Chapter 3

Quantum description of dechanneling by Dislocations

3.1 Introduction:

Dislocations [1] are formed either by strain relaxation in the fabrication of semiconductor devices [2] or due to complete missing of atomic planes during the process of crystal growth or ion-implantation. As a result of this, one may notice distortion in the crystallographic channels. This distortion decreases with increasing distance from the dislocation core. The crystallographic channels in the vicinity of the dislocation are distorted heavily. However, as shown in Fig. (3.1), the channels outside a particular region of radius \( r_0 \) around the dislocation core (called dechanneling cylinder), are distorted to a lesser extent and result in only moderate modification in the motion of the channeled particles. These distortions affect the spectrum of channeled flux, even though the energy loss of well channeled particles is not significantly affected [3].

The effects of dislocations on charged particle propagation along major crystallographic directions and planes have been studied for some time. Dechanneling induced by the isolated linear dislocations was first studied by Quere [4]. From the balance of the restoring force due to the continuum potential of the atomic strings and the centrifugal deflecting force arising from the bending of the planar channel, he derived a simple analytical expressions for the diameter of the dechanneling cylinder, around
Chapter III: Quantum description of the dislocation core.

Fig. 3.1: The planar channels that are distorted due to presence of a dislocation. Here $R_{mc}$ is minimal radius of curvature of a typical channel situated at a distance $r_0$ from the dislocation.

This classical treatment was successfully refined in a series of studies which describe the effect of the ion trajectories and extended them to the case of dislocation loops [5], formed due to higher dislocation concentration. The results of such theories apply to the characterization of the defective layers, if the defects actions simply superpose with out interacting. This classical approach has been used extensively and shown to describe experimental results [6], reasonably well.

However, as discussed in the previous chapters, the dechanneling of light particles due to presence of the defects should be described quantum mechanically [7, 2], because they cannot be regarded as being localized but rather as an extended wave in
Chapter III: Quantum description of the crystal [9]. In case of point defects, the related effects due to impurity scattering have been studied by evaluating quantum mechanically the corresponding scattering cross-sections [1]. Similar quantum treatment for the effects of extended defects like dislocations has not been given so far. In chapter 2, we studied the dechanneling effects due to stacking faults, quantum mechanically, where the effects of obstruction are suitably incorporated in transition matrix elements of wavefunctions. The model gave reasonable description of dechanneling. This stimulated us for further development of these models to handle the distortion effects of the planar channel due to dislocations. Here one requires much more rigorous treatment of the dechanneling problem. At the same time, these quantum dechanneling calculations involve complicated analytical as well as numerical calculations. In this chapter, we restrict ourselves to the simplest case of screw dislocations of low concentrations so that there is no nucleation of dislocation loops. We present a model quantum mechanical calculation for the dechanneling effects due to distortions of the planar channel situated away from the dislocation core and there by we evaluate the dechanneling probabilities due to these dislocations.

3.2 Basis of the present model:

For the case of stacking faults, the effects on the propagating particle are of obstruction type and the treatment was simple whereas for the case of dislocations the channels are distorted. Hence these distortion effects on channeling are incorporated by introducing an energy term \((-x)\) due to transverse deflecting centrifugal force. Here ‘\(E\)’ is average energy in the curved part of the channel with radius of curvature ‘\(R\)’ and ‘\(x\)’ is the position of the particle in transverse direction.
Chapter III: Quantum description of...

As shown in Fig. (3.2), the standard displacement equations for the case of screw dislocation are given by

\[ u_1 = u_2 = \theta; \text{ and } u_3 = \frac{b}{s}, \]

The corresponding critical distance \( r_0 \) of such a channel (say A) from the dislocation core with Burger's vector '6' is calculated by taking the displacement perpendicular to A i.e., with \( u = u_3 \cos \varphi \). Choosing the channel along the \( z \)-direction (which is same as direction of propagation of the particle), the corresponding curvature was estimated from the second derivative of this displacement equation given by

\[ u = \frac{b}{2\pi} \cos \varphi \tan^{-1} \left( \frac{z \cos \varphi}{r_o} \right); \quad \frac{1}{R} = \frac{d^2u}{dz^2} \]

Fig. 3.2 : The displacements of a channel A situated at a distance of \( r_o \) from a screw dislocation along the axis \( x_3 \). Here \( \varphi \) is the angle made by the channel with \( x_1x_2 \) plane.

By solving the above displacement equations for screw dislocation, the mean dechanneling radius is obtained in terms of minimal radius of curvature which is given by [4]

\[ r_0 = \sqrt{\left( \frac{bR_{mc}}{10} \right)} \]
with ‘b’ as the Burgers vector. Here, the critical minimum radius of curvature $R_{\text{mc}}$ of channels (below which the particle will dechannel completely) is obtained by equating the deflecting centrifugal force to the restoring force due to planar potential, evaluated at the minimum distance of approach $a_{T,F}$ [11]. The amount of distortion present in a channel depends on the average concentration of the dislocations ‘$n$’, one can make an estimate for the farthest distance from the dislocation in terms of dislocation concentration ($r_{o}^{\text{max}} = 1/2(n^{1/2})$).

