3.1 Introduction to Crystal Defects and Dechanneling

One of the main applications of ion channeling is the studies of various kinds of defects. It is well known that real crystals are never perfect. The most common kinds of defects found in solids are point defects which include lattice vacancies, interstitials, color centres etc, line defects like edge dislocations, screw dislocations etc and plane defects like grain boundaries, stacking faults etc.

A particle propagating through real solids can ‘see’ the presence of the defects through their effects in the solids. Classically, particles can see the presence of defects either by direct obstruction of the particle path or through the distortion produced
in the crystal or even both. When the projectile directly hits the defect sites or is scattered in the potential field of the defects obstructing the open channels and the trajectory gets modified as a consequence, the effects are said to be of obstruction type. Examples are stacking faults, interstitial atoms, grain or twin boundaries. If, on the other hand, the defects give rise to distortion in a certain region of the crystal, disturbing the regularity of the material in that region, the effects are of distortion type. The most important example here is that of dislocations. These two qualitatively different types of defects give rise to obstruction dechanneling and distortion dechanneling respectively.

Dechanneling may also be caused by a combination of both the types of defects. In such cases dechanneling is neither purely of obstruction type nor of distortion type. This phenomena is called composite dechanneling. This happens because of the fact that the defects produced in the solid are not uniquely of one type but a combination of different kinds of defects or because the defect itself gives rise partially to obstruction effects and partially to distortion effects. Examples are gas bubbles [51, 52], Guinier-Preston zones [53], voids and antiphase boundaries. The simultaneous use of channeling, back scattering and TEM [54] can correlate the dechanneling observations with damage configurations.

Classically, the dechanneling effects depend on the transverse energy. Transverse energy is increased when the particles are in the vicinity of the defects and when it exceeds a critical value \( (E\psi^2) \), the particles get dechanneled [55]. Quantum mechanically, this transverse energy is quantized. Due to the influence of defects, transverse energy is increased and the particles go to one of the excited states. If this influence is strong, the particles go above the barrier, and are no longer bounded. Therefore quantum mechanically, dechanneling means transition from bound state to scattering state due to the increase in transverse energy.
Such effects and transitions to scattering states leading to dechanneling take place due to distortions in the channels situated in the vicinity of dislocation core. Here the atomic rows and planes exhibit curvature which alters the trajectory of the channeled particle and can dechannel the particle altogether if the curvature is large enough to severely modify the trajectory. This distortion is maximum near the dislocation core and decreases as one moves away from the core [56]. Thus one can think of a cylindrical region around the dislocation axis, called ‘dechanneling cylinder’ [57]. Figure 3.1 illustrates how the distortion of channels outside a particular region of radius $r_0$ around the dislocation core; i.e., the dechanneling cylinder, decreases. The effects of dislocations are introduced through the curvature of the channels. The effect of this curvature is to introduce a transverse centrifugal force on the propagating particles. This force should therefore be combined with the force due to the continuum potential (longitudinal).

Figure 3.1: The dislocation affected planar channel. $R_{mc}$ is the minimal radius of curvature of the channel at a distance $r_0$ from the dislocation core.
Classical description of the dislocation effects on the channeling of positrons in the planar and axial cases [58, 59] has also been used to estimate the effects of such defects on the overall rate of energy loss of channeled particles. The corresponding quantum mechanical treatment of the effects of dislocations on channeling were given later [47, 60, 61]. In these investigations, a detailed relativistic framework was used to derive dechanneling probability and its energy dependence.

In this chapter, we consider a quantum mechanical model for the effects of dislocations on the initially well-channeled particles in a planar channel by considering both the transverse and longitudinal motion of the particles in the channel. We first consider the effects on positron planar channeling and later on electron channeling.

## 3.2 Electron and Positron Channeling

As mentioned in chapter 1, positively charged particles channeling along various crystallographic directions are bound to oscillate between the atomic rows or planes of atoms and are repelled by these rows or planes during its propagation. The corresponding transverse motion can be described by harmonic oscillator potential with equally spaced energy levels. On the other hand, the negatively charged particles like electrons are attracted towards the atomic planes or axes and cross them. Hence the electrons have increased probability for hard collisions with atoms and the transverse potential is approximated to one dimensional hydrogen atom [62]. Hence one can say that the continuum potential is simply the negative of that governing the motion of positrons. Figure 3.2 shows the transverse potentials of both positrons and electrons. Also Figure 3.3 illustrates the motion of electrons along a string of atoms. This helical motion of negatively charged particles is named "rosette motion" [50, 63, 64, 65, 66].
Figure 3.2: Planar potentials for 54.5 MeV positrons and electrons along (110) planes of Si and C respectively. For positrons the energy levels are equally spaced, whereas for electrons, it is not equally spaced.
3.3 Effects of Dislocations on Positron Channeling

We consider a typical channel at some distance from the dislocation core, outside the dechanneling cylinder so that the motion is influenced by the distortions but does not result in complete dechanneling. When the particles enter from an undistorted region of the channel to the distorted region, they see the curvature of the channel and experience additional centrifugal force. This results in modification of their trajectory following the curvature. The model is shown in Figure 3.4. The whole channel is divided into four regions. The dislocation affected parts of the channel are regions II and III. \( \rho_0 \) corresponds to the radial co-ordinate of the channel center as measured from the origin and \( \varphi_0 \) is the corresponding angular co-ordinate.
3.3.1 Shift in Potential Minima

