Dechanneling by dislocations: A time-dependent approach

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The motion of positrons in the planar channel surrounded by two atomic planes gives rise to descrete energy levels in the transverse potential. The transitions from these bound states to scattering states due to lattice distortions in the planar channel are described using a time-dependent centrifugal-energy term. The resulting expressions for dechanneling probabilities and hence for the dechanneling cross section for initially well channeled particles has been estimated, and qualitative features like dechanneling radius, energy dependence, etc., are discussed. [S0163-1829(99)04113-2]

I. INTRODUCTION

The motion of charged particles transmitted through single crystals (so-called channeling) is governed by correlated small-angle soft collisions with rows or planes of atoms. This channeling phenomena and its several applications in defects and radiation damage have been studied extensively within the framework of classical mechanics.[1–3] Furthermore, as the particle velocity increases, the quantal corrections to the classical description are negligible. However, when the particle wavelength is comparable to the lattice period, the wave interference effects are dominant.[4,5] It is well established that the motion of positively charged particles (like positrons) in the transverse direction can be described by the harmonic oscillator where as in the case of electron channeling the shape of the transverse potential is an inverted parabola;[6] and the transverse motion of the electrons is confined within the cusp-shaped potential centered around the axis or plane of atoms.

In recent years the problem of particle motion in a one-dimensional periodic potential acquired a special significance in connection with the quantum theory of light particles (like positron) and their propagation in crystals because of their sensitiveness and importance in probing various kind of defects present in the solid.[7] During the propagation of positrons in a planar channel (surrounded by two planes), the transverse motion is nearly harmonic. Quantum mechanically, the longitudinal and transverse components are separated out[8] with the transverse motion being described by a one-dimensional Schrödinger equation with a harmonic-oscillator potential and the solution gives rise to quantized transverse energies. Hence, a number of quantum states are formed and the transverse energy assumes a series of descrete values. In such a potential, the energies less than the height of the barrier namely below barrier states represent the initially channeled particles.

On the other hand, the states with energies above the potential barrier are basically dechanneling states and lead to dechanneling phenomena: In the case of dislocations the dechanneling is mainly due to the distortions of the planar channel and these distortions give rise to additional centrifugal energy in the transverse direction which eventually increases the transverse energy of the particle beyond the potential barrier to cause dechanneling. Classically this corresponds to centrifugal force exceeding the restoring force and shifting of the equilibrium axis away from the geometrical axis of the plane or axis.[9] Quantum mechanically, this is equivalent to the scattering of bound states from the corresponding perturbation potential to the scattering states. In a recent work we have used a sudden approximation to treat this problem for stacking faults[10] and dislocations.[11] The dechanneling mechanism in the case of dislocations was described with the assumption that the curvature of the planar channel near the dislocation is nearly constant and the overall length of the curved portion is on the order of the particle wavelength. We studied the dechanneling process, in the frame of bound-bound transitions in the planar channel induced by the sudden appearance of the curved channel. Here we extend that approach to a more realistic model by relaxing the sudden approximation and using the time-dependent perturbation theory. These calculations show that scattering states play a vital role in dechanneling because of the occurrence of additional bound states in the planar channel with a change in curvature. Even though the constant curvature model and the sudden approximation helped in a better quantum-mechanical understanding of the dechanneling mechanism, the consideration of the nonuniformity of the curvature during the propagation of the particle as done now is obviously more appropriate. It has also been shown here that under suitable semiclassical approximations, the well-known results are obtained.

II. TIME-DEPENDENT APPROACH

In the present calculations the nonuniformity effects in curvature mentioned above are taken in terms of a time-dependent force term which causes a transition from the bound state to the scattering state. The dechanneling phenomena under this situation are governed by the transition of the particle from a bound state (harmonic oscillator) to a scattering state (plane wave). The time-dependent centrifugal energy term[11] is modified in the relativistic case and is given by

$$V_R(x,t) = -\frac{mb}{\pi}\frac{\gamma^3 v_z^3 rt}{(r^2+\gamma^2 v_z^2 t^2)^2}x, \tag{1}$$

where $\gamma = 1/\sqrt{1-v_z^2/c^2}$, b is the Burgers vector, r is the distance of the channel from the dislocation, and x is the transverse coordinate. As we notice, due to the asymmetric nature of the above distortion term V_R, first-order perturbation theory will not give any shift in energy, hence the effect of dislocation on the positron is small for sufficiently small curvatures. On the other hand, it induces a transition from a bound state to a scattering state for larger curvatures and this corresponds to dechanneling.

