Channeling and Channeling radiation from Imperfect crystals with Dislocations, Stacking Faults and Anharmonic interactions

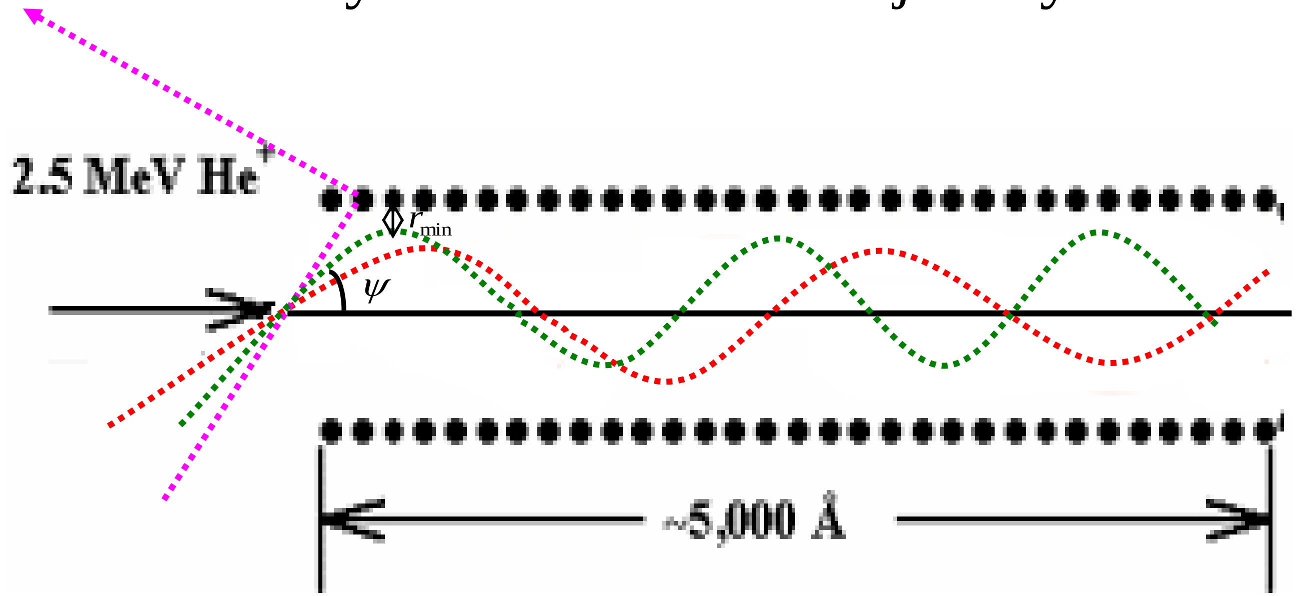
A.P. Pathak[a] **,S.V. S. Nageswara Rao**[a] **and V.S. Vendamani**[a,b]

[a]*School of of Physics,University of Hyderabad, Hyderabad,500046 India.*
[b]*Department of Physics, Pondicherry University, Puducherry 605014, India.*


Jammu &
Kashmir
Himachal
Pradesh
Punjab
Uttaranchal
DELHI
Rajasthan
Uttar
Pradesh
Arunachal
Pradesh
Sikkim
Assam
Nagaland
Megalaya
Manipur
Bihar
Tripura
Mizoram
Gujarat
Madhya
Pradesh
Jharkhand
West
Bengal
Chhattisgarh
Kolkata
(Calcutta)
Orissa
Mumbai
(Bombay)
Maharashtra
HYDERABAD
Andhra
Pradesh
Goa
Karnataka
Chennai(Madras)
Lakshwdeep
Tamil
Nadu
Kerala
Andaman & Nicobar