We consider the particle motion in the four regions separately, considering both the longitudinal and transverse motions. The Schrodinger equation for planar channeling for a particle of mass $m$ moving in region I (perfect channel) can be written as,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)\Psi^I(x,z) + \frac{1}{2}m\omega^2x^2\Psi^I(x,z) = E^I\Psi^I(x,z) \quad (3.1)$$

where $E^I$ is the total energy and can be written as $E^I = E^I_T + E^I_L$ (with $E^I_T$ and $E^I_L$, the energy components associated with the transverse and longitudinal motion, respectively).

$$E^I_T(n,\omega) = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$E^I_L = \frac{\hbar^2 k^2}{2m} \quad (3.2)$$

where $\omega$ is the characteristic frequency obtained from the harmonic approximation to the planar potential

$$V_p(x) = V_0 x^2 \quad (3.3)$$
i.e.,
\[ \omega = \sqrt{\frac{2V_0}{m}} \]  
\tag{3.4}

After separation of variables, the equation of motion in the transverse and longitudinal directions can be written as,
\[ -\frac{\hbar^2}{2m} X''^I(x) + \frac{1}{2} m \omega^2 x^2 X^I(x) = E^I_T X^I(x) \]  
\tag{3.5}
\[ -\hbar^2 \frac{Z''^I(z)}{2m} = E^I_L Z^I(z) \]  
\tag{3.6}

whose solutions are given by,
\[ X^I(x) = \frac{\exp(-x^2/2\alpha^2)}{\sqrt{2^n n! \alpha \sqrt{\pi}}} H_n(x/\alpha) \]  
\tag{3.7}
\[ Z^I(z) = A e^{ikz} + B^{-ikz} \]  
\tag{3.8}

where
\[ \alpha = \sqrt{\frac{\hbar}{m\omega}} \]

The total wave function for the region I can be written as
\[ \Psi^I(x, z) = X^I_n(x - x_0) \ Z^I(z) \]  
\tag{3.9}

where \( x_0 \) is the initial amplitude of the channelon. Assuming that an initially well-channeled particle coming from left, interacts and undergoes reflections at the boundary (between I and II regions), the actual wavefunction in the first region has the effects of excited states also. Hence the total wavefunction can be written as,
\[ \Psi^I(x, z) = A_0 X^I_0 e^{ik_0 z} + \sum_{n=0} B_n X^I_n e^{-ik_n z} \]  
\tag{3.10}

Now consider the dislocation affected parts of the channel. We have two curved regions which are due to the centrifugal force proportional to \( \mu^2/\rho^2 \), where \( \mu \hbar \) is the angular momentum with \( \mu^2 = l(l + 1) \) with \( l \) as the orbital angular momentum quantum number and \( \rho \) is the radius of curvature of the channel.
In the second region of the channel, the Schrödinger equation is written in terms of the polar co-ordinates $\rho$ and $\varphi$ and is given by,

$$-rac{\hbar^2}{2m} \nabla_{\rho,\varphi}^2 \Psi^{II}(\rho, \varphi) + V(\rho) \Psi^{II}(\rho, \varphi) = E^{II} \Psi^{II}(\rho, \varphi)$$  \hspace{1cm} (3.11)

where the potential in this region is given by,

$$V(\rho) = \frac{1}{2} m \omega^2 (\rho - \rho_0)^2$$  \hspace{1cm} (3.12)

Here the distance '$x$' in the transverse direction is replaced by $\rho - \rho_0$, the corresponding distance in the $\rho$-direction. In this region, the $x, y, z$ components are written in terms of $\rho$ and $\varphi$ and are given by,

$$x = \rho \cos \varphi$$
$$y = y$$
$$z = \rho \sin \varphi$$

The particle motion is in the $x$-$z$ plane. Therefore, the '$y$' component remains the same. Now, Eqn. (3.11) can be re-written as,

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right] \Psi^{II}(\rho, \varphi) + \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 \Psi^{II}(\rho, \varphi) = E^{II} \Psi^{II}(\rho, \varphi)$$  \hspace{1cm} (3.13)

Separating variables gives azimuthal equation,

$$F''^{II}(\varphi) = -\mu^2 F^{II}(\varphi)$$  \hspace{1cm} (3.14)

with solution

$$F^{II}(\varphi) = C e^{i\mu \varphi} + D e^{-i\mu \varphi}$$  \hspace{1cm} (3.15)

and radial equation,

$$R''^{II}(\rho) + \frac{2m}{\hbar^2} \left[ E^{II} - \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 - \frac{\hbar^2 \mu^2}{2m \rho^2} \right] R^{II}(\rho) = 0$$  \hspace{1cm} (3.16)
From the above equation, we can write the effective potential in the region II as,

\[ V_{\text{eff}}(\rho) = \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 + \frac{\hbar^2 \mu^2}{2 m} \rho^2 \]  
(3.17)

Putting \( \xi = \rho - \rho_0 \),

\[ V_{\text{eff}}(\xi) = \frac{1}{2} m \omega^2 \xi^2 + \frac{\hbar^2}{2 m} \frac{\mu^2}{(\xi + \rho_0)^2} \]