3.2.1 Relativistic expression for the curvature:

The analytical expression (for curvature) so obtained in the previous section is appropriate for non-relativistic heavy ions like protons, $\alpha$-particles, etc. So it is quite obvious that above expression is no longer valid for relativistic particles, hence these relativistic effects are to be incorporated suitably to obtain an equivalent relativistic expression for the curvature. Here we consider the motion of the positrons described in the rest frame of the particle. In this frame the particle "sees" continuum potential $\gamma V(x)$ in the transverse direction because of the fact that for the relativistic energies, the continuum potential in the transverse space is enhanced by a factor of 7 ($= 1/\sqrt{1 - v^2/c^2}$), due to length contraction in the direction of propagation. We denote the longitudinal co-ordinate in this relativistic case as $(Z)(= z/\gamma$ with $z$ being that in non-relativistic case). When the particle enters into the distorted portion, the motion of the particle is modified due to the influence of the curvature and in this distorted part of the channel, the corresponding relativistic displacement equation along $Z$ is obtained as follows:

$$Z \rightarrow \frac{z}{\gamma} \Rightarrow \frac{d}{dz} = \frac{d}{dZ} \Rightarrow \frac{d^2}{dz^2} = \gamma^2 \frac{d^2}{dZ^2} \Rightarrow \frac{1}{R} = \frac{d^2u}{dZ^2} = \gamma^2 \frac{d^2u}{dz^2} \bigg|_{z=\gamma Z} \quad (3.2)$$
Chapter III: Quantum description of

So the modified continuum potential as “seen” by the particle becomes 7

this is given by

$$
\gamma V_{\text{eff}} = \gamma V(x) - \gamma^2 m v_Z^2 \left\{ \frac{b}{\pi} \frac{r(\gamma Z)}{(r^2 + \gamma^2 Z^2)^2} \right\} x
$$

(3.3)

The expression for dechanneling radius \( r_0 \) in terms of minimal critical radius of curvature \( R_{mc} \) is obtained by equating the restoring force \(-\gamma \frac{dV}{dy}\) to the maximum value of the deflecting force due to curvature \( \gamma^2 \frac{2E}{R_{mc}} \). Using this procedure [11] and Eqn. (1.20), we have

$$
V(y) = \frac{2V_0 a_{T,F}}{(y + a_{T,F})} \quad \text{with} \quad V_0 = \pi Z_1 Z_2 e^2 C a_{T,F} N_p
$$

$$
\Rightarrow -\gamma \frac{dV}{dy} \bigg|_{a_{T,F}} = \gamma \frac{V_0}{2a_{T,F}}
$$

$$
-\gamma \frac{dV}{dy} = \gamma^2 \frac{2E}{R_{mc}} \Rightarrow \frac{V_0}{2a_{T,F}} = 2E \frac{\gamma}{R_{mc}} \Rightarrow \frac{R_{mc}}{\gamma} = \frac{4E}{\pi Z_1 Z_2 e^2 C N_p} \Rightarrow R_{mc} \rightarrow \frac{R_{mc}}{\gamma}
$$

The deflection force term on the other hand leads to modification in \( r_0 \) given by

$$
r_0 = \sqrt{\frac{\gamma^2 b}{10}} \frac{R_{mc}}{\gamma} \Rightarrow r_0 \rightarrow \sqrt{\frac{\gamma b R_{mc}}{10}} = \sqrt{\gamma} \ r_0
$$

One may notice that, due to these relativistic effects \( r_0 \) in Eqn. (3.1) is enhanced by a factor of \( \sqrt{\gamma} \). Here we evaluate dechanneling probabilities and discuss their variation with channel distance \( r_0 \) (given by Eqn. (3.1)) from the dislocation core.

Like in the stacking fault case, the quantum description requires as to calculate the transition probability among the energy levels in the transverse continuum potential. These transitions are induced by the distortion created due to dislocations. As before, we use harmonic oscillator model for transverse potential and sudden approximation for transitions. The coupling constant \( \alpha \) (appearing in the normal harmonic oscillator model potential \( \alpha = \sqrt{\frac{m + \omega}{\hbar}} \)) will change to \( \alpha' \) in the distorted portion because the oscillation frequency of the particle gets modified in this distorted portion, due to modification of net force constant.
Chapter III: Quantum description of.

The centrifugal energy term in the distorted portion is to be added to the well-known continuum potential (surrounding the channel), which acts as a restoring force [12, 11]. The channels within that critical region are distorted heavily, which eventually leads to dechanneling of most of the particles arriving in that region. However, the regions outside that core region are only moderately affected; channeling and continuum model is still valid and used extensively by incorporating the effects of distortion through above mentioned centrifugal force term. The situation in these regions is similar to that found in the bending of beams by bent crystal channeling [15] explained with continuum model. The condition is that bending should be less than critical angle for channeling. The force constant in the distorted channel is different from that in the straight channel and as a result of that, all the particles coming in the channels with radius of curvature less than $R_{nc}$ will get dechanneled. This modified force constant is obtained with the consideration of the harmonic approximation to above effective planar potential in the distorted part. This analysis is appropriate for the channels that are situated far away from the dislocation which in turn implies that we are dealing with crystals of low dislocation concentrations (typically $10^6$ to $10^8$ per cm$^2$).

Classically, the initially well-channeled particle in undistorted region starts oscillating about the axis of the distorted channel. Once it enters into the distorted portion, the potential minimum (about which the particle oscillates) is shifted due to curvature, reducing the available space for transverse motion in the channel. The expression for this shift (say ‘$\alpha_r$’) in the distorted channel is obtained with an approximation namely, neglecting fourth and higher order terms of $x/L$ which implies that we are dealing with those channel which are not heavily distorted (i.e., not very close to dislocation axis). This in turn introduces a maximum error of about 6%. The effects of distortion on the continuum potential will be discussed in the following section.
3.2.2 Effects of distortion on the force constant:

The effective potential in the distorted part of the channel is given by [12]

$$V_{\text{eff}} = \frac{4V_0La_{T,F}}{L^2 - x^2} - \frac{2E}{R} x$$

(3.4)

