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The effects of stacking faults on dechannelling—a quantum mechanical calculation

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Abstract. A quantum mechanical treatment of the effects of stacking faults on dechannelling is given. A simple harmonic model for the planar potential due to two planes surrounding the channel, and the corresponding bound states in the potential are considered. At the stacking fault boundary, these states make transitions for which the probabilities have been calculated, using the 'sudden approximation'.

1. Introduction

Most of the work on dechannelling caused by defects is based on several simplifying assumptions, restricting the validity of the results. For example, although qualitatively the results on the energy dependence of dechannelling, etc, are reliable, quantitatively the accuracy is poor. Therefore more work, possibly using quantum mechanical and/or field theoretical techniques, is needed to treat the whole defect problem in a more accurate way. The classical description of dechannelling caused by defects already given in earlier studies [1–4] demonstrates that protons, α-particles and other heavy ions behave classically, and the results obtained by using the classical description are in fairly good agreement with experimental results. However, electrons, positrons, mesons, etc, should be treated quantum mechanically [5] since quantum and diffractional effects [6] are important for these light particles. The dipole approximation [7, 8] is valid for the study of channelling radiation in the MeV range. In such a consideration of heavy ions and high-energy electrons/positrons the number of quantum levels increases ($n \propto \sqrt{\gamma m}$) [9] and the motion becomes more classical. However, quantum effects are dominant when the number of quantum states supported in the potential well is small [10]. So it will be very interesting to have a quantum description of the effects of defects on channelling in solids. In this spirit a quantum mechanical formulation is developed and a description for dechannelling is given, with stacking faults as a special case. The assumption of the separability of transverse and longitudinal motion is fairly accurate, and we continue to use it in the quantum description also.

In this work, keeping in mind the earlier discussions about the choice of interatomic potentials for the study of defects, the power-law potential [11–13] proposed by Pathak *et al* has been used. We consider positrons of energy 12.25 MeV ($\gamma = 25$) channelled along Al(111) with stacking faults, with the specific assumptions that the crystal is otherwise pure and clean, etc. The appropriate dechannelling probabilities are calculated.

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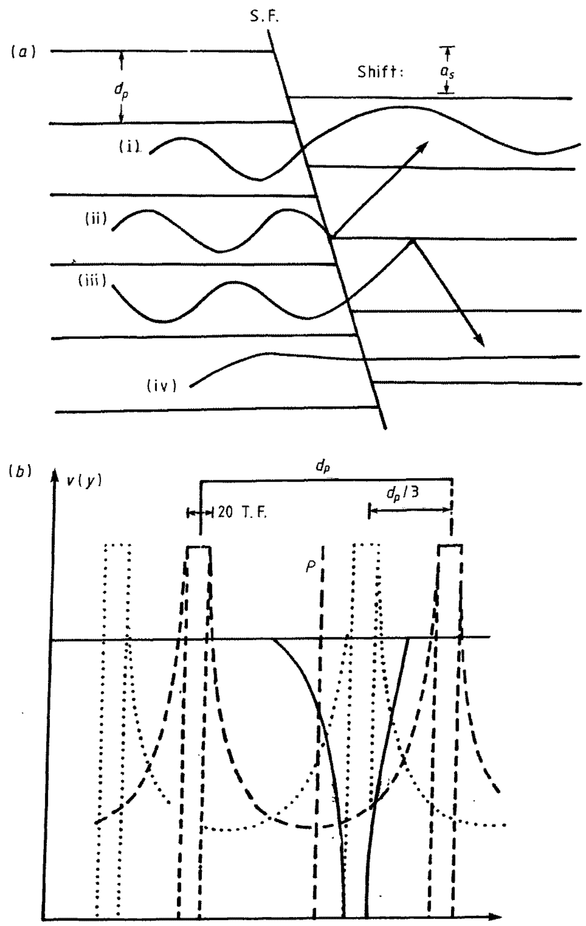

Figure 1. (a) The stacking fault situation involving (i) improved channelling, (ii) dechannelling at the fault, (iii) dechannelling after the fault, and (iv) the particle becoming well channelled (with zero amplitude) due to the various phases in which the incident particle is approaching the stacking fault region. (b) The obstruction of potential valleys present on one side by the potential hills at the S.F., corresponding to a typical FCC crystal, where the shift is usually $d_p/3$.