Since \( \xi \ll \rho_0 \), we may expand \( V_{\text{eff}} \) to second order around \( \xi = 0 \),

\[ V_{\text{eff}}(\xi) = V(0) + \left( \frac{dV_{\text{eff}}}{d\xi} \right)_{\xi=0} \xi + \frac{1}{2} \left( \frac{d^2V_{\text{eff}}}{d\xi^2} \right)_{\xi=0} \xi^2 \]  
(3.18)

Putting \( a = \sqrt{\frac{\mu^2}{m} \rho_0} \),

\[ V_{\text{eff}} = \frac{\hbar^2}{2m} \left[ \frac{a^4 \xi^2}{\lambda} + \frac{\mu^2}{(\xi + \rho_0)^2} \right] \]  
(3.19)

The above equation gives,

\[ V(0) = \frac{\hbar^2 \mu^2}{2m \rho_0^2} \]  
(3.20)

\[ \frac{dV_{\text{eff}}}{d\xi} = \frac{\hbar^2}{2m} \left[ 2a^4 \xi - \frac{2\mu^2}{(\xi + \rho_0)^3} \right] \]  
(3.21)

\[ \frac{d^2V_{\text{eff}}}{d\xi^2} = \frac{\hbar^2}{2m} \left[ 2a^4 + \frac{6\mu^2}{(\xi + \rho_0)^4} \right] \]  
(3.22)

Substituting the above values in Eqn. (3.18), we get the effective potential for the region II given by,

\[ V_{\text{eff}}(\xi) = \frac{\hbar}{2m} \left[ \frac{\lambda}{\rho_0^4} \right] (\xi - a_p)^2 + U_{\text{min}} \]  
(3.23)

where

\[ \lambda = a^4 \rho_0^4 + 3 \mu^2 \]

\[ a_p = \frac{\mu^2 \rho_0}{\lambda} \]

\[ U_{\text{min}} = \frac{\mu^2 (\lambda - \mu^2)}{\rho_0^2 \lambda} = \frac{2m}{\hbar^2} V_{\text{min}} \]

This equation of effective potential (Eqn. (3.23)) corresponds to a harmonic oscillator with frequency,

\[ \omega' = \frac{\hbar}{m} \left( \frac{\lambda}{\rho_0^4} \right)^{1/2} \]  
(3.24)
The qualitative shape of the potential is shown in Figure 3.5. It is observed that the effect of centrifugal force shifts the potential curve; the new curve is centered at $a_p$ with a shift $V_{min}$ in energy minimum. Furthermore, the effective transverse potential is no longer completely harmonic.

![Figure 3.5: The shape of the effective potential in the third region of the dislocation affected channel (region II) for positrons.](image)

The wavefunction for region II can be written as,

$$
\Psi^{II}(\rho, \varphi) = \sum_{m=0}^{\infty} R_{m}^{II} \left[ C_{m} e^{i\mu \varphi} + D_{m} e^{-i\mu \varphi} \right]
$$

(3.25)

Putting $\eta = \xi - a_p = \rho - \rho_0 - a_p$, the radial equation in Eqn. (3.16) can now be written as,

$$
R''^{II}(\eta) + \left[ \frac{\hbar^2}{2m} E^{II} - \frac{\lambda}{\rho_0^2} \eta^2 + U_{min} \right] R^{II}(\eta) = 0
$$

(3.26)

with solution,

$$
R_{n'}^{II}(\eta) = \left( \frac{m \omega'}{\pi \hbar} \right)^{1/4} \frac{1}{(2^{n'} n')^{-1/2}} H_{n'}(b \eta) e^{-b^2 \eta^2 / 2}
$$

(3.27)

where $b = (m \omega' / \hbar)^{1/2}$. 

60
For the third region, the Schrödinger equation in polar coordinates becomes,

$$-\frac{\hbar^2}{2m} \left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right] \Psi^{III}(\rho, \varphi) + \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 \Psi^{III}(\rho, \varphi) = E^{III} \Psi^{III}(\rho, \varphi)$$

(3.28)

Separating variables gives azimuthal equation,

$$F''^{III}(\varphi) = -\mu^2 F^{III}(\varphi)$$

(3.29)

with solution,

$$F^{III}(\varphi) = Ge^{i\mu\varphi} + He^{-i\mu\varphi}$$

and radial equation,

$$R''^{III}(\rho) + \frac{2m}{\hbar^2} \left[ E^{III} - \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 + \frac{\hbar^2 \mu^2}{2m \rho^2} \right] R^{III}(\rho) = 0$$

(3.30)

The effective potential, in the third region can be written as

$$V'_{eff}(\rho) = \frac{1}{2} m \omega^2 (\rho - \rho_0)^2 - \frac{\hbar^2 \mu^2}{2m \rho^2}$$

(3.31)

Using the Eqn. (3.18), the corresponding equations for (3.20 to 3.22) are given by,

$$V'(0) = -\frac{\hbar^2 \mu^2}{2m \rho_0^2}$$

(3.32)

$$\frac{dV'_{eff}}{d\xi} = \frac{\hbar^2}{2m} \left[ 2a^4 \xi + \frac{2\mu^2}{(\xi + \rho_0)^3} \right]$$

(3.33)

$$\frac{d^2V'_{eff}}{d\xi^2} = \frac{\hbar^2}{2m} \left[ 2a^4 - \frac{6\mu^2}{(\xi + \rho_0)^4} \right]$$