Ion Channeling

- Scattering process
- Influence of crystal lattice on the trajectory of ions

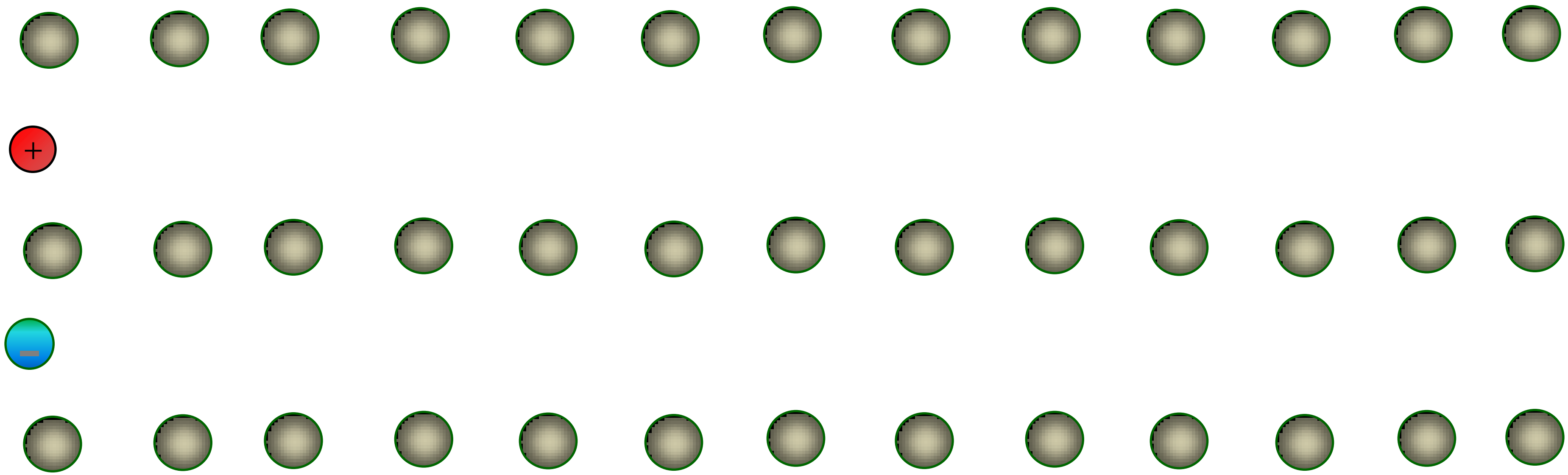


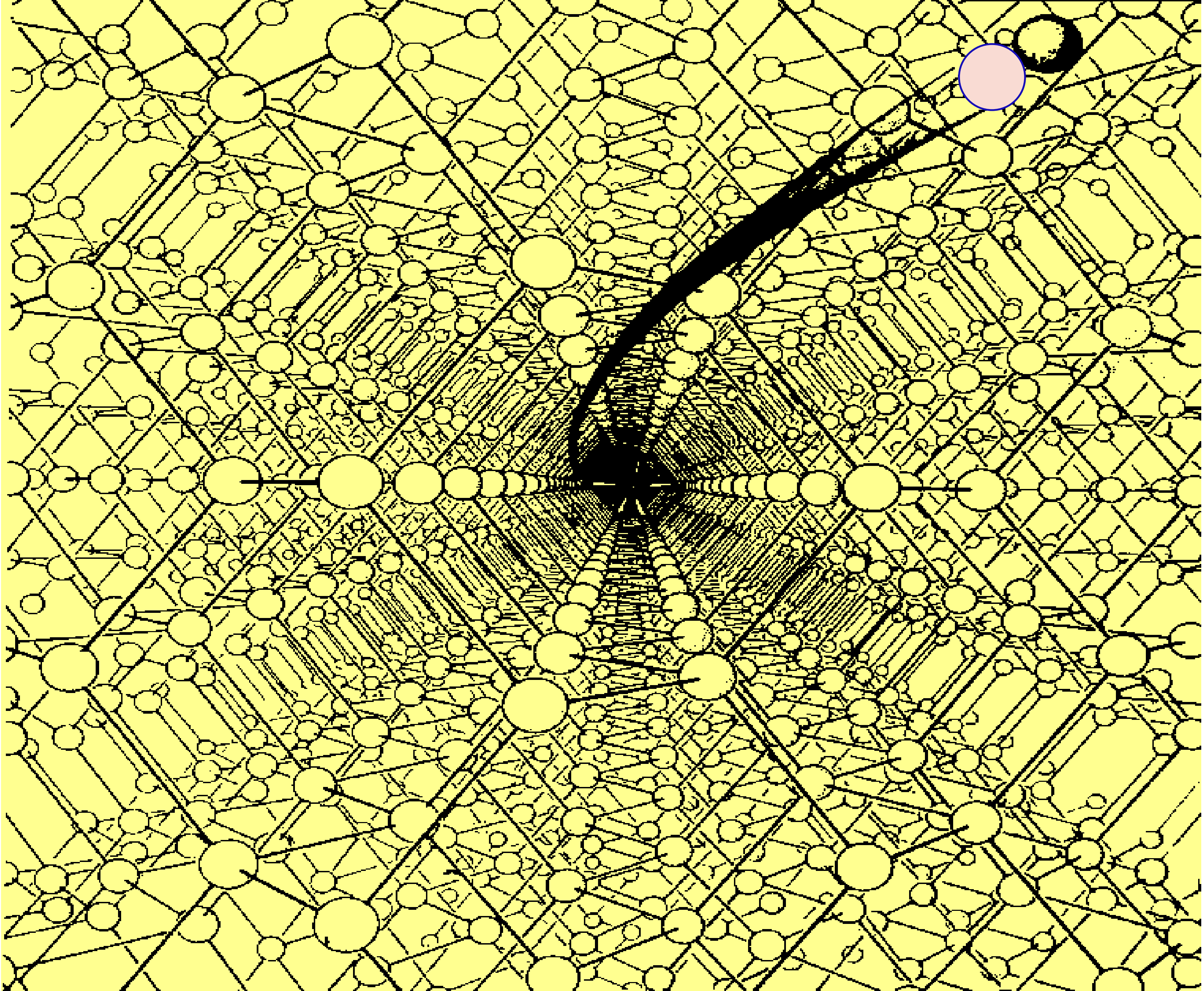