2. The quantum description

A stacking fault (S.F.) is an example of an obstruction to particle motion along crystallographic channels without any distortion, as shown in figure 1(a). At the stacking fault, the potential valleys present on one side (say, on the left) are obstructed by the potential hills on the other side of the fault (say, on the right) as shown in figure 1(b). For any charged particle managing to pass through the stacking fault, the longitudinal component of its energy is not much affected, but the transverse energy [14, 15] undergoes a change. Since the transverse potential for positrons (or any positive particles) is well approximated by a harmonic potential, the presence of a stacking fault is described by two similar harmonic potentials but shifted by the amount of the stacking shift. The available space for the particle just at the fault is slightly reduced because of the shifting of the atomic plane. Since the coupling constant α is a measure of the force constant of the harmonic potential it changes to α', and this is due to the fact that the force constant is modified due to the reduction of the effective planar channel width available for crossing the fault, as shown in figure 1. The channelling phenomena in this situation are governed by the overlap integral of the wave functions corresponding to the left-hand channel and the right-hand channel. Assuming that the stacking shift is a_s w.r.t. the left-hand channel as shown in figure 1(a), we can write

$$\psi_i = \psi_L = \left(\frac{\alpha}{\sqrt{\pi}2^n\, n!}\right)^{1/2} \exp\left(\frac{-\alpha^2 x^2}{2}\right) H_n(\alpha x) \tag{1}$$

$$\psi_f = \psi_R = \left(\frac{\alpha'}{\sqrt{\pi}2^m\, m!}\right)^{1/2} \exp\left(\frac{-\alpha'^2 (x+a_s)^2}{2}\right) H_m(\alpha' x + \alpha' a_s). \tag{2}$$

The matrix element is given by

$$\langle \psi_i | \psi_f \rangle = \left(\frac{\alpha\alpha'}{\pi 2^{m+n} m! n!}\right)^{1/2} I_{n,m}$$

where

$$I_{n,m} = \int_{-\infty}^{\infty} \exp\left\{-\frac{1}{2}[\alpha^2 x^2 + \alpha'^2 (x+a_s)^2]\right\} H_n(\alpha x) H_m(\alpha' x + \alpha' a_s)\ \mathrm{d}x. \tag{3}$$

Here n and m represent harmonic oscillator states corresponding to the initial state (the left-hand part of the channel before the fault) and the final state (after the fault) respectively.

2.1. The 'sudden' approximation [16]

Since the energy of the incident particle is high, the time spent by the charged particle at the interface between the two channels is very small compared to the time spent by it in either of the channels (i.e., left or right). Hence one can use the 'sudden' approximation [16] so that the wave functions on either side of the fault are identical in coupling terms. That means that the discontinuity at the boundary cannot be 'seen' during channelling, and α' equals α in expression (3).

If we write

$$\psi_i(x) = |n\rangle \qquad \text{and} \qquad \psi_f(x) = |m\rangle$$

then under the sudden approximation the overlap integral $\langle \psi_i | \psi_f \rangle$ can be written as

$$\langle n|m\rangle = \frac{1}{\sqrt{\pi 2^{m+n} m! n!}} \exp\{-\alpha^2 a_s^2/4\} \int_{-\infty}^{\infty} \exp\left\{-\left(t + \frac{b}{2}\right)^2\right\} H_n(t) H_m(t+b)\ \mathrm{d}t \tag{4}$$

where $b = \alpha a_s$ and $\alpha x = t$. The general expression for $\langle n|m\rangle$ is obtained by evaluating the above integral and we get

$$\langle n|m\rangle = \frac{\exp(-\alpha^2 a_s^2/4)}{\sqrt{2^{m+n} m! n!}} \left(\sum_{r=\max(0,m-n)}^{m} (-1)^{n-m+r} 2^{m-r} m_{c_r}\ \frac{n!}{(n-m+r)!}\ (b)^{n-m+2r}\right). \tag{5}$$