The maximum number of quantum states in undistorted continuum potential is $n_{\max}\approx 3$ for a specific case of 12.25 MeV ($\gamma=25$) positrons channeled along Al(111). The initial and final wave functions of the positron are given by

$$\psi_n(x,y,z) = \frac{1}{L}\left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} \exp(ik_z z)\exp(ik_y y) \times \exp\left(-\frac{1}{2}\alpha^2 x^2\right) H_n(\alpha x),$$

$$\psi_f(x,y,z) = L^{-3/2}\exp(i\mathbf{k}_f\cdot\mathbf{r}).$$

Here the coupling constant α is given by $\sqrt{(m_\perp \omega/\hbar)}$ with transverse mass $m_\perp(=\gamma m)$ and the oscillation frequency $\omega = \sqrt{k/\gamma m}$, respectively.[10,11]

The distortions of the planar channel shifts particle motion in the transverse direction (x) whereas in the z direction the propagation is nearly constant. The expression for dechanneling probability of a particle with initial bound state $|n\rangle$ (due to channel distortion) to a final scattering state is given by

$$\chi_n = \frac{1}{\hbar^2}\left|\int V_R^{fn} e^{i\omega_{fn}t}dt\right|^2 \quad \text{with} \quad V_R^{fn} = \langle \psi_f | V_R(x,t) | \psi_n\rangle. \tag{2}$$

Due to scattering, the particle goes to continuum of states and the dechanneling probability can be obtained by considering the transitions to a group of closely spaced states. Hence, total dechanneling probability to any one of final states is obtained by integration over density of final states, i.e.,

$$\overline{\chi_n} = \alpha\left(\frac{L}{2\pi}\right)^3 \int \chi_n dq dk_f^y dk_f^z \tag{3}$$

with $q = k_f^x/\alpha$. The straightforward integration in k space leads to the expression

$$\overline{\chi_n} = \left(\frac{\alpha^2}{2\pi\sqrt{\pi}2^n n!}\right)\left(\frac{mb}{2\hbar}\right)^2 \left\{\int \omega_{fn}^2 \exp\left\{\frac{-2\omega_{fn} r}{\gamma v_z}\right\} e^{-q^2} \times \left|\int x e^{-(1/2)\alpha^2(x+x_o)^2} H_n(\alpha x)dx\right|^2 dq\right\},$$

where $\omega_{fn} = [E_f(q) - E_n/\hbar]$ and $x_o = iq/\alpha$.

Here E_f is final energy background in which the particle propagates after getting dechanneled. Because the remaining integrand has a pronounced maximum at $q = q_{\max}$, the term $\omega_{fn}^2 \exp(-2\omega_{fn} r/\gamma v_z)$ is assumed to be constant with $\omega_{fn}(q)\rightarrow\tilde{\omega}$, where $\tilde{\omega}$ depends on n and is given by $\omega_{fn}(q_{\max})$. Since $E_f(q) \gg E_n$, we assume that $\tilde{\omega}$ is independent of n and the above equation can be rewritten as

$$\overline{\chi_n} = \left(\frac{\alpha^2}{2\pi\sqrt{\pi}2^n n!}\right)\exp\left\{\frac{-2\tilde{\omega} r}{\gamma v_z}\right\}\left(\frac{mb\tilde{\omega}}{2\hbar}\right)^2 \times \left\{\int e^{-q^2}\left|\int x e^{-(1/2)\alpha^2(x+x_o)^2} H_n(\alpha x)dx\right|^2 dq\right\}. \tag{4}$$

Using the Rodrigues formula for H_n and incorporating the appropriate expressions, we obtain the total dechanneling probability $\overline{\chi_n}$ and it is given by

$$\overline{\chi_n} = (2n+1)\overline{\chi_0} \quad \text{with} \quad \overline{\chi_0} = \left(\frac{m\tilde{\omega}b}{2\sqrt{2}\hbar\alpha^2}\right)\exp\left(-\frac{2\tilde{\omega}r}{\gamma v_z}\right).$$

The above expression for $\overline{\chi_0}$ is obtained with specific reference to initially well channeled particles.

