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Dechanneling of electrons by stacking faults – a model quantum mechanical calculation

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Abstract

A quantum mechanical treatment for dechanneling of fast moving electrons by stacking faults is given. One dimensional hydrogen atom model is used for planar potential due to an atomic plane and corresponding bound states in the transverse potential are considered. At the stacking fault boundary, the electrons in these states make transitions for which probabilities have been calculated, using sudden approximation. Some numerical results using mathematica have been presented and applications to channeling radiation problem are briefly discussed.

1. Introduction

Channeling and back-scattering experiments with energetic ions have been widely employed for defect studies [1]. The simultaneous use of these techniques with TEM [2] is a promising procedure to correlate the dechanneling observations with the defect configurations. However, recent experiments [3] on TEM and channeling suggest that TEM is useful for the samples with thickness $\leqslant 10^3$ Å and positron channeling is more appropriate and can be a substitute for TEM to probe bulk crystals (for thicknesses ≈ μm). Dechanneling of particles, especially electrons and positrons are effective technique as different types of defects may be separated out on the basis of the qualitative energy dependence of dechanneling cross-sections [4–6].

Classically, the dechanneling effects caused by defects are explained on the basis of change in transverse energy while encountering defects.

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Though these classical dechanneling results give reliable energy dependence, detailed dynamics of the particle during its passage through defected region is not so clear. Hence it is important to have a complete quantum mechanical description of the particle during its passage through the defected region. The quantized nature of the transverse motion of these light particles has been nicely revealed by channeling radiation spectroscopy [7]. Since then these light particles have been used for channeling radiation and probing various defects in crystals [8–11]. Particularly the quantum mechanical studies [12] and the experiments involving these light particles [13] have highlighted the importance of channeling radiation. Quantitative comparisons and detailed quantum calculations are to be carried out by incorporating various factors (like initial population and redistribution of these population after the stacking interface) [14].

The time dependent formulation of positron channeling provided important results especially in connection with dechanneling widths which show good agreement with experimental data [15,16] and subsequent extension to bent crystal channeling for beam extraction process [17–20] has given good support to the model. However, for the case of electrons similar quantum treatment has not been given though some discussion on the subject has been found in the literature [21]. In the present quantum description, the obstruction effects caused by stacking faults are considered as perturbation and the dechanneling probabilities are obtained using sudden approximation. In the next section we describe the theory and formulation and in Section 3 the results are discussed.

2. Dechanneling by stacking faults

A planar channeling model for electrons reported by our group earlier [14] has been utilized for the present dechanneling calculations also. Stacking fault (SF) is an example of obstruction dechanneling. At the stacking fault the potential valleys present on the one side of the fault (say left) are completely shifted w.r.t those on the other side (say right) and the amount of this stacking shift is denoted by 'b'. During the process of its passage through the stacking fault, the electron makes a transition from a well defined initial state $|n\rangle$ to a final state $\langle m|$ (right side of the fault). The channeling phenomenon under this situation is governed by the matrix element of the wave functions representing the transverse motion on either side of the fault. Transition amplitudes are obtained using sudden approximation. Recently this has been used extensively for the positron dechanneling calculations and shown to be fairly appropriate, especially for energetic light ions [12,14]. In the present quantum description we use this approximation to obtain dechanneling probabilities. The maximum number of quantum states $n_{\max}$ available in the attractive transverse potential well is estimated by equating the total quantized transverse energy to the depth of the potential well [14,22] and this is given by

$$E_n = -\frac{\gamma m U_0^2}{2\hbar^2 n_{\max}^2} = \frac{U_0}{x_{\max}} \Rightarrow n_{\max} = \left(\frac{\gamma m U_0 x_{\max}}{2\hbar^2}\right)^{1/2}. \tag{1}$$