Applications

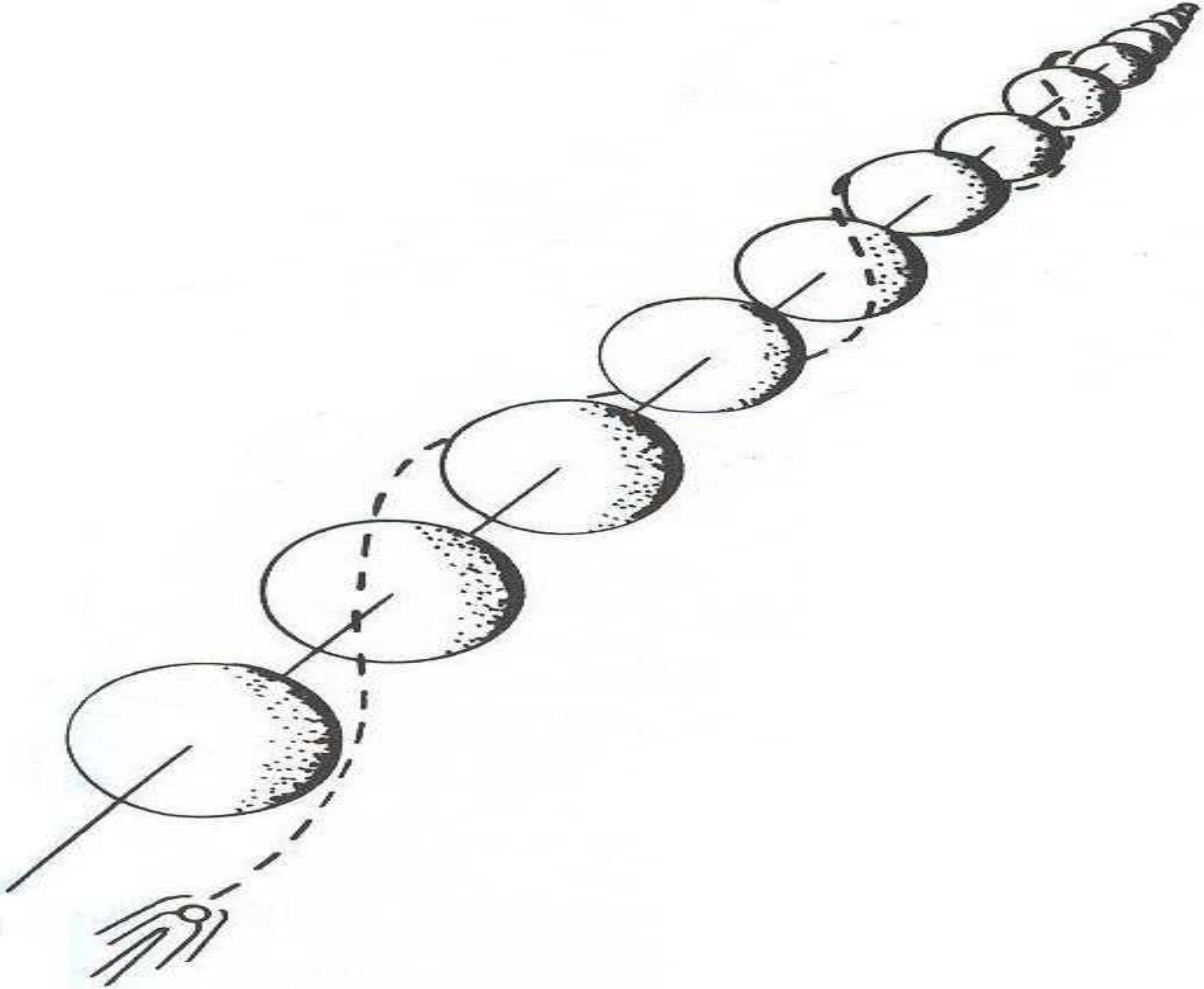
- Defects in crystals
- Structural and crystalline order
- Location of impurity atoms

