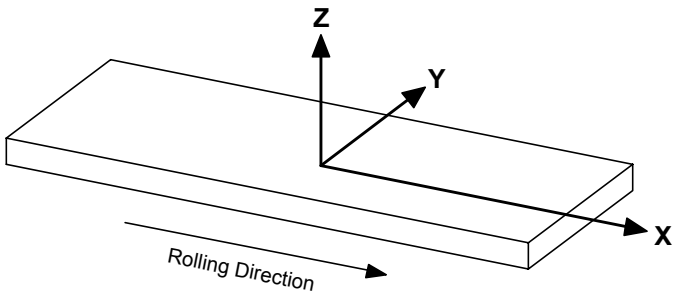

Figure A1 Definitions of the directions X, Y and Z. X is along the rolling direction, Y in the transverse direction and Z parallel to the substrate normal.

There are several equivalent methods of describing a rotation between two co-ordinate systems which will be suitable in describing crystallographic textures :

Euler Angles

Initially the two co-ordinate systems are considered to be coincident, as shown in figure A2(a). To reach their final position, the crystal co-ordinates are rotated by an angle φ_1 about the Z′ axis, then by ϕ about X′ (in its new position) and finally by φ_2 about Z′ in its new orientation. This is demonstrated in figure A2.

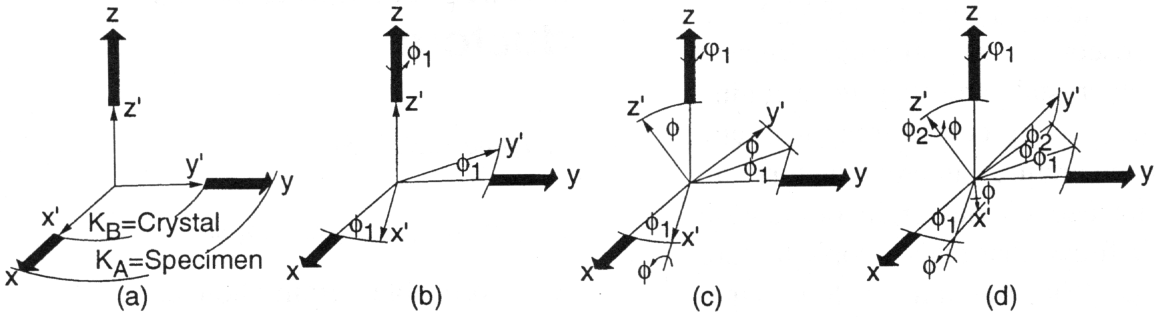

Figure A2 Rotations of the crystal axes by the Euler angles [250].

If these rotations are represented as $g_{\varphi 1}^{(Z')}$, $g_{\Phi}^{(X')}$ and $g_{\varphi 2}^{(Z')}$ respectively, then a product notation may be used to describe the successive rotations :

$$g = g_{\varphi 2}^{(Z')} \cdot g_{\Phi}^{(X')} \cdot g_{\varphi 1}^{(Z')} \tag{A2}$$

Rotation axis and angle

For any two sets of crystal and sample orientations, there will be an axis about which a rotation may be made which will bring the two into coincidence. This rotation is represented by the rotation axis (which may be described using 2 parameters) and the angle of rotation (one further parameter). The rotation axis is often represented by its spherical polar co-ordinates ψ and ϕ, and the rotation angle as ω. Thus

$$g = \{\psi, \phi, \omega\} \tag{A3}$$

The Pole Figure

One may represent orientation by describing a crystal direction in the sample co-ordinates. This is not a complete description however as the angle of rotation about this axis must also be specified, thus it is necessary to examine more than one pole in order to completely assess the crystal orientation.

Note that when an X-Ray pole figure is measured, the distribution of the plane normals is investigated. In general the direction [*hkl*] is not perpendicular to the (*hkl*) plane, and thus for

non-cubic systems, a (*hkl*) pole figure does not necessarily show the distribution of the [*hkl*] crystal directions.

If a plane normal is represented by a vector **r**, with components $\mathbf{r}_x$, $\mathbf{r}_y$ and $\mathbf{r}_z$ in the sample co-ordinate system, then the spherical (pole figure) co-ordinates of the pole are given by :

$$\cos\psi = r_z \tag{A4}$$

$$\sin\phi = \frac{r_y}{\sqrt{(1-r_z{}^2}} \tag{A5}$$

$$\cos\phi = \frac{r_x}{\sqrt{(1-r_z{}^2}} \tag{A6}$$

Miller Indices

Simple orientation relationships may be described using the Miller indices (hkl) and the crystal direction [UVW]. One simply specifies the crystal plane parallel to the plane of the rolled tape and the crystal direction parallel to the rolling direction. Hence the "cube texture" may be described by :

$$\mathsf{g} = (001)\,[100] \tag{A7}$$

Matrix Representation

Any rotation may of course be represented by a matrix. One may use the direction cosines relative to the ND and RD considered above h′, k′, l′ and u′, v′, w′ and those of the TD, r′, s′, t′ to represent **g** as :

$$\mathbf{g} = \begin{bmatrix} u' & r' & h' \\ v' & s' & k' \\ w' & t' & l' \end{bmatrix} \tag{A8}$$