We have taken specific example of 10 MeV ($\gamma = 20$) electrons channeled in Si along (1 1 0) planes with stacking faults for which $n_{\max} = 3$ and these bound states are $|1\rangle$, $|2\rangle$ and $|3\rangle$. This simple estimate reflects the fact that there are many more eigen states in the attractive potential well and the exact calculation of all the quantum states available for the particle require detailed first principle calculation of the interaction potential. However, one can realize that the quantum states present deep inside the well are more responsible for the direct dechanneling mechanism. The probability for a particle with initial state $|i\rangle$ to occupy any one of the available final states $\langle f|$ (i.e. the probability for particle to remain channeled after the fault) is obtained by the equation.

$$P_i = \sum_{f=1}^{3} |\langle\psi_f(x+b)|\psi_i(x)\rangle|^2. \tag{2}$$

The corresponding dechanneling probability of the electron during the process of its transmission is obtained by $\chi_i = 1 - P_i$.

The initial state of the particle $|i\rangle$ is fixed, it can be 1, 2, or 3. The state $|i\rangle = |1\rangle$ is ground state and corresponds to initially well channeled particle, $|2\rangle$ and $|3\rangle$ are first and second excited states respectively. The matrix elements are evaluated from the integral [14],

$$\langle m|n\rangle = C_n C_m \int_{-\infty}^{\infty} \mathrm{Exp}\left(-\frac{1}{A_0 mn}[n|x+b| + m|x|]\right) \{x+b\}\{x\} \times L_m^1\left(\frac{2|x+b|}{mA_0}\right) L_n^1\left(\frac{2|x|}{nA_0}\right) \mathrm{d}x, \tag{3}$$

where C_n and C_m are normalization constants. The individual transition amplitudes $|\langle m|n\rangle|^2$ are obtained by splitting the integral into various intervals, i.e.

$$\int_{-\infty}^{\infty} \ldots \mathrm{d}x \Rightarrow \int_{-\infty}^{-b} \ldots \mathrm{d}x + \int_{-b}^{0} \ldots \mathrm{d}x + \int_{0}^{\infty} \ldots \mathrm{d}x. \tag{4}$$

3. Results and discussion

The calculations involving integrations are carried out using Mathematica™. In the straight channel configuration i.e. $b = 0$ the diagonal matrix elements are unity (see Figs. 1–3 and the non-diagonal elements are zero as expected. The electron remains in the same state implying the perfect crystal situation and the particle makes no transition. The presence of stacking faults (finite b) enables the particle to make transitions to other states, while crossing over to the right side of the fault.

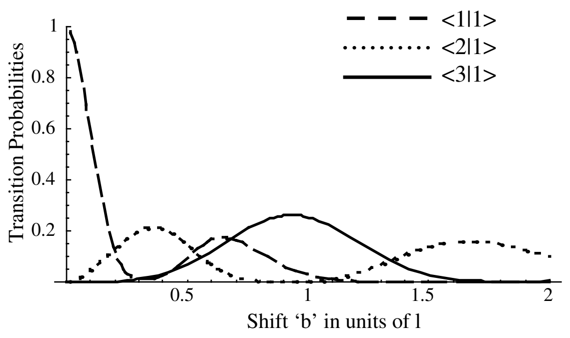

Fig. 1. The variation of channeling probabilities for electron initially in the state $|1\rangle$ going to various final states after encountering the stacking shift.

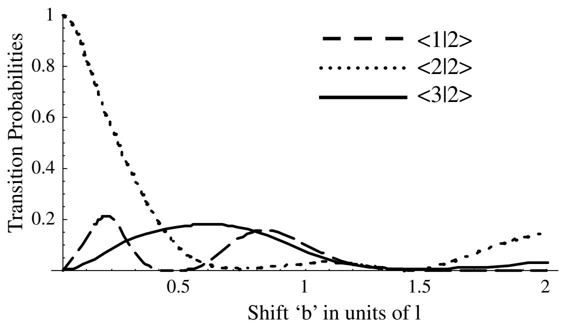

Fig. 2. The variation of channeling probabilities for electron initially in the state $|2\rangle$ going to various final states after encountering the stacking shift.