The transition/channelling probability, in general, is then obtained through the expression $p_{m\to n} = |\langle n|m\rangle|^2 = p_{n\to m}$, and the number of quantum states in the harmonic potential well can be calculated using the equation

$$\left(n_{\max} + \frac{1}{2}\right)\overline{h}\omega = \frac{1}{2} k_1 x_{\max}^2. \tag{6}$$

In the above equations,

$$\alpha = \sqrt{\frac{m\omega}{\hbar}} \qquad \omega = \sqrt{\frac{k_1}{\gamma m}}.$$

γm is the relativistic mass [18], and $x_{\max} = d_p/2 - a_{T.F.} = l - a_{T.F.}$. To calculate the force constant, we consider the planar potential [12, 13, 17]

$$V(x) = 2\pi z_1 z_2 e^2 C a_{T.F.}^2 Np\left(\frac{1}{l + a_{T.F.} - x} + \frac{1}{l + a_{T.F.} + x}\right).$$

This can be expanded around $x = 0$, and we get

$$V(x) = V_0 + \frac{1}{2}k_1 x^2$$

where

$$V_0 = \frac{4\pi z_1 z_2 e^2 C a_{T.F.} Np}{(l + a_{T.F.})} \qquad k_1 = \frac{2V_0}{(l + a_{T.F.})^2}.$$

In the above equations d_p is the interplanar distance, $a_{T.F.}$ is the Thomas–Fermi screening radius, C is the Lindhard constant given by $\sqrt{3}$, z_1 and z_2 are the atomic numbers of the projectile particle and the target atom respectively, and $Np = Nd_p$, N being the bulk density of atoms in the crystal. Using the above expressions, the number of quantum states for positrons channelled along (111) planes in an aluminium target has been calculated to be $n_{\max} = 3$.

2.2. *Dechannelling probabilities*

The initial state of the particle is fixed (in the left-hand part of the channel). It can go on to occupy any one of the states in the right-hand-side channel (after the fault). All of the possibilities that one can expect are

$$\begin{array}{cccc} 0 \longrightarrow 0 & 0 \longrightarrow 1 & 0 \longrightarrow 2 & 0 \longrightarrow 3 \\ 1 \longrightarrow 0 & 1 \longrightarrow 1 & 1 \longrightarrow 2 & 1 \longrightarrow 3 \\ 2 \longrightarrow 0 & 2 \longrightarrow 1 & 2 \longrightarrow 2 & 2 \longrightarrow 3 \\ 3 \longrightarrow 0 & 3 \longrightarrow 1 & 3 \longrightarrow 2 & 3 \longrightarrow 3. \end{array}$$

The probability for a particle to remain channelled after the fault is given by

$$p_n = \sum_{m=0}^{3} |\langle n|m\rangle|^2. \tag{7}$$

The dechannelling probability is defined as

$$\chi_n = 1 - p_n. \tag{8}$$

The initial state of the particle $|n\rangle$ is fixed, and it can be 0, 1, 2, or 3.

One can find the matrix elements and the channelling probabilities for various states, by substituting appropriate values of n and m in (5), and some numerical results for specific cases have been given in table 1.

Table 1. The variation of the dechannelling probabilities for positrons in Al with the stacking shift for various initial states.