(3.34)

which give the effective potential in the IIIrd region as,

$$V'_{eff}(\xi) = \frac{\hbar}{2m} \left[ \left( \frac{\lambda'}{\rho_0} \right) (\xi - a'_p)^2 + U'_{min} \right]$$

(3.35)

where

$$\lambda' = a^4 \rho_0^4 - 3\mu^2$$

$$a'_p = \frac{\mu^2 \rho_0}{\lambda'}$$

$$U'_{min} = -\frac{\mu^2 (\lambda' + \mu^2)}{\rho_0^2 \lambda'} = -\frac{2m \lambda'}{\hbar^2 \lambda'_{min}}$$
The potential equation; Eqn. (3.35) corresponds to a harmonic oscillator with frequency,

\[
\omega'' = \frac{\hbar}{m} \left( \frac{\lambda'}{\rho_0^3} \right)^{1/2}
\]  

(3.36)

The shape of this potential is shown in Figure 3.6. It is observed that the effect of the centrifugal force shifts the potential curve as in region II, but in a direction opposite to it. The new curve is centered at \( a' \rho \) with a negative shift of \( V_{min}' \) in energy minimum.

It is observed from the above calculations that the curvature of the channel induces a shift in the equilibrium axis for channeling which changes the frequency of oscillation from \( \omega \) to \( \omega' \) and \( \omega'' \) in the first and second regions of the curved channel respectively.

![Figure 3.6: The shape of the effective potential in the second region of the dislocation affected channel (region III) for positrons.](image)
The total wavefunction in the third region can be written as

$$\Psi^{III}(\rho, \varphi) = \sum_{m=0} R_{m}^{III} \left[ G_{m} e^{i\mu \varphi} + H_{m} e^{-i\mu \varphi} \right]$$

where

$$R_{m}^{III}(\eta') = \left( \frac{m \omega''}{\pi \hbar} \right)^{1/4} (2^{n'} n'!)^{-1/2} H_{m}(b' \eta') e^{-b'^{2} \eta'^{2}/2}$$

with $b' = (m \omega''/\hbar)^{1/2}$ and $\eta' = \xi + \alpha'_{p} = \rho - \rho_{0} + \alpha'_{p}$.

In the fourth region (i.e., the perfect channel), there will be only the transmitted wave and the wave function in this region is given by,

$$\Psi^{IV}(x, z) = X^{IV}_{n} I_{n} e^{ik_{n} z}$$

### 3.3.2 Channeling and Dechanneling Probabilities

Now we proceed to find the reflection and transmission coefficients. We have 4 regions and 3 boundaries separating them. The boundary conditions across these regions are given by the following equations,

$$\Psi^{I}|_{z=0} = \Psi^{II}|_{\varphi=0}$$

$$\frac{\partial \Psi^{I}}{\partial z} \bigg|_{z=0} = \frac{1}{\rho_{0}} \frac{\partial \Psi^{II}}{\partial \varphi} \bigg|_{\varphi=0}$$

$$\Psi^{II}|_{\varphi=\varphi_{0}} = \Psi^{III}|_{\varphi=0}$$

$$\frac{\partial \Psi^{II}}{\partial \varphi} \bigg|_{\varphi=\varphi_{0}} = \frac{\partial \Psi^{III}}{\partial \varphi} \bigg|_{\varphi=0}$$

$$\Psi^{III}|_{\varphi=\varphi_{0}} = \Psi^{IV}|_{z=t}$$

$$\frac{1}{\rho_{0}} \frac{\partial \Psi^{III}}{\partial \varphi} \bigg|_{\varphi=\varphi_{0}} = \frac{\partial \Psi^{IV}}{\partial z} \bigg|_{z=t}$$
We use the above boundary conditions in the wavefunction of the 4 regions given by the equations, (3.10), (3.25), (3.37) and (3.39).

Eqn. (3.40) \[ AX^I + BX^I = R^I_m(C + D) \] (3.46)

Eqn. (3.41) \[ \frac{k\rho_0}{\mu} AX^I - BX^I = R^I_m(C - D) \] (3.47)

Eqn. (3.42) \[ R^I_m[C e^{i\mu\varphi_0} + De^{-i\mu\varphi_0}] = R^I_{m}(G + H) \]

which gives,

\[ G + H = \langle R^I_{m}|R^I_{m} > [C e^{i\mu\varphi_0} + De^{-i\mu\varphi_0}] \] (3.48)

Eqn. (3.43) \[ R^I_m[C e^{i\mu\varphi_0} - De^{-i\mu\varphi_0}] = R^I_{m}(G - H) \]

which gives,

\[ G - H = \langle R^I_{m}|R^I_{m} > [C e^{i\mu\varphi_0} - De^{-i\mu\varphi_0}] \] (3.49)

Eqn. (3.44) \[ R^{III}_m[G e^{i\mu\varphi_0} + He^{-i\mu\varphi_0}] = IX^{IV} e^{ikt} \] (3.50)

Eqn. (3.45) \[ \frac{i\mu R^{III}_m}{\rho_0}[G e^{i\mu\varphi_0} - He^{-i\mu\varphi_0}] = ikIX^{IV} e^{ikt} \] (3.51)

From the above equations we need to find $\left| \frac{B}{A} \right|^2$ which gives the reflection co-efficient.