Expanding this around the shifted minimum, $a_r$

$$V_{\text{eff}}(x) = V_{\text{eff}}(a_r) + (x - a_r) \left. \frac{dV_{\text{eff}}}{dx} \right|_{x=a_r} + \frac{1}{2} (x - a_r)^2 \left. \frac{d^2V_{\text{eff}}}{dx^2} \right|_{x=a_r}$$

$$\frac{dV_{\text{eff}}}{dx} = 0 \Rightarrow a_r = \sqrt{\left(\frac{B^2}{L^2}\right) + \frac{L}{2} \frac{B}{L}; B = \frac{RV_0a_{T,F}}{E}, L = l + a_{T,F}}$$

$$\Rightarrow V_{\text{eff}}(x) = V_{\text{eff}}(a_r) + \frac{1}{2} (x - a_r)^2 \left. \frac{d^2V_{\text{eff}}}{dx^2} \right|_{x=a_r}$$

(3.5)

The effective force constant is obtained as

$$k_1^{\text{eff}} = \frac{8V_0a_{T,F}L}{(L^2 - a_r^2)^3} \left[ L^2 + 3a_r^2 \right]$$

Hence the maximum number of bound states in the distorted part ($j_{\text{max}}$) is obtained as

$$j_{\text{max}} = \frac{1}{2} \left[ \sqrt{\frac{\gamma m8V_0a_{T,F}L}{(L^2 - a_r^2)^3} \left( L^2 + 3a_r^2 \right) \left( \frac{l - a_{T,F} - a_r}{\hbar} \right)^2 - 1} \right]$$

(3.6)

From the prescription given in the previous chapter, we have

$N_p = 0.0394649a_o^{-2}, V_0 = \pi Z_Z^2 e^2 C a_{T,F}, N_p = 0.9671975 \text{ a.u.}$

$L = l + a_{T,F} = 2.2094091a_o + 0.3466437a_o = 2.5560528a_o; l - a_{T,F} = 1.8627654a_o.$

$$\Rightarrow j_{\text{max}} = \frac{1}{2} \left[ \sqrt{\frac{171.39505}{(6.5334059 - a_r^2)^3} \left( 6.5334059 + 3a_r^2 \right) \left( 1.8627654 - a_r \right)^2} - 1 \right]$$

As a consequence of change in the force constant of harmonic motion in the distorted portion, coupling constant gets modified to $\alpha'$. So from the Eqn. (3.6),

$$\alpha'^2 = \frac{\sqrt{\gamma m8V_0a_{T,F}L} \left( L^2 + 3a_r^2 \right)^3 \gamma m8V_0a_{T,F}}{L^3} \frac{1 + 3(a_r/L)^2}{1 - (a_r/L)^2}$$
When $a_r \to 0$, we notice $\alpha' \to a$ indicating that the shift in the potential (induced by the curvature) reflects in the modification of resulting force constant. This is as expected because when the channel becomes straight the coupling term will be as it was in the straight channel. Here we introduce a transition parameter $\tau (= \alpha'/\alpha)$ as we did in the earlier chapter. As shown in Fig. (3.3), $r \to 1 \Rightarrow a_r \to 0$ and this happens when the channel becomes straight (radius of curvature $R \to \infty$). Here onwards we call this ‘$\tau$’ as distortion parameter to take care of distortion effects.

\[
\tau^2 \alpha^2 \text{ where } \alpha^2 = \sqrt{\frac{\gamma m_8 V_0 a_{T,F}}{L^3}} \quad \text{and } \tau^2 = \sqrt{\frac{1 + 3(a_r/L)^2}{1 - (a_r/L)^2}}
\]

\[= \tau^2 \alpha^2 \text{ where } \alpha^2 = \sqrt{\frac{\gamma m_8 V_0 a_{T,F}}{L^3}} \quad \text{and } \tau^2 = \sqrt{\frac{1 + 3(a_r/L)^2}{1 - (a_r/L)^2}}
\]

Fig. 3.3 : The variation of distortion parameter $\tau (= \alpha'/\alpha)$ as a function of distance from the dislocation.
3.3 Theory and formulation:

Using those concepts discussed in the previous sections, a quantum mechanical formulation is developed for the effects of dislocations on planar dechanneling of positrons, with specific reference to screw dislocations. Here we use analysis similar to that given in the previous chapter and corresponding bound states in the straight channel are considered with $n_{\text{max}} = \ell_{\text{max}}$. This $\ell_{\text{max}}$ is calculated by equating total transverse energy to the depth of the continuum potential well; these details are given in forthcoming sections. The channeling/dechanneling phenomena under this situation is governed by the overlap integrals of the appropriate wave functions in various regions of distortion. As shown in Fig. (3.4), there are three boundaries, which the particle has to cross during its passage through the distorted channel, to find itself again in straight channel.

![Diagram](image)

**Fig. 3.4**: a) Typical planar channel of some finite curvature $R$, $a_r$ is the shift in equilibrium position due to distortion. b) Straight model channel replacing the channel of part (a).