Shift in units of l	Dechannelling probabilities χ_0	χ_1	χ_2	χ_3
0.00	0.00	0.00	0.00	0.00
0.10	0.00	0.07	0.07	0.17
0.20	0.00	0.21	0.29	0.46
0.30	0.00	0.33	0.57	0.56
0.40	0.01	0.38	0.71	0.51
0.50	0.04	0.38	0.62	0.52
0.60	0.10	0.37	0.43	0.60
0.70	0.22	0.36	0.32	0.63
0.80	0.39	0.35	0.37	0.61
0.90	0.56	0.38	0.48	0.63
1.00	0.72	0.47	0.56	0.69

2.3. The dechannelling effects at the fault

In the quantum mechanical treatment we start with a wave function describing the incident particle (ψ_L) coming from the left. This wave function is of the form of a wave packet along the longitudinal direction (z) and a harmonic oscillator in the transverse direction (x). When this packet reaches the fault, the general transverse planar potential can be described by an expression of the form

$$V(z,x) = \frac{1}{2}k_1 x^2 H(z_0 - z) + \frac{1}{2}k_1 (x + a_s)^2 H(z - z_0)$$

where $H(z)$ is a step function which equals one for positive arguments and zero for negative arguments. The solution of the Schrödinger equation for this potential is different in two parts of the crystal, i.e., for $z < z_0$ and for $z > z_0$. At the boundary $z = z_0$, part of this wave function is reflected and part is transmitted. The general solution for the left-hand part is of the form

$$\psi_L(z,x) = (A\exp(\mathrm{i}kz) + B\exp(-\mathrm{i}kz))\varphi_n(x).$$

Similarly the wave function corresponding to the transmitted particle after the fault will take the form

$$\psi_R(z,x) = C\exp(\mathrm{i}k'z)\varphi_m(x + a_s).$$

So one can match the wave functions [16] at the stacking fault ($z = z_0$), which gives the reflected flux (N_r) and the transmitted flux (N_t) in terms of the incident flux (N_i) at the fault. The corresponding reflection and transmission coefficients are given by

$$R = \frac{N_r}{N_i} = \left(\frac{k - k'}{k + k'}\right)^2 \qquad T = \frac{N_t}{N_i} = \frac{4kk'}{(k + k')^2}|\langle m|n\rangle|^2. \tag{9}$$

It is evident from the above expressions that there are some particles which are neither in the left-hand part of the channel nor in the right-hand part. These particles will not experience the standard harmonic potential since they have already come out of the channel. These may be dechannelled particles which hit the fault and depart from the channel. This situation corresponds to dechannelling at the fault. So one can define the dechannelling coefficient (D) in terms of the dechannelled flux N_d ($=N_i - (N_r + N_t)$) as

$$D = \frac{N_d}{N_i} = \frac{4kk'}{(k+k')^2}(1 - p_{n\to m}). \tag{10}$$

Since the total energy of the positron is very high, the positron cannot recognize the presence of the fault during the passage through the fault unless it hits the fault directly. The longitudinal momentum is therefore likely to be unaltered, and so k' equals k, and $R = 0$. So in the high-energy limit we get the same results as were obtained in the calculations described in the above sections.

2.4. The effects of periodicity in the transverse space [7]

The transverse potential is in principle a periodic function with period d_p; hence the wave functions are of Bloch type. One can estimate the periodicity effect due to the remaining wells by evaluating the dipole momentum. An estimate is given here for the contribution of the remaining wells at $n = 1$ obtained using equation (3.8) of reference [7]; we get

$$\bar{\alpha}_x - \alpha_x = -0.001\,0511.$$

Therefore the contribution of the other wells to the dipole momentum ($\bar{\alpha}_x$) is negligibly small when compared to the dipole momentum coresponding to a single well ($\alpha_x \approx 1.001$); hence the periodicity effects are likely to be negligible for our channelling/dechannelling probability calculations.

3. Results and conclusions

We have developed a quantum theory of dechannelling due to defects with special reference to stacking faults. The theory is valid as long as the number of quantum states supported by the transverse potential due to the two planes is small. This happens for light particles like positrons for which, to the best of our knowledge, no previous calculations exist.