From Equations (3.46) and (3.47), we get,

\[ C = \frac{1}{2} \langle R^I_{m}|X^I > \left[ A \left( 1 + \frac{k\rho_0}{\mu} \right) + B \left( 1 - \frac{k\rho_0}{\mu} \right) \right] \] (3.52)

\[ D = \frac{1}{2} \langle R^I_{m}|X^I > \left[ A \left( 1 - \frac{k\rho_0}{\mu} \right) + B \left( 1 + \frac{k\rho_0}{\mu} \right) \right] \] (3.53)

which gives the value of $\frac{B}{A}$ as,

\[ \frac{B}{A} = \frac{\frac{k\rho_0}{\mu} \left( \frac{C}{D} + 1 \right) - \left( \frac{C}{D} - 1 \right)}{\frac{k\rho_0}{\mu} \left( \frac{C}{D} + 1 \right) + \left( \frac{C}{D} - 1 \right)} \] (3.54)
From equations (3.48) and (3.49) we have,

\begin{align}
G &= <R_m^{II} | R_m^{II}> C e^{i \mu \varphi_0} \\
H &= <R_m^{III} | R_m^{III}> D e^{-i \mu \varphi_0}
\end{align}

The above equations (3.55) and (3.56) give,

\[ \frac{C}{D} = \frac{G}{H} e^{-2i \mu \varphi_0} \]  

Finally from equations (3.50) and (3.51) we have

\[ \frac{G}{H} = \frac{\mu + k \rho_0 e^{-2i \mu \varphi_0}}{\mu - k \rho_0} \]

Substituting Eqn. (3.58) in (3.57), we get the value of \( \frac{C}{D} \) as,

\[ \frac{C}{D} = \frac{\mu + k \rho_0 e^{-4i \mu \varphi_0}}{\mu - k \rho_0} \]

Substituting Eqn. (3.59) in Eqn. (3.54), we get,

\[ \frac{B}{A} = \frac{(k^2 \rho_0^2 - \mu^2)[1 - e^{-4i \mu \varphi_0}]}{(k^2 \rho_0^2 + \mu^2)[1 - e^{-4i \mu \varphi_0} - 2k \rho_0 \mu [1 - e^{-4i \mu \varphi_0}]} \]

Now substituting,

\[
1 - e^{-4i \mu \varphi_0} = 2ie^{2i \mu \varphi_0} \sin(2 \mu \varphi_0) \\
1 + e^{-4i \mu \varphi_0} = 2ie^{2i \mu \varphi_0} \cos(2 \mu \varphi_0)
\]

and solving, we get the reflection co-efficient as

\[ \frac{|B|^2}{|A|} = |R|^2 = \frac{(-\mu^2 + k^2 \rho_0^2)^2 \sin^2(2 \mu \varphi_0)}{4k^2 \mu^2 \rho_0^4 \cos^2(2 \mu \varphi_0) + (\mu^2 + k^2 \rho_0^2)^2 \sin^2(2 \mu \varphi_0)} \]

The transmission co-efficient is given by,

\[ 1 - |R|^2 = |T|^2 = \frac{4k^2 \rho_0^2 \mu^2}{4k^2 \mu^2 \rho_0^4 \cos^2(2 \mu \varphi_0) + (\mu^2 + k^2 \rho_0^2)^2 \sin^2(2 \mu \varphi_0)} \]
The reflection and transmission co-efficients given in the above equations give us the values of dechanneling and channeling probabilities respectively. These can be written, in terms of energy as

\[ |R|^2 = \frac{(-\mu^2 \hbar^2 + 2mE\rho_0^2)^2 \sin^2(2\mu\phi_0)}{8mE\mu^2\rho_0^2 \cos^2(2\mu\phi_0) + (\mu^2 \hbar^2 + 2mE\rho_0^2)^2 \sin^2(2\mu\phi_0)} \]  

(3.63)

\[ |T|^2 = \frac{8mE\rho_0^2 \mu^2}{8mE\mu^2\rho_0^2 \cos^2(2\mu\phi_0) + (\mu^2 \hbar^2 + 2mE\rho_0^2)^2 \sin^2(2\mu\phi_0)} \]  

(3.64)

The dependence of these probabilities on the parameters \(E\) and \(\rho_0\) are given in figures 3.7 and 3.8, taking the average values of \(\sin^2(2\mu\phi_0)\) and \(\cos^2(2\mu\phi_0)\) as 0.5. Here \(\rho_0\) is inversely related to the density of dislocations.

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Figure 3.7: The \(E\) and \(\rho_0\) dependence of dechanneling probability for positrons.

Now let us consider the case of maximum and minimum dechanneling probabilities. The maximum dechanneling takes place when the value of \(\rho_0\) is very small, i.e., when the curvature of the channel is very large. The figures 3.7 and 3.8 also show the channeling and dechanneling probabilities for the least value of \(\rho_0\) which
Figure 3.8: The $E$ and $\rho_0$ dependence of channeling probability for positrons.

gives maximum dechanneling and minimum channeling probabilities. The minimum dechanneling takes place at $\varphi_0=0$, i.e., when the channel is straight. The maximum value of $\varphi_0$ is found to be $\pi/(4\sqrt{2})$.

3.4 Effects of Dislocations on Electron Channeling

Here, we consider the effects of dislocations on planar channeling of electrons. Electrons, as mentioned in section 3.3, are confined to move around the planes or axes where their potential minima lies. Just like in the case of positron case, both the transverse and longitudinal motion of the particles are considered.

