Transmission and Reflection Coeficients at a Model Grain Boundary

In general, we shall regard a grain boundary (GB) as a two-dimensional surface separating regions of different crystal orientations. If the local curvature of this surface is much larger than the electron de Broglie wavelength, then for the purpose of calculating the transmission of such an electron we can regard the GB as a plane separating two crystals – left (L) and right (R) – rotated in a different way with respect to a coordinate frame, fixed with respect to GB.

Our discussion will be confined to semiconductors like Si and Ge, in which isoenergetic surfaces in the conduction band are ellipsoids of revolution. Consider an electron moving within one such ellipsoid. The electron kinetic energy operator $\hat{H}$ and the velocity operator $\hat{\mathbf{V}}$ are given by

$$\hat{H} = -\frac{\hbar^2}{2m} (M^{-1})_{\alpha\beta}\, \partial^\alpha \partial^\beta \;, \tag{A.1}$$

$$\hat{V}_\alpha = -\frac{i\hbar}{m} (M^{-1})_{\alpha\beta}\, \partial^\beta \;, \tag{A.2}$$

where $\partial^\alpha \equiv \partial/\partial r_\alpha$ and $\mathbf{M}^{-1}$ is the normalized effective mass tensor, which has the form

$$\mathbf{M}^{-1} = \begin{bmatrix} m/m_t & 0 & 0 \\ 0 & m/m_t & 0 \\ 0 & 0 & m/m_l \end{bmatrix}$$

with respect to the principal axes of a chosen ellipsoid, m is the reduced effective mass,

$$m \equiv \frac{3 m_t m_l}{2 m_l + m_t} \;, \tag{A.3}$$

and m_l and m_t are the longitudinal and the transverse effective masses, respectively. With respect to an arbitrary fixed frame, the rotated tensor $\mathbf{M}^{-1}$ is given by

$$\mathbf{M}^{-1} = \begin{bmatrix} a & d & c \\ d & \bar{a} & \bar{c} \\ c & \bar{c} & b \end{bmatrix} \;, \tag{A.4}$$

where

$$a \equiv M_{xx} = 1 + \Delta(3\sin^2\theta\cos^2\phi - 1) \;; \tag{A.5a}$$

$$b \equiv M_{zz} = 1 + \Delta(3\cos^2\theta - 1) \;; \tag{A.5b}$$

$$c \equiv M_{zx} = M_{xz} = (3\Delta/2)\,\sin 2\theta\cos\phi \;; \tag{A.5c}$$

$$d \equiv M_{xy} = M_{yx} = (3\Delta/2)\,\sin^2\theta\cos 2\phi \;; \tag{A.5d}$$

and the quantities $\bar{a}$ and $\bar{c}$ are obtained by the substitution $\phi \rightarrow \bar{\phi} = \pi/2 - \phi$ in the expressions for a and c, respectively. The angles θ and ϕ, specifying the transformation, represent the polar angles of the ellipsoid's axis of rotation relative to the fixed frame and the parameter Δ describes the ellipsoid's excentricity:

$$\Delta \equiv \frac{m_t - m_l}{2m_l + m_t} \ . \tag{A.6}$$

In what follows, the fixed frame will be defined in such a way that its z axis is normal to the GB plane and the zx plane is the plane of electron motion. For an electron moving with a wave vector $\mathbf{q} = (q_x, q_z)$, the kinetic energy $H(\mathbf{q})$ and the normal velocity component $V_z(\mathbf{q})$ are given by

$$H(\mathbf{q}) = -\frac{\hbar^2}{2m} \left(a\, q_x^2 + b\, q_z^2 + 2c\, q_x q_z \right) , \tag{A.7}$$

$$V_z(\mathbf{q}) = -\frac{i\hbar}{m} \left(b\, q_z + c\, q_x \right) . \tag{A.8}$$

Consider an electron moving within an ellipsoid (centered at $\mathbf{k}_i^{(L)}$) whose orientation is characterized by the polar angles $\theta_i^{(L)}$ and $\phi_i^{(L)}$ of its axis of revolution $\mathbf{n}_i^{(L)}$. The electron is incident on the GB with a wave vector $\mathbf{q} = \mathbf{k} - \mathbf{k}_i^{(L)}$, where $\mathbf{k}$ is the electron crystal momentum. In principle, neither the transmitted nor the reflected waves will correspond to a definite ellipsoid. We shall calculate the GB transmission probability under a simplifying assumption that the reflected wave belongs to the same ellipsoid as the incident wave.