Table 2. A comparison of the dechannelling probabilities for a stacking shift of $d_p/3$ obtained from a classical calculation with those from the present quantum description.

	The present quantum calculations			
The classical calculation [12]	χ_0	χ_1	χ_2	χ_3
0.28	0.17	0.36	0.34	0.63

The dechannelling probabilities for various initial states χ_0, χ_1, χ_2, and χ_3 as a function of the stacking shift are given in figures 2(a), 2(b), 3(a), and 3(b). The dechannelling probabilities depend on the intial state. If the particle after passing through the fault goes to a state which is the same as the initial state, then the transition probability is a maximum corresponding to the shift $a_s = 0$, as expected because the channel is straight and the particle will propagate without any obstruction, which can also be seen through the vanishing of the dechannelling coefficient ($D = 0$). The channelling probability for a given initial state is very sensitive to the stacking shift. If the final state is different from the initial state, the channelling probability drastically oscillates with the stacking shift a_s as shown in figures 4 and 5. There are some combinations of $\langle n|m\rangle$ which lead to maximum dechannelling.

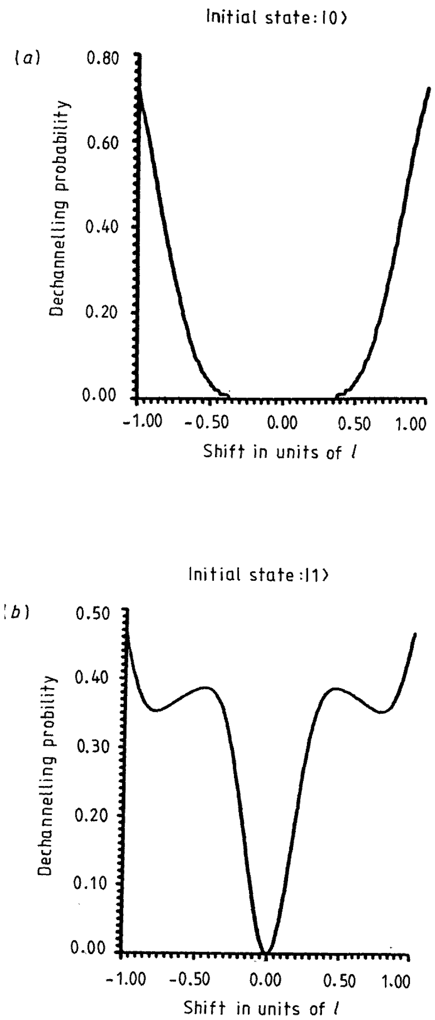

Figure 2. (a) The variation of the dechannelling probability with the stacking shift corresponding to the initial state $|0\rangle$ in the left-hand channel. (b) The variation of the dechannelling probability with the stacking shift corresponding to the initial state $|1\rangle$ in the left-hand channel.