3.4.1 Shift in Potential Minima

The Schrodinger Equation for planar channeling for a particle of mass $m$ moving in region I (perfect channel) can be written as:

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) \Psi^I(x, z) + U(x) \Psi^I(x, z) = E^I \Psi^I(x, z)$$  \hspace{1cm} (3.65)
For electron the transverse potential is given by [62, 67, 68],

\[ U(x) = - \frac{V_0}{x + a_{TF}} \]  

(3.66)

where

\[ V_0 = 2\pi Z_1 Z_2 e^2 N d_p C a_{TF}^2 \]  

(3.67)

After separation of variables, the total wavefunction for region I becomes,

\[ \Psi_I(x, z) = A_0 X_0^I e^{ik_0 z} + \sum_{n=0} B_n X_n^I e^{-ik_0 z} \]  

(3.68)

Now consider the two regions in the channel which are affected by dislocation. These curved regions are due the centrifugal force proportional to \( \frac{\mu^2}{\rho^2} \).

The Schrodinger equation for the region II in terms of the polar coordinates \( \rho \) and \( \varphi \),

\[ -\frac{\hbar^2}{2m} \left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right] \Psi^{II}(\rho, \varphi) - \frac{V_0}{(\rho - \rho_0) + a_{TF}} \Psi^{II}(\rho, \varphi) = E^{II} \Psi^{II}(\rho, \varphi) \]  

(3.69)

Separating variables gives azimuthal equation,

\[ F''^{II}(\varphi) = -\mu^2 F^{II}(\varphi) \]  

(3.70)

with solution similar to that in the positron case (Eqn. (3.15)) and radial equation,

\[ R''^{II}(\rho) + \frac{2m}{\hbar^2} \left[ E^{II} + \frac{V_0}{(\rho - \rho_0) + a_{TF}} - \frac{\hbar^2 \mu^2}{2m \rho^2} \right] R^{II}(\rho) = 0 \]  

(3.71)

From the above radial equation, the effective potential for region II can be written as

\[ V_{eff}(\rho) = -\frac{V_0}{(\rho - \rho_0) + a_{TF}} + \frac{\hbar^2 \mu^2}{2m \rho^2} \]  

(3.72)

Keeping \( \xi = \rho - \rho_0 \) and simplifying the above equation we get the effective potential and is given by,

\[ V_{eff}(\xi) = \frac{\hbar^2}{2m} \left\{ \frac{\lambda_1^3}{\lambda_1^2 \rho_0^2 a_{TF}^3 [2\xi + \lambda_1]} - \frac{\lambda_1^2}{\lambda_1 \rho_0 a_{TF}^2} + \frac{\lambda_1^3}{\rho_0^2 a_{TF}^3} \right\} \]  

(3.73)
where

\[
\begin{align*}
\lambda_1 &= -2a^4 \rho_0^4 + 3\mu^2 a_{TF}^3 \\
\lambda' &= -a^4 \rho_0^4 a_{TF} + \mu^2 a_{TF}^3 \rho_0 \\
\lambda'' &= -2a^4 \rho_0^4 a_{TF}^2 + \mu^2 a_{TF}^3 \rho_0^2
\end{align*}
\]

(3.74) (3.75) (3.76)

From Eqn. (3.73) we can see a shift in the minimum of the potential, which is due to the shift in the equilibrium axis due to dislocations. Figure 3.9 shows the potential shift in this region. The wavefunction of region II can be written in a form given by Eqn. (3.25),

\[
\Psi_{III} = \sum_{m=0} R_m [C_m e^{i\mu \phi} + D_m e^{-i\mu \phi}]
\]

(3.77)

Figure 3.9: The shift in potential due to dislocations for electrons.

Similarly, proceeding to the region III, the Schrodinger equation can be written as

\[
\begin{align*}
-\frac{\hbar^2}{2m} \left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right] \Psi_{III}(\rho, \phi) - \frac{V_0}{(\rho - \rho_0) + a_{TF}} \Psi_{III}(\rho, \phi) &= E_{III} \Psi_{III}(\rho, \phi)
\end{align*}
\]

(3.78)
Separating variables gives azimuthal and radial equations as,

\[ F''''(\phi) = -\mu^2 F'''(\phi) \quad (3.79) \]

\[ R''''(\rho) + \frac{2m}{\hbar^2} \left[ E''' + \frac{V_0}{(\rho - \rho_0)} + \frac{\hbar^2 \mu^2}{2m \rho^2} \right] R'''(\rho) = 0 \quad (3.80) \]

The effective potential for region III can be written as

\[ V_{\text{eff}}(\rho) = -\frac{V_0}{(\rho - \rho_0)} + \frac{\hbar^2 \mu^2}{2m \rho^2} \quad (3.81) \]

which, upon simplification,

\[ V_{\text{eff}}(\xi) = \frac{\hbar}{2m} \left\{ \frac{\lambda_2^3}{\lambda_2^2 \rho_0^6 a_{TF}^3 [2\xi + \frac{\lambda_2}{\lambda_2^3}]} - \frac{\lambda_2^2}{\lambda_2^3 \rho_0^6 a_{TF}^3} + \frac{\lambda_2^2}{\rho_0^6 a_{TF}^3} \right\} \quad (3.82) \]

where

\[ \lambda_2 = -3a^2 \rho_0^2 \rho_0^2 \]

\[ \lambda_2' = -2a^4 \rho_0^2 \rho_0^2 \rho_0^2 \]