The overall transmission coefficient can be written in the following approximate form:

$$T_i(\mathbf{q}) = \sum_{j=1}^{N} \xi(\mathbf{k}_i^{(L)}, \mathbf{k}_j^{(R)})\, t_{ij}(\mathbf{q}\, ;\, \mathbf{n}_i^{(L)}, \mathbf{n}_j^{(R)}) , \tag{A.9}$$

where N is the number of equivalent ellipsoids in the Brillouin zone. In the above expression, the coefficients t_{ij} describe the transmission amplitudes calculated in the ‘‘plane-wave approximation’’, i.e. ignoring the difference in the locations of equivalent minima on both sides of the boundary, while taking account the different orientations $\mathbf{n}_j^{(R)}$ not related by symmetry to $\mathbf{n}_i^{(L)}$. Without a detailed calculation of the band-structure in the presence of a GB it is impossible to estimate the coupling between different valleys, expressed by the coefficients ξ. It is probably a good approximation to assume as we did in (A.9) that $\xi \neq \xi(\mathbf{q})$, i.e. that the entire dependence on the electron wave vector is contained in the coefficients t_{ij} which we shall now proceed to calculate.

Consider first the reflected wave. It is clear that since in general the GB is not a plane of reflection symmetry for the hamiltonian (A.1), plane waves with $\mathbf{q}_1 = (q_x, q_z)$ and with $\mathbf{q}_2 = (q_x, -q_z)$ correspond to different energies. Because of the translational invariance of GB in the x direction, the wave vector of the reflected wave is of the form $\mathbf{q}^{(r)} = (q_x, q_z^{(r)})$, where $q_z^{(r)}$ is determined by the conservation of energy, $H(q_x, q) = H(q_x, q_z^{(r)})$, giving

$$q_z^{(r)} = -q_z - 2\left[c^{(L)}/b^{(L)}\right] q_x \ . \tag{A.10}$$

Elastic reflection occurs at an angle β which does not coincide with the incident angle α (cf. Fig. 1). From eqs. (A.10) and (A.5) one easily finds that

$$\tan\beta = \tan\alpha + \frac{(m_l - m_t)\, \sin 2\theta_i^{(L)}\, \cos\phi_i^{(L)}}{m_l \sin^2\theta_i^{(L)} + m_t \cos^2\theta_i^{(L)}} \ . \tag{A.11}$$

The wave vector of a transmitted wave $\mathbf{q}^{(t)} \equiv (q_x, q_z^{(t)})$ is again determined by the conservation of energy:

$$H^{(L)}(q_x, q) = H^{(R)}(q_x, q_z^{(t)}) \;, \tag{A.12}$$

which reduces to a quadratic equation of the form

$$[q_z^{(t)}]^2 + 2P\, q_z^{(t)} + Q = 0 \;, \tag{A.13}$$

determining $q_z^{(t)} = -P \pm \sqrt{P^2 - Q}$, where

$$\begin{aligned} P &= \frac{c^{(R)} q_x}{b^{(R)}} \;, \\ Q &= \frac{q_x^2 (a^{(R)} - a^{(L)}) - q_z^2 b^{(L)} - 2c^{(L)} q_x q_z}{b^{(R)}} \;. \end{aligned} \tag{A.14}$$

The discriminant $P^2 - Q$ may become negative for certain range of wave-vectors; this implies an exponential decay of the wave across the boundary. This phenomenon is quite analogous to the complete internal reflection of light at the boundary of two media with different refractive index.

With the knowledge of the transmitted and reflected wave vectors, $\mathbf{q}^{(t)}$ and $\mathbf{q}^{(r)}$, we can determine the transmission (t) and the reflection (r) coefficients for the channel corresponding to the passage of electron from the i-th valley on the L side of the GB to the j-th valley on the R side – assuming no other channels present. This is done by matching the wavefunction and the normal component of the velocity across the boundary; the latter condition expresses the conservation of flux (note that in the present problem $|t|^2 + |r|^2 \neq 1$). Since the particle is assumed incident from the left, we take

$$\begin{aligned} \Psi^{(L)}(\mathbf{r}) &= \exp(\mathrm{i}\, \mathbf{q}\cdot\mathbf{r}) + r \exp(\mathrm{i}\, \mathbf{q}^{(r)}\cdot\mathbf{r}) \;, \\ \Psi^{(R)}(\mathbf{r}) &= t \exp(\mathrm{i}\, \mathbf{q}^{(t)}\cdot\mathbf{r}) \;. \end{aligned} \tag{A.15}$$