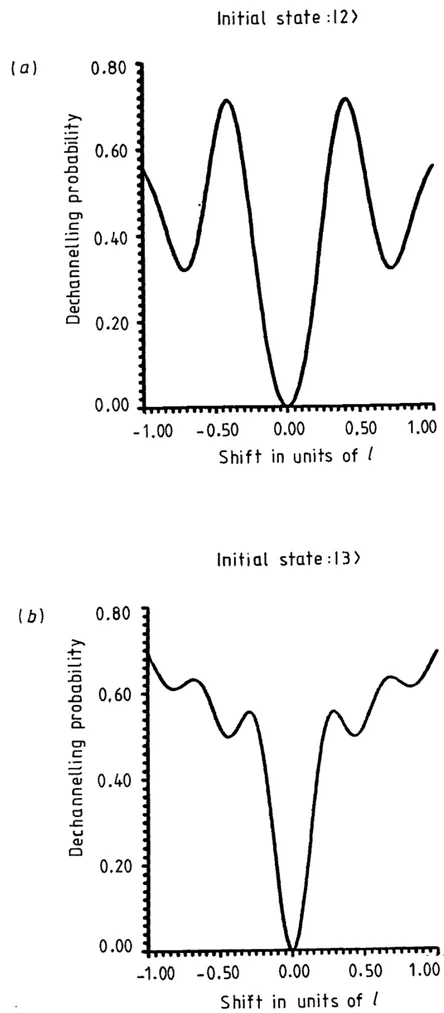

Figure 3. (a) The variation of the dechannelling probability with the stacking shift corresponding to the initial state $|2\rangle$ in the left-hand channel. (b) The variation of the dechannelling probability with the stacking shift corresponding to the initial state $|3\rangle$ in the left-hand channel.

These may be called dechannelling states. If the particle happens to be in these dechannelling states, then, whatever the shift may be, there is very high tendency for dechannelling of the particle in general, and at the fault in particular. In the present case these are $1 \leftrightarrow 3$, $2 \leftrightarrow 0$, and $3 \leftrightarrow 0$; see figures 4(a), 4(b), and 5(b). Detailed experiments are needed to see the precise effects of this kind of behaviour.

These points indicate that there is another important parameter, i.e., the phase in which the particle is approaching the stacking fault boundary. This can also be seen explicitly

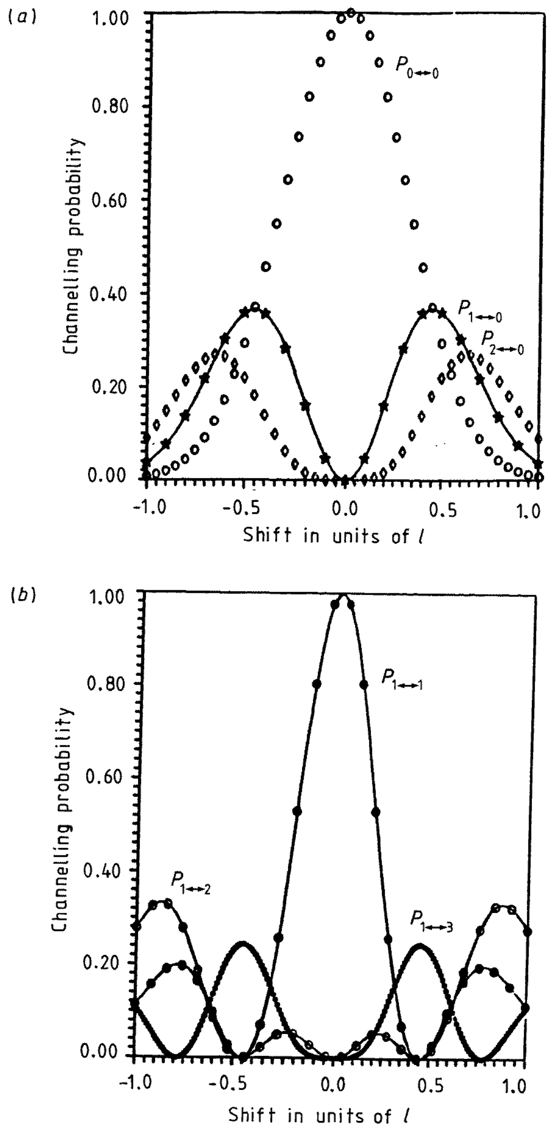

Figure 4. (a) The channelling probability as a function of the stacking shift a_s in units of l for various matrix elements symbolically denoted by ○: $|\langle 0|0\rangle|^2$; ★: $|\langle 1|0\rangle|^2$; and ◊: $|\langle 2|0\rangle|^2$. (b) The channelling probability as a function of the stacking shift a_s in units of l for various matrix elements symbolically denoted by ●: $|\langle 1|1\rangle|^2$; ○: $|\langle 1|2\rangle|^2$; and ★: $|\langle 1|3\rangle|^2$.