Corresponding to a given initial state (say $|n\rangle$), the dechanneling probability is maximum for those channels which are situated below the dechanneling radius r_n (i.e., the critical distance of the channel from the dislocation below which the particle completely gets dechanneled) and this happens for $\tilde{\omega} = \gamma v_z/r$. Invoking $\overline{\chi_n}(r_n) = 1$ for $r \leqslant r_n$, an estimate of the upper bound for the dechanneling radius with reference to a particle of the initial state $|n\rangle$ is obtained as

$$r_n^{(u)} \approx \left(n+\frac{1}{2}\right)\frac{b}{2.718}\sqrt{\frac{\gamma E}{2E_n}}, \tag{5}$$

where $2E = mv_z^2$ and the quantized transverse energy $E_n = (n+1/2)\hbar\omega$.[11]

However, one will be curious to have an estimate for the minimum distance of the channel from the dislocation. By exploring the possibility that a particle gets dechanneled when its transverse energy approaches the critical transverse energy, an equivalent expression for the minimum critical distance is obtained by replacing E_n with total transverse energy, $E_\perp = (n_{\max}+1/2)\hbar\omega = E_{n_{\max}} = E_3$. Hence, we get lower bound for r_n as $r_n^{(l)}$ given by

$$r_n^{(l)} \approx \left(n+\frac{1}{2}\right)\frac{b}{2.718}\sqrt{\frac{\gamma E}{2E_\perp}}. \tag{6}$$

Figure 1 shows clearly these two limits for $|n\rangle = |0\rangle$ (i.e., initially well-channeled particles). Obviously this is of prac-

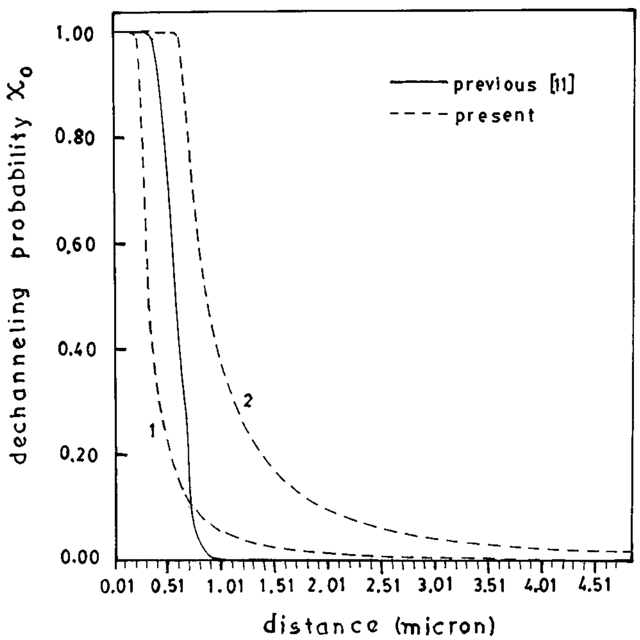

FIG. 1. Variation of dechanneling probability for initially well channeled particles ($\overline{\chi_0}$) with channel distance from the dislocation. $\overline{\chi_0}$ corresponding to the lower and upper bounds are denoted as 1 and 2, respectively.

tical interest and provides the definition for the dechanneling radius and at the same time, to a certain extent, enables us to relax the approximations mentioned above.

The dechanneling cross section with reference to an initial state $|n\rangle$ is obtained by the expression

$$\overline{\lambda_n} = \int \chi_n(r)dr = 2r_n. \tag{7}$$

The dechanneling widths $\overline{\lambda_n}$ are estimated using Eqs. (6) and (7) for positrons along Al(111) and results are given in Table I(a).