The above equation (3.82) shows a shift in the potential minimum, but in the reverse direction of that of region II and the shifts in both the regions are in accordance with the direction of the centrifugal force. The wavefunction of region III can be written as,

\[ \Psi^{III}(\rho, \phi) = \sum_{m=0} R_{m}^{III} \left[ G_{m} e^{i\mu \phi} + H_{m} e^{-i\mu \phi} \right] \quad (3.86) \]

The fourth region is the perfect channel as discussed in the previous section and the wavefunction is,

\[ \Psi^{IV}(x, z) = X_{n}^{IV} I_{n} e^{i k_{n} z} \quad (3.87) \]
To find the reflection and transmission coefficients, we use the boundary conditions across the 3 boundaries are given by equations (3.40) to (3.45). From these we get $|R|^2$ and $|T|^2$ as,

$$|R|^2 = \frac{(-\mu^2 + k^2 \rho_0^2)^2 \sin^2(2\mu \varphi_0)}{4k^2 \mu^2 \rho_0^2 \cos^2(2\mu \varphi_0) + (\mu^2 + k^2 \rho_0^2)^2 \sin^2(2\mu \varphi_0)}$$  \hspace{1cm} (3.88)

$$|T|^2 = \frac{4k^2 \rho_0^2 \mu^2}{4k^2 \mu^2 \rho_0^2 \cos^2(2\mu \varphi_0) + (\mu^2 + k^2 \rho_0^2)^2 \sin^2(2\mu \varphi_0)}$$  \hspace{1cm} (3.89)

These give the dechanneling and channeling probabilities respectively. The variation of these co-efficients with the value of $\rho_0$ and incident energy $E$ is given in figures 3.10 and 3.11.

![Figure 3.10: Variation of the reflection co-efficient / dechanneling probability with $\rho_0$ and Incident energy $E$ of electron](image)

The above equations (3.88) and (3.89) look similar to those of the positron channeling case since we consider the same channel with same dislocation effects. From the figures 3.7 and 3.10, and from 3.8 and 3.11, it is found that for electron channeling,
Figure 3.11: Variation of the transmission coefficient / channeling probability with $\rho_0$ and Incident energy $E$ of electron

channeling starts at a smaller value of $\rho_0$ compared to that of positron channeling. It means that at a particular value of $\rho_0$, the probability of the particles to dechannel is less for electrons when compared to positrons. This is due to the fact that the electrons have its transverse motion bound to an atomic row or plane of atoms.

3.4.2 Spectral Distribution of Radiation Intensity

The eigen spectrum of electron channeling is given by [67, 68],

$$|E_n| = \frac{V_0^2}{2\hbar^2(n + \delta n)^2}$$  

(3.90)

$$\delta n = 2a_T/a_{TF}$$  

(3.91)

$$a_T = \sqrt{a_{TF}^2 + u^2}$$  

(3.92)

where $u^2$ is the mean-square vibrational amplitude. The additional centrifugal force due to the dislocation changes the spectrum. This change in energy due to channeling of electrons in a dislocation affected channel for various materials and various
energies are given in Table 1 and compared with that in a straight channel for a value of $\rho_0 = 0.5 \times 10^{-7}$ m.

Table 1: The change in energy (in eV) for various materials for electrons channeling along the (110) direction at different incident energies for a value of $\rho_0 = 0.5 \times 10^{-7}$ m.

<table>
<thead>
<tr>
<th>Material</th>
<th>50 MeV</th>
<th>20 MeV</th>
<th>10 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>2.83 $\times 10^{-3}$</td>
<td>2.861 $\times 10^{-3}$</td>
<td>0.93 $\times 10^{-3}$</td>
</tr>
<tr>
<td>Cu</td>
<td>3.257 $\times 10^{-3}$</td>
<td>3.293 $\times 10^{-3}$</td>
<td>1.3 $\times 10^{-3}$</td>
</tr>
</tbody>
</table>

Now we consider the effects of dislocations on the spectral distribution of the radiation intensity. The probability of transition from an initial state ($i$) to a final state ($f$) of the electron per unit time is determined by the well-known formula,

$$W_{fi} = \frac{4\pi^2 e^2}{\hbar V} \sum_{\vec{q}} |\vec{q}|^{-1} |\vec{\alpha}_{fi} \cdot \vec{e}_k|^2 \delta(\omega_{fi} - \omega) \tag{3.93}$$

Where $V$ is the volume of the system, $\vec{q}$ and $\vec{e}_k$ are the wave vector and polarization vector of a quantum of electromagnetic field as discussed in chapter 2.

$$\hbar \omega_{fi} = E_{ni} - E_{nf} \tag{3.94}$$

The matrix elements $\vec{\alpha}_{fi}$ are given by

$$\vec{\alpha}_{fi} = \delta_{\sigma_i \sigma_f} \delta_{p_{iy} p_{fy} + m_y} \vec{D}_{fi} \tag{3.95}$$

$$\vec{D}_{fi} = -ix_{fi}(\Omega_{fi}, 0, q_x \beta) \tag{3.96}$$

$$x_{fi} = \int_{-\infty}^{\infty} x S_{niE_i}(x) S_{mfE_f}(x) \, dx \tag{3.97}$$
where $S_{nE}$ are oscillatory wavefunctions which obeys the Schrödinger equation given by

$$\left[-\frac{\hbar^2}{2E} \frac{d^2}{dx^2} + U(x)\right]S_{nE}(x) = ES_{nE}(x) \quad (3.98)$$