Here $I, II, III$ are various portions of distortion and $a_r$ is the equilibrium position about which the particle will oscillate.
These boundaries are not so sharply well defined. However, for simplicity of the present (model) calculations, we use sudden approximation to calculate the transition probabilities across these three boundaries and in what follows, we will identify these boundaries as 3 interfaces (denoted by I, II, & III). The wavefunction of the particle in different regions may be written as,

\[ \psi_i = \psi_I = \left( \frac{\alpha}{\sqrt{\pi i!}} \right)^{1/2} \exp \left\{ -\frac{\alpha^2 x^2}{2} \right\} H_i(\alpha x) \] (3.7)

\[ \psi_j = \psi_J = \left( \frac{\alpha'}{\sqrt{\pi j!}} \right)^{1/2} \exp \left\{ -\frac{\alpha'^2 (x + a_r)^2}{2} \right\} H_j(\alpha' x + \alpha'a_r) \] (3.8)

\[ \psi_k = \psi_K = \left( \frac{\alpha'}{\sqrt{\pi 2^k k!}} \right)^{1/2} \exp \left\{ -\frac{\alpha'^2 (x - a_r)^2}{2} \right\} H_k(\alpha' x - \alpha'a_r) \] (3.9)

\[ \psi_f = \psi_R = \left( \frac{\alpha}{\sqrt{\pi f!}} \right)^{1/2} \exp \left\{ -\frac{\alpha^2 x^2}{2} \right\} H_f(\alpha x) \] (3.10)

As described in section 2.2 of previous chapter, the maximum number of quantum states supported by a planar channel (surrounded by two planes) is estimated from the equation given by

\[ \left( i_{\text{max}} + \frac{1}{2} \right) \hbar \omega = \frac{1}{2} k x_{\text{max}}^2. \] (3.11)

The maximum number of quantum states in undistorted continuum potential \( i_{\text{max}} = f_{\text{max}} \) is taken as 3. However, the number of quantum states available in the distorted portions '1' and '2' is estimated using Eqn. (3.6) which is found to be

\[ i_{\text{1}}^{(1)} = k_{\text{2}}^{(2)} \] corresponding to a channel situated at a distance of \( 15r_0 \) from the dislocation \( (r_0 \text{ obtained from Eqn.}(3.1) \) and for the present case of \( \text{Al}(111), b \) is taken as 2.86A). As shown in Fig. (3.5), this \( j_{\text{max}}^{(1)} \) approaches to \( i_{\text{max}} \) for those channels at the farthest distance from the core.
Chapter III: Quantum description of

3.3.1 Channeling probabilities across(I) interface:

The channeling probability of the particle with initial state $\psi_i$ to cross first interface and to be in state $\psi_j$ in distorted part, can be defined as

$$p_{i \rightarrow j} = |\langle \psi_j^{(1)} | \psi_i \rangle|^2$$

(3.12)

where subscript ‘1’ on the state denotes the relevant wave function corresponds to distorted channel after I interface.

We have

$$|\langle j^{(1)} | i \rangle|^2 = \left( \frac{\alpha \alpha^l}{\pi 2^{j^{(1)}+i^{(1)}}!} \right) \exp \left\{ - \left( \frac{\alpha l^2}{\alpha^2 + \alpha l^2} \right) \alpha^2 a_r^2 \right\}$$

$$\times \left| \int_{-\infty}^{\infty} \exp \left\{ - \frac{1}{2} \left( \alpha^2 + \alpha^2 \right) \left[ x + \frac{\alpha l^2}{\alpha^2 + \alpha l^2} \right] \right\} H_j (\alpha^l x + \alpha^l a_r) H_i (\alpha x) \right|^2$$
Chapter III: Quantum description of

For example consider,

i) $|\langle 0^{(1)}|0 \rangle|^2$:

$$ = \left( \frac{\alpha \alpha'}{\pi} \right) \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} \times \left| \int_{-\infty}^{\infty} \exp \left\{ - \frac{1}{2} \left( \alpha^2 + \alpha'^2 \right) \left[ x + \frac{\alpha'^2}{\alpha^2 + \alpha'^2} a_r \right] \right\} \ H_0 \left( \alpha x + \alpha' a_r \right) \ H_0 \left( \alpha x \right) \right|^2 $$

$$ = \frac{2\alpha \alpha'}{\alpha^2 + \alpha'^2} \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} $$

$$ |\langle 0^{(1)}|0 \rangle|^2 \Rightarrow 2 \left( \frac{\tau}{1 + \tau^2} \right) \exp \left\{ - \frac{\tau^2}{1 + \tau^2} \alpha^2 a_r^2 \right\} $$

ii) $|\langle 1^{(1)}|0 \rangle|^2$:

$$ = \left( \frac{\alpha \alpha'}{2\pi} \right) \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} \times \left| \int_{-\infty}^{\infty} \exp \left\{ - \frac{1}{2} \left( \alpha^2 + \alpha'^2 \right) \left[ x + \frac{\alpha'^2}{\alpha^2 + \alpha'^2} a_r \right] \right\} \ H_1 \left( \alpha x + \alpha' a_r \right) \ H_0 \left( \alpha x \right) \right|^2 $$

$$ = \frac{4\alpha \alpha'}{\alpha^2 + \alpha'^2} \left( \alpha'^2 a_r^2 \right) \left( \alpha^2 / \alpha^2 + \alpha'^2 \right)^2 \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} $$

$$ |\langle 1^{(1)}|0 \rangle|^2 \Rightarrow \left( \frac{4\tau}{1 + \tau^2} \right) \left( \frac{\tau}{1 + \tau^2} \right)^2 \alpha^2 a_r^2 \exp \left\{ - \frac{\tau^2}{1 + \tau^2} \alpha^2 a_r^2 \right\} $$

iii) $|\langle 2^{(1)}|0 \rangle|^2$:

$$ = \left( \frac{\alpha \alpha'}{8\pi} \right) \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} \times \left| \int_{-\infty}^{\infty} \exp \left\{ - \frac{1}{2} \left( \alpha^2 + \alpha'^2 \right) \left[ x + \frac{\alpha'^2}{\alpha^2 + \alpha'^2} a_r \right] \right\} \ H_2 \left( \alpha x + \alpha' a_r \right) \ H_0 \left( \alpha x \right) \right|^2 $$