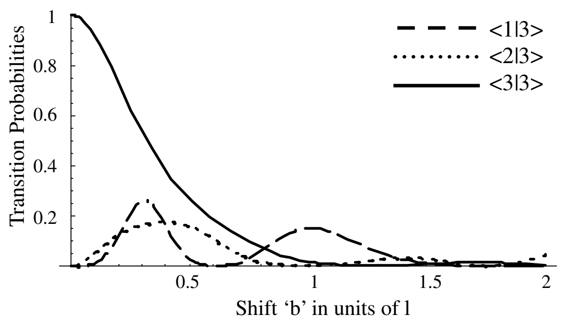

Fig. 3. The variation of channeling probabilities for electron initially in the state $|3\rangle$ going to various final states after encountering the stacking shift.

Channeling/dechanneling probabilities are very much sensitive to the stacking shift for initially well-channeled particles (see Fig. 4 (χ_1)). This behavior confirms our assumption that the well-channeled particles are more responsible for dechanneling process particularly for obstruction type model discussed in these calculations. The channeling probabilities corresponding to excited states (Fig. 4 – χ_2 and χ_3) decrease more slowly. It is also seen in Fig. 4 that the minimum of the channeling probabilities moves towards higher shift for excited states. This is in contrast to positron case where the excited states dechanneling

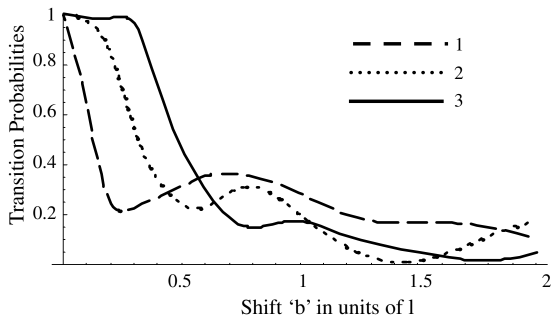

Fig. 4. The variation of total channeling probability (χ_1, χ_2 and χ_3) with stacking shift, where the initial state of the electron (in the left part of the channel) is $|1\rangle$, $|2\rangle$ and $|3\rangle$.

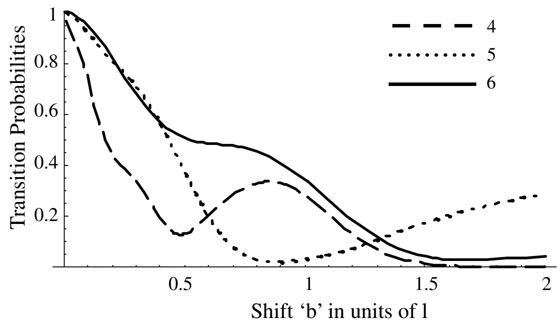

Fig. 5. The variation of total channeling probability (χ_4, χ_5 and χ_6) with stacking shift, where the final state of the electron (in the right part of the channel) is $|1\rangle$, $|2\rangle$ and $|3\rangle$.

probabilities drastically oscillate with shift while the total channeling probability for ground state is almost gaussian in shape [12]. This reflects the fact that the dechanneling of electrons and positrons is qualitatively different because of their opposite charges and this is revealed clearly in the present quantum mechanical calculations. The electron motion is always confined to the atomic plane whereas for positrons; the transverse motion is confined within the parabolic potential valley surrounded by the crystal planes. Ground state for channeled electron ($|1\rangle$) is localized about the plane while the excited states extend over to the either side of the atomic plane. Particles in excited states of the transverse energy spectrum propagate with higher amplitudes as compared to those in ground state. As a result the channeling probabilities corresponding to these cases are more sensitive to stacking shift and oscillate.