Let us define a vector of polarization $\vec{e}_1$ in the plane having the wave vector $\vec{q}$ and the $z$-axis and a vector $\vec{e}_2 \perp \vec{e}_1$ in the plane having the axes $x$ and $y$. If $\varphi$ and $\theta$ are the azimuth and polar angle of the wave vector $\vec{q}$,

$$\vec{e}_1 = (\cos \theta \cos \varphi, \cos \theta \sin \varphi, -\sin \theta) \quad (3.99)$$
$$\vec{e}_2 = (-\sin \varphi, \cos \varphi, 0) \quad (3.100)$$

The summation in Eqn. (3.93) is written in the integral form as

$$W_{f i} = \frac{e^2}{2\pi \hbar} \int \left(|\vec{\alpha}_{fi} \cdot \vec{e}_1|^2 + |\vec{\alpha}_{fi} \cdot \vec{e}_2|^2\right) |\vec{q}|^{-1} \delta(\omega_{fi} - \omega) d\vec{q} \quad (3.101)$$

Solving we get the transmission probabilities as

$$\frac{dW_{f i}}{d\Omega} = \frac{e^2 x_{fi}^2 \Omega_{fi}^3}{2\pi \hbar (1 - \beta \cos \theta)^5} \left[(1 + \beta)^2 - 2(1 + \beta) \frac{\omega}{\omega_{0fi}} + 2(1 + \beta)^2 \left(\frac{\omega}{\omega_{0fi}}\right)^2\right] \quad (3.102)$$

$$\frac{dW_{f i}}{d\omega} = e^2 x_{fi}^2 \Omega_{fi}^2 \frac{\omega}{2\hbar \beta^3} \left[1 + \beta^2 - 2(1 + \beta) \frac{\omega}{\omega_{0fi}} + 2(1 + \beta)^2 \left(\frac{\omega}{\omega_{0fi}}\right)^2\right] \quad (3.103)$$

$$\frac{dI_{f i}}{d\Omega} = \frac{e^2 x_{fi}^2 \Omega_{fi}^2 \omega}{2\pi (1 - \beta \cos \theta)^5} \left[(1 - \beta \cos \theta)^2 - (1 - \beta^2) \sin^2 \theta \cos^2 \varphi\right] \quad (3.104)$$

$$\frac{dI_{f i}}{d\omega} = e^2 x_{fi}^2 \Omega_{fi}^2 \frac{\omega}{2\beta^3} \left[1 + \beta^2 - 2(1 + \beta) \frac{\omega}{\omega_{0fi}} + 2(1 + \beta)^2 \left(\frac{\omega}{\omega_{0fi}}\right)^2\right] \quad (3.105)$$

where

$$\omega_{0fi} \approx 2\Omega_{fi} \gamma^2 \quad (3.106)$$

The spectral intensity of radiation of a channeled electron in the case of a straight and dislocation affected channels are plotted in figures 3.12 and 3.13 with

$$s = \frac{3e^2 x_{fi}^2}{8\beta^3 \gamma^2} \quad (3.107)$$
It is found that the change in the effective potential and frequency of oscillations proportionally changes the spectral distribution of radiation intensity. But the change is small and owes to the small dechanneling probability of electrons due to its motion in a symmetry direction (around the strings of atoms).

Figure 3.12: Spectral distribution of radiation intensity

3.5 Results and Discussions

We have developed a quantum mechanical model for the effects of dislocations on positron and electron channeling. The effects of centrifugal force developed due to the distorted channel have been discussed by including the effects of longitudinal motion of the particle using polar co-ordinates. The shift in potential due to the additional influence of longitudinal motion is thus found, in this dynamic formalism. The transverse potential and the frequency of channeling radiation in the perfect channel and the two regions of dislocation affected channels are also calculated. The wave functions for the transverse and longitudinal motions are calculated by using continuity of wave functions and their derivatives at the three boundaries. The reflection and
transmission coefficients are found using these boundary conditions which are the
dechanneling and channeling probabilities respectively.

Comparing the positron and electron channeling cases, it is found from the figures
3.7 and 3.10 and also 3.8 and 3.11 that, for a given radius of curvature of the channels,
the dechanneling probability is less for electrons than that for positrons. This is due
to the property of electron channeling, where the transverse motion of electrons is
bound to an atomic row or plane of atoms. Hence the dechanneling of the particles is
less in this case when compared to the positively charged particles where transverse
oscillation is between two planes or several rows of atoms. Due to this, the effects of
dislocations are lesser for an electron channeling case than that for positrons.

For the electron case, the energy change is calculated for few materials like Si and
Cu and for various incident energies and are given in Table 1. A comparison with
the straight channel values is also made here. The change in spectral distribution

Figure 3.13: Spectral distribution of radiation intensity, showing clearly the fractional
change due to the effects of dislocations
of radiation intensity is also calculated as seen from Figures 3.12 and 3.13. With the dechanneling probability being small for electrons, the spectral distribution of radiation intensity also has only small influence from the dislocations.

Summing up, the quantum mechanical model developed here for the effects of dislocations is applicable for channeling of both positive and negatively charged particles. This model is general and is likely to be basis for the explanation of the channeling/dechanneling phenomena due to any kind of distortion effects in crystalline materials.