This representation is useful as the result of successive rotations is given by the product of the corresponding matrices. Thus the transformation made by the Euler rotations may be represented by a single matrix :

The three individual rotations are represented by

$$g_{\varphi 1}(Z') = \begin{bmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{A9}$$

$$g_{\phi}(X') = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{bmatrix} \tag{A10}$$

$$g_{\varphi 2}(Z') = \begin{bmatrix} \cos\varphi_2 & \sin\varphi_2 & 0 \\ -\sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{A11}$$

and given that :

$$g(\varphi_1,\phi,\varphi_2) = g(\varphi_2).g(\phi).(g\varphi_1) \tag{A12}$$

$$g(\varphi_1\phi\varphi_2) = \begin{bmatrix} \cos\varphi_1\cos\varphi_2 - \sin\varphi_1\sin\varphi_2\cos\phi & \sin\varphi_1\cos\varphi_2 + \cos\varphi_1\sin\varphi_2\cos\phi & \sin\varphi_2\sin\phi \\ -\cos\varphi_1\sin\varphi_2 - \sin\varphi_1\cos\varphi_2\cos\phi & -\sin\varphi_1\sin\varphi_2 + \cos\varphi_1\cos\varphi_2\cos\phi & \cos\varphi_2\sin\phi \\ \sin\varphi_1\sin\phi & -\cos\varphi_1\sin\phi & \cos\phi \end{bmatrix} \tag{A13}$$

Another useful orientation description, that of a rotation axis and angle may also be represented by a matrix. To do this it is necessary to transform the Z axis into the rotation direction, then perform the required rotation, before carrying out the inverse of the initial transformation.

$$\mathsf{g}\,(\mathbf{d},\omega) = \mathsf{g}^{-1}(Z\rightarrow\mathbf{d}) \cdot \mathsf{g}_{\omega}^{(Z)} \cdot \mathsf{g}(Z\rightarrow\mathbf{d}) \tag{A14}$$

$$g(d,\omega) = \begin{bmatrix} (1-d_1^{\,2})\cos\omega + d_1^{\,2} & d_1d_2(1-\cos\omega) + d_3\sin\omega & d_1d_3(1-\cos\omega) - d_2\sin\omega \\ d_1d_2(1-\cos\omega) - d_3\sin\omega & (1-d_2^{\,2})\cos\omega + d_2^{\,2} & d_2d_3(1-\cos\omega) + d_1\sin\omega \\ d_1d_3(1-\cos\omega) + d_2\sin\omega & d_2d_3(1-\cos\omega) - d_1\sin\omega & (1-d_3^{\,2})\cos\omega + d_3^{\,2} \end{bmatrix} \tag{A15}$$

where

$$d_1 = \sin\psi\,\cos\phi \tag{A16}$$

$$d_2 = \sin\psi\,\sin\phi \tag{A17}$$

$$d_3 = \cos\psi \tag{A18}$$

Considering the trace of the matrix g.

$$Tr[\mathbf{g}] = g_{11} + g_{22} + g_{33} \tag{A19}$$

$$Tr[\mathbf{g}] = d_1^{\,2} + d_2^{\,2} + d_3^{\,2} + \cos\omega(1-d_1^{\,2}+1-d_2^{\,2}+1-d_3^{\,2}) \tag{A20}$$

But as ***d*** is a unit vector,

$$d_1^{\,2} + d_2^{\,2} + d_3^{\,2} = 1 \tag{A21}$$

$$Tr[\mathbf{g}] = 1 + 2\cos\omega \tag{A22}$$

Hence the value of ω is easily deduced from a given rotation matrix. It is this value ω which is used to quantify the "misorientation angle", in this case between the crystal and the sample axes.

Misorientation of two crystallites

If two grains A and B have orientation matrices g_A and g_B respectively, then the rotation from one to the other is described by the matrix g_{AB} such that

$$\mathsf{g}_{AB} = \mathsf{g}_A^{-1}\,\mathsf{g}_B \tag{A23}$$

Indeed as the matrices are derived from orthogonal axes, the matrices are themselves orthogonal, therefore

$$g^{-1}=g^{T} \tag{A24}$$

$$g_{AB} = g_A^{T}\, g_B \tag{A25}$$

Thus we can again calculate the misorientation angle, this time between the two grains, from the trace of the matrix g_{AB}.

Note that the final thing to consider here is that the angle and axis produced from the matrix calculation is one of many which are symmetrically equivalent. For the cubic system, of interest here, there are 24 equivalent forms. Thus the calculation must be carried out for each and the smallest value of the misorientation angle is used.