From the condition $[\Psi^{(L)} = \Psi^{(R)}]_{z=0}$, one has the usual $t = 1 + r$. The velocity matching, $[\hat{V}_z \Psi^{(L)} = \hat{V}_z \Psi^{(R)}]_{z=0}$, results in an equation of the form

$$A\, t - B\, r = C \;, \tag{A.16}$$

where

$$A(\mathbf{q}\,;\, \mathbf{n}_i^{(L)}, \mathbf{n}_j^{(R)}) = b^{(R)} q_z^{(t)} + c^{(R)} q_x \tag{A.17a}$$

$$B(\mathbf{q}\,;\, \mathbf{n}_i^{(L)}) = b^{(L)} q_z^{(r)} + c^{(L)} q_x \tag{A.17b}$$

$$C(\mathbf{q}\,;\, \mathbf{n}_i^{(L)}) = b^{(L)} q_z + c^{(L)} q_x \tag{A.17c}$$

Using eq. (A.10), it is easy to show that, in general, $B = -C$. Consequently, the transmission coefficient $t_{ij}(\mathbf{q})$ is given by

$$t_{ij}\,(\mathbf{q}) \equiv t\,(\mathbf{q}\,;\,\mathbf{n}_i^{(L)},\mathbf{n}_j^{(R)}) = \frac{2C}{A-B}\ . \tag{A.18}$$

Consider a specific example of a Σ_3 twin boundary, which is the lowest energy and therefore the most commonly occuring GB in polycristalline Si. In this structure the two crystals L and R are mirror images of one another in the GB plane which is a [111] crystallographic plane. Consider transitions between the two ellipsoids, illustrated in Fig. 2. The polar angles of the initial ellipsoid's axis of revolution are $\theta_i^{(L)}, \phi_i^{(L)}$ where $\cos\theta_i^{(L)} = \pm(1/3)^{1/2}$ and $\phi_i^{(L)}$ is arbitrary (determined by the plane of electron motion). Then the possible orientations of $\mathbf{n}_j^{(R)}$ are

$$\theta_j^{(R)} = \theta_i^{(L)} \quad \text{and} \quad \phi_j^{(R)} = \phi_i^{(L)} + \pi \qquad (j=1)\ ;$$
$$\theta_j^{(R)} = \pi - \theta_i^{(L)} \quad \text{and} \quad \phi_j^{(R)} = \phi_i^{(L)} \qquad (j=2)\ ;$$
$$\theta_j^{(R)} = \theta_i^{(L)} \quad \text{and} \quad \phi_j^{(R)} = \phi_i^{(L)} \pm 2\pi/3 \qquad (j=3,4)\ ;$$
$$\theta_j^{(R)} = \pi - \theta_i^{(L)} \quad \text{and} \quad \phi_j^{(R)} = \phi_i^{(L)} \pm 2\pi/3 \qquad (j=5,6)\ ;$$

It turns out that for $j=1,2$ the transmission coefficient equals unity. From eqs. (A.5) one finds

$$a^{(R)} = a^{(L)} = 1-\Delta + 2\Delta\cos^2\phi_i^{(L)}\ ;$$
$$b^{(R)} = b^{(L)} = 1\ ;$$
$$c^{(R)} = -c^{(L)} = \sqrt{2\Delta}\cos\phi_i^{(L)} \equiv c\ .$$

Equation (A.10) then gives

$$q_z^{(r)} = -q_z + 2c\,q_x\ , \tag{A.19}$$

and from eqs. (A.14) we find $P^2 - Q = (q_z - cq_x)^2$, whence, in light of the fact that $q_z - cq_x = -q_z^{(r)} > 0$, we find

$$q_z^{(t)} = q_z - 2c\,q_x = -qr\ . \tag{A.20}$$

Substituting these expression into eq. (A.18) for the transmission coefficient we find

$$t_{ij} = 1 \quad (j=1,2)\ . \tag{A.21}$$

The situation is different for the transmission into the valleys $j = 3-6$.