Classically, that above $E_\perp$ is equivalent to the critical transverse energy, given by $E_\perp^c \approx E\psi_p^2$, where ψ_p is the planar critical angle.[1] So for the case of nonrelativistic positive particles and other heavy ions ($\gamma=1$), and one may replace $E_\perp$ by the equivalent classical expression, an estimate of the corresponding dechanneling width for initially well-channeled particles ($\overline{\lambda}$) can be obtained as

$$\overline{\lambda} = \frac{b}{2.718}\sqrt{\frac{E}{4\pi Z_1 Z_2 e^2 N_p a_{T.F}}} = 0.3\overline{\lambda}_{\text{Quere}}\sqrt{\frac{b}{a_{T.F}}} = (0.44)\overline{\lambda}_{\text{Quere}} Z_2^{1/6}\sqrt{b}, \tag{8}$$

where b is in Å . Using the above equation, the dechanneling width for He ions has also been estimated and compared with existing theory and experimental data.[13] These details are given in Table I(b), showing reasonable agreement.

TABLE I. (a). Dechanneling widths for positrons in Al for various initial states. (b). Dechanneling width for He in Al. (Here E is expressed in MeV.)

(a)

Particulars of the crystal	Dechanneling widths in μm			
	$\overline{\lambda_o}$	$\overline{\lambda_1}$	$\overline{\lambda_2}$	$\overline{\lambda_3}$
Al(111), $b=2.86$ Å	0.47	1.41	2.35	3.3

(b)

Particulars of the crystal	Dechanneling width ($\overline{\lambda}$) in Å		
	Experimental (Ref. 13)	Quere	Present
Al(111), $b=2.86$ Å	$85\sqrt{E}$	$79\sqrt{E}$	$90\sqrt{E}$

III. RESULTS AND CONCLUSIONS

The expressions for the dechanneling radius and hence for the dechanneling width is derived. These expressions are qualitatively similar to the expression obtained by equating the deflecting force to the restoring force.[12] In the present calculation we obtain an expression for the dechanneling width purely on the basis of quantum-mechanical considerations. By incorporating appropriate limits in the present expression for the dechanneling width, an equivalent classical expression is obtained. For example, in the case of a heavy nonrelativistic particle here $\gamma \approx 1$, the above expression is identical to the one obtained in classical analysis.[2,12] The present procedure provides a simple and convenient way to estimate the order of magnitude of the effect and its scaling with particle energy and planar potential. This expression is very close to that obtained by Quere's classical analysis where the continuum model and the phase dependence of the approaching particle are considered. Quantitatively the present calculation may overestimate the actual dechanneling width by a numerical factor and this may be because of the semiclassical approximation, namely, the maximization of dechanneling probability and fixing $\tilde{\omega}$ correspondingly. However, one may set an appropriate numerical constant to fit with the experimental data as was done by Lindhard for his power-law potential ($C=\sqrt{3}$).

The result also confirms the results of earlier work[11] where one can notice that $r_0 \propto \sqrt{\gamma E}$, hence one can say qualitatively that the dechanneling cross section is linear with E and for higher energies this will be slower than E, etc., and it is $\propto \sqrt{E}$ as proposed in the case of heavy particles which in the classical framework[2,3] are obtained as semiclassical limits. These results also make uniform the qualitative energy dependence, i.e., the dechanneling cross section varies linearly with E at relativistic energies as confirmed by the bent crystal channeling experiments done by Carrigan.[14] He also mentioned that increasing the bending is in ''some sense'' like raising the atomic number of the crystal. From Eq. (8) one can see that the dechanneling radius increases with Z_2, which means that the critical region increases with Z_2, which in turn implies that the channels are distorted heavily. So the present theory shows that the bending increases with Z_2 and hence is also applicable for the channeling studies with bent crystals. So one may infer that materials with higher values of Z_2 are appropriate for bending of beams. Figure 1 shows a comparison of the present calculation with previous work.[11] As expected, the dechanneling probability falls off sharply (for a large curvature, i.e., large distortion) as compared to that obtained with bound-bound transitions in the sudden approximation. On the other hand, for sufficiently smaller curvatures, the dechanneling probability decreases slowly as compared to that obtained with bound-bound transitions. We expect the present theory to be valid for a wider range of dislocation concentrations. The quantum-mechanical results under suitable limits reproduce the known classical results qualitatively. The quantitative agreement is also satisfactory as seen from Table I. This gives us confidence in the basic concepts applied to this complicated problem. We hope to carry out further refinements and improvements of this simple model in the near future.

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