$$ = \frac{\alpha \alpha'}{4(\alpha^2 + \alpha'^2)} \left[ \frac{\alpha^2 - \alpha'^2}{\alpha^2 + \alpha'^2} + 4\alpha'^2 a_r^2 \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right)^2 \right]^2 \exp \left\{ - \left( \frac{\alpha'^2}{\alpha^2 + \alpha'^2} \right) \alpha^2 a_r^2 \right\} $$

$$ |\langle 2^{(1)}|0 \rangle|^2 \Rightarrow \left( \frac{\tau}{4(1 + \tau^2)} \right) \left[ \frac{(\tau^2}{1 + \tau^2} \right]^2 \alpha^2 a_r^2 \exp \left\{ - \frac{\tau^2}{1 + \tau^2} \alpha^2 a_r^2 \right\} $$

$$ = |\langle 0^{(1)}|2 \rangle|^2 $$
Chapter III: Quantum description of .......... 7b

By incorporating appropriate Hermite functions in the overlap integral one can obtain the other expressions for these transition amplitudes. The details of these expressions are given in the APPENDIX. Here it can easily be verified that $|\langle i | j^{(1)} \rangle|^2 = |\langle j^{(1)} | i \rangle|^2$. The corresponding probability for the particle with initial state $|i\rangle$ (in the straight part of the channel), to occupy any one of the states $|j^{(1)}\rangle$ ($j_{\text{max}} < i_{\text{max}}$) in the distorted portion I is:

$$p_i^I = \sum_{j=0}^{2\text{max}} |\langle j^{(1)} | i \rangle|^2$$  \hspace{1cm} (3.13)

So the dechanneling probability at (I) is $\chi_i^I = 1 - p_i^I \cdot$

3.3.2 Channeling probabilities across (II) interface:

The channeling probability of the particle with intermediate state $|j\rangle$ to cross second interface and to occupy a state $|k\rangle$ can be defined as

$$p_{j\rightarrow k} = |\langle \psi_k^{(2)} | \psi_j^{(1)} \rangle|^2$$  \hspace{1cm} (3.14)

Here subscript '2' denotes the wave function in second part of distorted channel after crossing 'II' interface.

Corresponding probability of the particle to occupy any one of the states $|k\rangle$ ($k_{\text{max}} < i_{\text{max}}$) is:

$$p_{j^{(1)}} = \sum_{k=0}^{k_{\text{max}}} |\langle k^{(2)} | j^{(1)} \rangle|^2; \chi_{j^{(1)}} = 1 - p_{j^{(1)}}$$  \hspace{1cm} (3.15)

To evaluate various matrix elements in this case, we make use of the general expression obtained for $(j \& k)$ in the previous chapter and one may notice here that $|\langle k^{(2)} | j^{(1)} \rangle|^2 = |\langle j^{(2)} | k^{(1)} \rangle|^2$. These details are given in APPENDIX - II.
3.3.3 Channeling probabilities across (III) interface:

The channeling probability of the particle with intermediate state \( |k\rangle \) to cross third interface and to occupy any one of the states \( |f\rangle \) \(( f < i \rangle \) is:

\[
P^\text{III}_k = \sum_{f=0}^{3} |\langle f | k^{(2)} \rangle|^2; \chi^\text{III}_k = 1 - p^\text{III}_k
\]

with

\[
p^0_{k(3) \rightarrow f} = |\langle f | k^{(2)} \rangle|^2
\]

For Example,

\[
p^\text{(3)}_{0(2) \rightarrow 0} = |\langle 0 | 0^{(2)} \rangle|^2 = 2 \frac{\tau}{1 + \tau^2} \exp \left\{ - \frac{\tau^2}{1 + \tau^2} a_r^2 \right\} = |\langle 0^{(1)} | 0 \rangle|^2
\]

The details of these expressions are given in the APPENDIX - I. Further, it can be shown that \( |\langle f | k^{(2)} \rangle|^2 = |\langle j^{(1)} | i \rangle|^2 \) for the same quantum numbers of ‘\( k \)’ and ‘\( j \)’. The transition probability for the passage of initially well channeled particle through dislocation will be product of the transition probabilities across various parts of the channel, where the effects of distortion are suitably incorporated. The general expression for the total channeling probability of the particle with a specific initial state \( |i\rangle \) so that the particle feels itself again in the straight channel with final state \( |f\rangle \) (after passing through the various portions of distortion) has been obtained and is given by [15]

\[
p_{i \rightarrow f} = \sum_{k^{(2)} = 0}^{k_{\text{max}}} \left( p^\text{(2)}_{k^{(2)} \rightarrow f} \left[ \sum_{j^{(1)} = 0}^{j_{\text{max}}} p_{i \rightarrow j^{(1)}} \times p_{j^{(1)} \rightarrow k^{(2)}} \right] \right) = p_{f \rightarrow i}
\]

The total channeling probability for initially well channeled particle, to find itself again in the straight channel after passing through various portions of the distortions is given by

\[
p_0 = \sum_{f=0}^{f_{\text{max}}=3} (p_0 \rightarrow f); \chi_0 = 1 - p_0
\]

These probabilities are calculated by incorporating the above equations and results are given in Fig. (3.6 - 3.8)
3.4 Results and Discussion:

We have developed a quantum theory of dechanneling due to defects with special reference to dislocations. The theory is valid as long as the number of quantum states supported by the transverse potential due to the two planes is small and is the case of light particles (like positrons) in Mev range. We studied the dechanneling processes by continuous distortions of the planar channels, mapping to three distinct regions and corresponding displaced and modified wavefunctions. This happens for channels far away from the dislocation which in turn implies applicability of present calculation to lower concentrations (i.e. no interaction between dislocations). On the other hand the channels close to the dislocation axis, the distortion is so heavy that one can not talk of crystallographic channels.