These calculations support the earlier predictions made for positrons. Particular combination of initial–final states yields negligibly small channeling probabilities irrespective of stacking shift. This concept of dechanneling states can also be applied for electron case where the transition amplitudes show oscillatory behavior. It is clear from Fig. 5 that the channeling/dechanneling at the fault will also depend upon the final states $\langle f|$. The total channeling probability (χ_4) for channeled particle to go to ground state after the fault decays faster (particularly at lower shifts) than to go to first and second excited states (χ_5 and χ_6). The overall probability of the particles remaining channeled decreases more slowly. Finally, from Figs. 6 and 4 we can conclude that fast exponential decay of transition probability for ground state (χ_1) is changed to moderate exponential decay for total channeling probability.

These predictions in fact explain the conclusions drawn by Park et al. [13,23] from their experiments in diamond crystals with and without the nitrogen platelets where the presence of these platelets are treated as stacking faults along (1 1 1), (1 1 0) planar directions while the effects encountered by channeled electrons and positrons are of distortion type in (1 0 0) direction. Some of these interesting features are explained as follows: the electron/positron radiation spectrum yields are affected by the platelets which clearly indicate that the positrons with smaller amplitudes (ground state particles) can survive after encountering the shift, while for electron case it shows higher

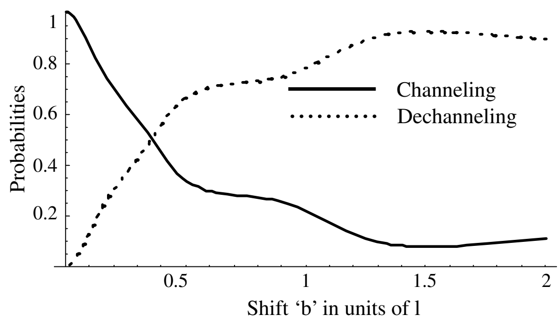

Fig. 6. The total channeling and dechanneling probability with stacking shift.

tendency to dechannel. The resolution of electron/positron radiation spectra in (100) direction is poor and only a bump can be noticed in the yield suggesting severe dechanneling due to distortions originated by the platelets [13,23]. These attenuation effects are severe and especially for positrons wave functions are localized along the middle axis of the planar channel and hence the re-adjustment to the distortion might be very difficult. Beam attenuation for positrons/electrons indicates the importance of relativistic effects on planar curvature. This has been discussed for dislocation case in earlier quantum mechanical formulation. We expect both these quantum and well-known classical estimates of dechanneling widths overestimate actual values obtained from the experiments. These effects are studied in single channel configuration by incorporating centrifugal force term in the distorted part. When centrifugal force dominates the harmonic coupling (present inside to steer the particle along the channel) the tunneling transitions [24] enable the particle to cross-over into neighboring atomic planes. The particles undergo re-channeling instead of getting dechanneled in its parent channel. These re-channeling effects are to be incorporated suitably using tunneling states and evaluating corresponding transition amplitudes. The electron data in similar situation indicates better yield compared the one noticed for positron case. Here some of the initially well channeled electrons propagate through these distortions and get channeled as they are steered along the atomic plane or axes.

In conclusion these quantum mechanical calculations give some insight into actual physics involved in dechanneling problems especially for electrons and their interaction with extended defects like stacking faults. This makes the problem more interesting to carry out further research work in both theoretical and experimental directions to check these predictions and utility of such models. The usefulness of such quantum mechanical calculations lies in the fact that the number of bound states increase with energy ($n_{\max} \propto \gamma m$ implying that for sufficiently high energies the number of bound states is large so that the quantal corrections are negligibly small) and classical descriptions are more appropriate. However for lower relativistic energies (few MeV e^- and e^+) these quantum mechanical effects are important. More rigorous and refined experiments are to be carried out for both electrons and positrons because of their importance in relativistic case. The channeling radiation studies can directly be used for defect characterization. Subsequently, detailed theoretical calculations are to be carried out in this direction by incorporating the population of electron states and their redistribution effects as influenced by these defects.

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