from equation (10), which indicates that the dechannelling at the fault will depend upon the final state that the particle will be in. The non-diagonal matrix elements vanish for zero shift. This implies that the well-channelled (oscillating) particle suddenly cannot exhibit oscillatory (minimum-amplitude) behaviour in the absence of stacking faults. The fate of the particle after the fault will be decided by the amount of the shift. This kind of

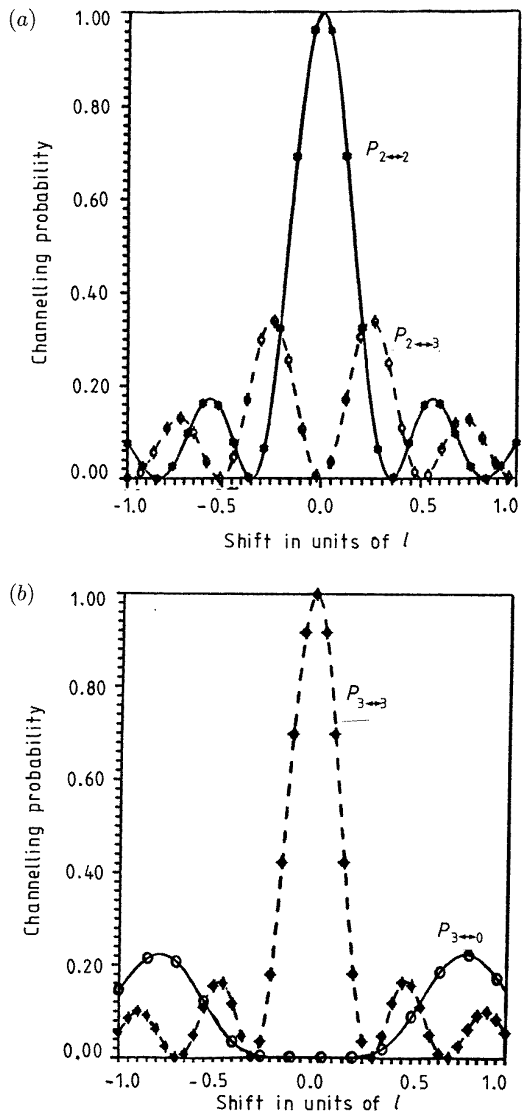

Figure 5. (a) The channelling probability as a function of the stacking shift a_s in units of l for various matrix elements symbolically denoted by ★: $|\langle 2|2\rangle|^2$; and ○: $|\langle 2|3\rangle|^2$. (b) The channelling probability as a function of the stacking shift a_s in units of l for various matrix elements symbolically denoted by ●: $|\langle 3|3\rangle|^2$; and ○: $|\langle 3|0\rangle|^2$.

dependence on the phase of the approaching particle has also been discussed in a classical analysis [11, 12].

Mory and Quere [11] discussed some experimental results for χ using a classical description. An attempt has been made to discuss those results using the present quantum description, and for that case, $n_{\max}$ turns out to be as large as 278. This clearly shows that for the α-particle-dechannelling situation a classical treatment will be good enough as far as the channelling aspects are concerned. A comparison of the present quantum mechanical calculation with the classical approach [12] for the specific situation of the standard stacking shift $d_p/3$ is shown in the table 2. Experiments on electron/positron dechannelling are needed to verify these results and to confirm the utility of the present quantum description. We do not expect the classical results to be valid for positron and electron dechannelling.

In conclusion, a general expression for the overlap integral $\langle n|m\rangle$ for arbitrary values of n and m is given for the first time, and is shown to have remarkable physical significance; it also reduces the number of laborious analytical calculations involving Hermite functions required—in particular, for the higher states. This general expression can be used elsewhere. The usefulness and completeness of this quantum mechanical formulation lies in the fact that this general expression is valid for various stacking shifts.

There is an interesting left–right symmetry inbuilt in the problem, which is not clearly realized in the classical description. More refined experiments are needed to check the predictions.

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