In Fig. 3.3, we show the variation of the distortion parameter ‘\( r \)’ with \( r_0 \). We notice that, for larger \( r_0 \) the radius of curvature (R) of distorted planar channel increases to infinity, \( a_r \to 0 \) and \( r \to 1 \) as expected because the coupling terms in the wavefunctions are identical, the particle recognizes the absence of distortions in those regions and obviously the non-diagonal matrix elements vanish for \( a_r = 0 \), implying that a well-channeled particle cannot suddenly go to oscillatory behaviour in an undistorted channel. In Fig. 3.5, we have shown variation of maximum number of allowed states in the distorted channel as a function of distance from the dislocation. The atomic planes at considerably larger distances from the core are distorted slightly and thus ‘\( r_0 \)’ carries the signature of the distortion effects. We notice that \( j_{\text{max}} \) approaches asymptotically to \( i_{\text{max}}(=3) \) as \( r_0 \) increases (i.e. the channel is almost straight). As mentioned earlier this depends on the concentration of dislocations, thus for lower concentrations we have a family of channels through which a particle can propagate successfully without much dechanneling. We consider the channels starting from \( 15r_0 \) (this corresponds to a
concentration $\approx 3 \times 10^8$ dislocations/cm$^2$, below this the channels are distorted heavily leading to formation of dislocation loops) to a farthest distance $50r_0$ (this dislocation concentration is typically $\approx 2 \times 10^7$/cm$^2$).

The results for channeling probabilities obtained from expressions (3.18) and (3.19) have been plotted in Figs. (3.6 & 3.7) for initially well channeled particle (i.e. ground state) and first excited state respectively. One may notice that at some values of $r_0$, there is sharp increase in the probability for individual transitions. This is result of change in the number of states supported in the distorted portions of channel (i.e., after I & II interfaces). This is also reflected in the overall dechanneling probabilities $\chi_0$ and $\chi_1$ respectively, because corresponding channeling probabilities approaches unity for the channels situated at the farthest from the dislocation axis, which means that slight dissociation of dislocations reduces their long range distortion as discussed in classical analysis.

Fig. 3.6: Influence of channel distance from the dislocation on channeling probabilities corresponding to initially well channeled particle ($\langle \psi \rangle = |0\rangle$).
As shown in Fig. (3.8), the overall dechanneling probabilities for initially well channeled particle (xₒ) always less for any channel as compared to χ₁ (particle initially in first excited state) because well channeled particle, even after making transitions to other excited states in distorted portions of the channel, manages to remain channeled for higher curvatures (lesser radii of curvatures) than does the initially excited (oscillating) particle. In the present simple model calculation these effects are manifested in natural way.
If the particle after passing through various portions of distortions goes to a state which is same as initial state, corresponding channeling/transition probability is much higher as compared to other transitions. This is expected and can also be seen through the asymmetric nature of the planar channel. The channeling probabilities corresponding to different initial and final states combination are very low, and approach zero as channel distance increases from the dislocation. So the dechanneling probability depends upon final state of the particle which in turn reflects the phase dependence of the approaching particle, near the distortion.
The equation (3.18) carries the signature of interesting left-right symmetry inbuilt in the problem which is not clearly realized in classical descriptions. Fig. (3.9) shows the energy dependence of dechanneling probabilities, for initially well channeled particles. At the lower end of these relativistic energies, it is linear variation and as energy increases to higher side of relativistic energy, the energy dependence tends to be slower than linear.

**Fig. 3.9** : Energy dependence of total dechanneling probability of initially well channeled particle ‘$x_0$’.
Chapter III: Quantum description of

APPENDIX -

Evaluation of individual transition amplitudes: $|\langle j^{(1)} | i \rangle|^2$

Here we denote $\beta = \frac{\tau}{1 + \tau^2}$, $\xi = \frac{\tau^2}{1 + \tau^2}$, and $E x = \exp\{-\xi a^2 a^*_r\}$; this notion makes the final expressions for transition amplitudes more compact. By substituting the Hermite functions corresponding to various states and evaluating the integrals, the expressions for individual transition amplitudes are obtained as:

\[
|\langle 0^{(1)} | 0 \rangle|^2 = 2 \beta E x
\]
\[
|\langle 1^{(1)} | 0 \rangle|^2 = 4 \beta^3 \alpha^2 a^*_r E x
\]
\[
|\langle 2^{(1)} | 0 \rangle|^2 = \frac{\beta}{4} \left[ 4 \beta^2 \alpha^2 a^*_r + 2 \left( \frac{1 - \tau^2}{1 + \tau^2} \right) \right]^2 E x
\]
\[
|\langle 3^{(1)} | 0 \rangle|^2 = \frac{\beta}{24} \left[ \alpha a_r \left( 24 \tau \xi^2 - 36 \tau \xi + 12 \tau \right) + \alpha^3 a^*_r \left( 8 \tau^3 \xi^3 + 24 \tau \xi^2 - 8 \tau^3 \right) \right]^2 E x
\]
\[
|\langle 0^{(1)} | 1 \rangle|^2 = 4 \beta \xi^2 \alpha^2 a^*_r E x
\]
\[
|\langle 1^{(1)} | 1 \rangle|^2 = 8 \beta^3 \left[ 1 - \xi \alpha^2 a^*_r \right]^2 E x
\]
\[
|\langle 2^{(1)} | 1 \rangle|^2 = \frac{\beta}{8} \left[ \alpha a_r \left( 24 \xi^2 - 20 \xi \right) + \alpha^3 a^*_r \left( 8 \tau^2 \xi^3 - 16 \tau^2 \xi^2 + 8 \tau^2 \xi \right) \right]^2 E x
\]
\[
|\langle 3^{(1)} | 1 \rangle|^2 = \frac{\beta}{48} \left[ (48 \beta \xi - 24 \beta) + \alpha^2 a^*_r \left( 96 \tau^3 \xi^3 - 16 \tau^3 \xi^2 + 72 \tau \xi \right) + \alpha^4 a^*_r \left( 16 \tau^3 \xi^4 + 48 \tau \xi^3 - 16 \tau^3 \xi \right) \right]^2 E x
\]
\[
|\langle 0^{(1)} | 2 \rangle|^2 = \frac{\beta}{4} \left[ 2 \left( \frac{1 - \tau^2}{1 + \tau^2} \right) + 4 \xi^2 \alpha^2 a^*_r \right]^2 E x
\]
\[
|\langle 1^{(1)} | 2 \rangle|^2 = \frac{\beta}{8} \left[ 8 \beta \xi^2 \alpha^3 a^*_r + 4 \beta \alpha a_r - 24 \beta \xi \alpha a_r \right]^2 E x
\]
\[
|\langle 2^{(1)} | 2 \rangle|^2 = \frac{\beta}{32} \left[ 48 \beta^2 + \alpha^2 a^*_r \left( 96 \tau^2 \xi^3 - 96 \tau^2 \xi^2 + 8 \tau^2 \xi + 16 \xi - 8 \tau^2 \right) + \alpha^4 a^*_r \left( 16 \tau^2 \xi^4 - 32 \tau^2 \xi^3 + 16 \tau^2 \xi^2 \right) - 4 \right]^2 E x
\]
Chapter III: Quantum description of

\[
|\langle 3^{(1)}|2 \rangle|^2 = \frac{\beta}{192} \left[ \alpha a_r \left( -480\beta\xi^2 + 432\beta\xi + 48\tau\xi^2 - 48\beta - 72\tau\xi + 24\tau \right) \\
+ \alpha^3 a_r^3 \left( -320\tau\xi^4 + 624\tau\xi^3 - 336\tau\xi^2 + 16r^3\xi^3 + 32\tau\xi + 48\tau\xi^2 - 16\tau^3 \right) \\
+ \alpha^5 a_r^5 \left( -32\tau^3\xi^5 - 96\tau\xi^4 + 32\tau^3\xi^2 \right) \right]^2 E \chi
\]

\[
|\langle 0^{(1)}|3 \rangle|^2 = \frac{\beta}{24} \left[ 12\xi \alpha a_r - 24\beta^2 \alpha a_r - 8\xi^3 \alpha^3 a_r^3 \right]^2 E \chi
\]

\[
|\langle 1^{(1)}|3 \rangle|^2 = \frac{\beta}{48} \left[ 24 \left( \frac{1 - \tau^2}{1 + \tau^2} \right) \beta + 96\beta\xi^2 \alpha^2 a_r^2 - 48\beta\xi\alpha^2 a_r^2 - 16\beta^3 \alpha^4 a_r^4 + 24\beta\xi\alpha^2 a_r^2 \right]^2 E \chi
\]

\[
|\langle 2^{(1)}|3 \rangle|^2 = \frac{\beta}{192} \left[ \alpha a_r \left( 144\xi^2 - 480\beta^2 \xi - 120\xi + 240\beta^2 \right) \\
+ \alpha^3 a_r^3 \left( -320\xi^4 + 48\tau^2\xi^3 + 400\xi^3 - 96\xi^2 - 96\tau^2\xi^2 + 48\tau^2 \xi \right) \\
+ \alpha^5 a_r^5 \left( -32\tau^2\xi^5 - 32\tau^2\xi^3 + 64\tau^2\xi^4 \right) \right]^2 E \chi
\]

\[
|\langle 3^{(1)}|3 \rangle|^2 = \frac{\beta}{1152} \left[ (960\beta^3 - 288\beta\xi - 144\beta \left( \frac{1 - \tau^2}{1 + \tau^2} \right) ) \\
+ \alpha^2 a_r^2 \left( 2880\beta\xi^3 - 3456\beta\xi^2 + 1008\tau\xi^2 + 864\beta\xi - 576\tau\xi^3 - 432\tau\xi \right) \\
+ \alpha^4 a_r^4 \left( 960\tau\xi^6 - 2016\tau\xi^4 - 96\tau^3\xi^4 + 288\tau^3\xi^3 + 1248\tau^3\xi^3 - 192\tau^2\xi^2 \\
- 288\tau^3\xi^2 + 96\tau^3\xi \right) + \alpha^6 a_r^6 \left( 64\tau^3\xi^6 - 192\tau^3\xi^5 + 192\tau^3\xi^4 - 64\tau^3\xi^3 \right) \right]^2 E \chi
\]
APPENDIX - II

Channeling probabilities across interface (II):

The wavefunctions in the regions (1) and (2) are given by $\varphi_j(\alpha'x + \alpha' a_s)$ and $\varphi_k(\alpha'x - \alpha' a_s)$ respectively. This is equivalent to shifting the origin so that the wavefunctions are about $x = 0$ and $x = 2a_s$ respectively. This enables us to make use of the general expression given in chapter 2. This can be shown mathematically as follows.

We have

$$\int_{-\infty}^{\infty} \varphi_j(x + a_s) \varphi_k(x - a_s) \, dx$$

Put $x - a_s = t$ (another variable)

$$\Rightarrow \int_{-\infty}^{\infty} \varphi_j(t + 2a_s) \varphi_k(t) \, dt$$

This expression is in the form of overlap integral, discussed in the chapter 2.

By replacing $\alpha$ with $\alpha'$ and $a_s$ with $2a_s$ in the results of the previous chapter, we obtain

$$|\langle 0^{(2)} | 0^{(1)} \rangle|^2 = \exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}$$

$$|\langle 1^{(2)} | 0^{(1)} \rangle|^2 = 2\tau^2 \alpha^2 a_r^2 \exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}$$

$$|\langle 2^{(2)} | 0^{(1)} \rangle|^2 = 2\tau^4 \alpha^4 a_r^4 \exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}$$

$$|\langle 3^{(2)} | 0^{(1)} \rangle|^2 = \frac{4\tau^6 \alpha^6 a_r^6}{3} \exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}$$

$$|\langle 0^{(2)} | 1^{(1)} \rangle|^2 = |\langle 1^{(2)} | 0^{(1)} \rangle|^2$$

$$|\langle 1^{(2)} | 1^{(1)} \rangle|^2 = \left( 1 - 2\tau^2 \alpha^2 a_r^2 \right) \exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}$$

$$|\langle 2^{(2)} | 1^{(1)} \rangle|^2 = \left( 4\tau \alpha a_r - 4\tau^3 \alpha^3 a_r^3 \right)^2 \frac{\exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}}{4}$$

$$|\langle 3^{(2)} | 1^{(1)} \rangle|^2 = \left( 24\tau^2 \alpha^2 a_r^2 - 16\tau^4 \alpha^4 a_r^4 \right)^2 \frac{\exp \left\{ -2\tau^2 \alpha^2 a_r^2 \right\}}{96}$$
\begin{align*}
|\langle 0|2 \rangle|^2 &= |\langle 2|0 \rangle|^2 \\
|\langle 1|2 \rangle|^2 &= |\langle 2|1 \rangle|^2 \\
|\langle 2|2 \rangle|^2 &= \left(2\tau^4\alpha^4 a_r^4 - 4\tau^2\alpha^2 a_r^2 + 1 \right)^2 \exp \left\{ -2\tau^2\alpha^2 a_r^2 \right\} \\
|\langle 3|2 \rangle|^2 &= \left(4\tau^5\alpha^5 a_r^5 - 12\tau^3\alpha^3 a_r^3 + 6\tau\alpha a_r \right)^2 \exp \left\{ -2\tau^2\alpha^2 a_r^2 \right\} / 6 \\
|\langle 0|3 \rangle|^2 &= |\langle 3|0 \rangle|^2 \\
|\langle 1|3 \rangle|^2 &= |\langle 3|1 \rangle|^2 \\
|\langle 2|3 \rangle|^2 &= |\langle 3|2 \rangle|^2 \\
|\langle 3|3 \rangle|^2 &= \left(3 - 18\tau^2\alpha^2 a_r^2 + 18\tau^4\alpha^4 a_r^4 - 4\tau^6\alpha^6 a_r^6 \right)^2 \exp \left\{ -2\tau^2\alpha^2 a_r^2 \right\} / 9
\end{align*}

One can easily notice here that $|\langle j^{(1)}|i \rangle|^2 = |\langle i|j^{(1)} \rangle|^2 \Rightarrow p_{i\rightarrow j^{(0)}} = p_{j^{(0)}\rightarrow i}$.

So we have

\begin{align*}
|\langle 1|0^{(2)} \rangle|^2 &= |\langle 0^{(1)}|1 \rangle|^2; \quad |\langle 2|0^{(2)} \rangle|^2 &= |\langle 0^{(1)}|2 \rangle|^2; \\
|\langle 3|0^{(2)} \rangle|^2 &= |\langle 0^{(1)}|3 \rangle|^2; \quad |\langle 0|1^{(2)} \rangle|^2 &= |\langle 1^{(1)}|0 \rangle|^2; \\
|\langle 1|1^{(2)} \rangle|^2 &= |\langle 1^{(1)}|1 \rangle|^2; \quad |\langle 2|1^{(2)} \rangle|^2 &= |\langle 1^{(1)}|2 \rangle|^2
\end{align*}

and

\begin{align*}
|\langle 3|1^{(2)} \rangle|^2 &= |\langle 1^{(1)}|3 \rangle|^2.
\end{align*}
References

[1] F. R. N. Nabarro Adv. in Phys. 1, 269 (1952);
J. Friedel, Dislocations (Pergamon, N. Y.), 1964.


Rad. Eff. 51, 127 (1980); A. P. Pathak, Phys. Lett. 55A, 104 (1975);
57A, 467 (1976).


Hiroshi Kudo J. Phys. Soc. Jpn. 40, 1640 (1976);


[8] L. N. S. Prakash Goteti and Anand P. Pathak


[10] Azher M. Siddiqui, V. Harikumar, L. N. S. Prakash Goteti and


*Nuclear Inst. and Meth. in Phys. Res.* B 48, 167 (1990);
M.A. Khumakov, *Nuclear Instrum. and Meth. in Phys. Res.* B 48, 167 (1990);
W. E. Gibson, I. J. Kim, M. Pisharody, S. M. Salman, C. R. Sun
G. H. Wang and R. Wijayawardana, J. S. Forster and I. V. Mitchell,
T. S. Nigmanov and E. N. Tsyganov, S. I. Baker, R. A. Carrigan Jr.,
and T. E. Toohig, V. V. Avdeichikov, J. A. Ellison, P. Siffert