Ref: L .C. Feldman and J.W. Mayer, Fundamentals of surface and Thin film Analysis, North-Holland,Newyork,(1986); A.P. Pathak, Nuclear instr. and methods in phys. Res. **R**

Ion Channeling







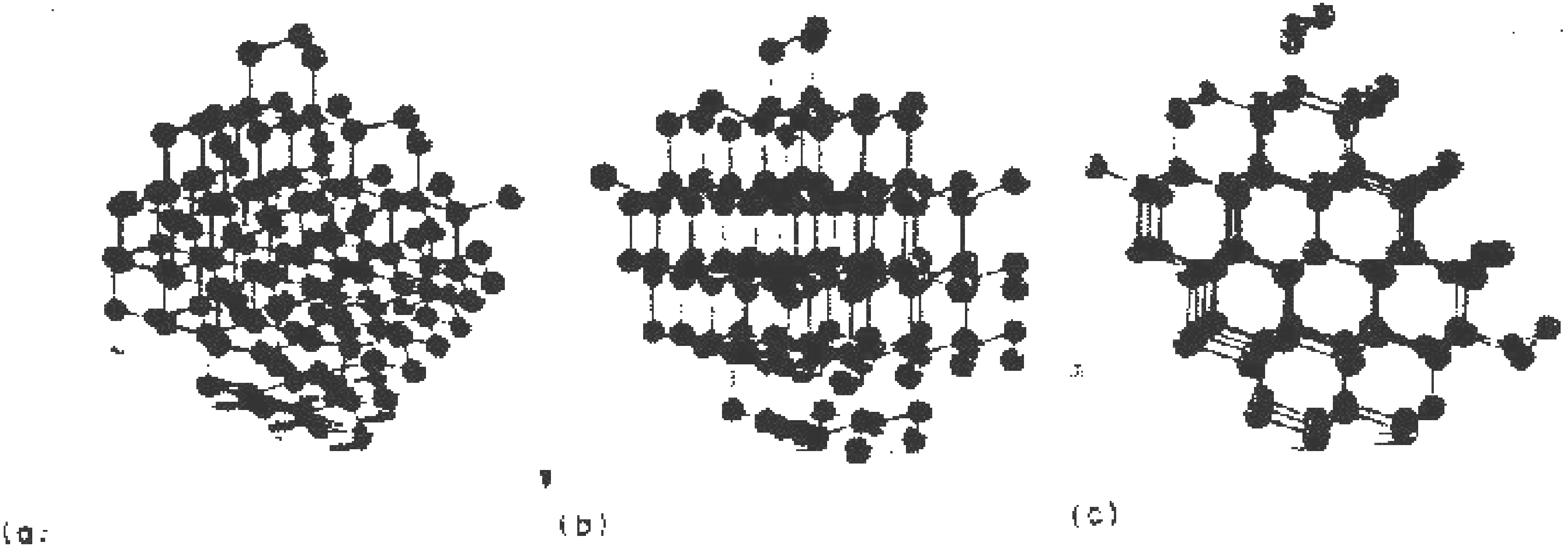
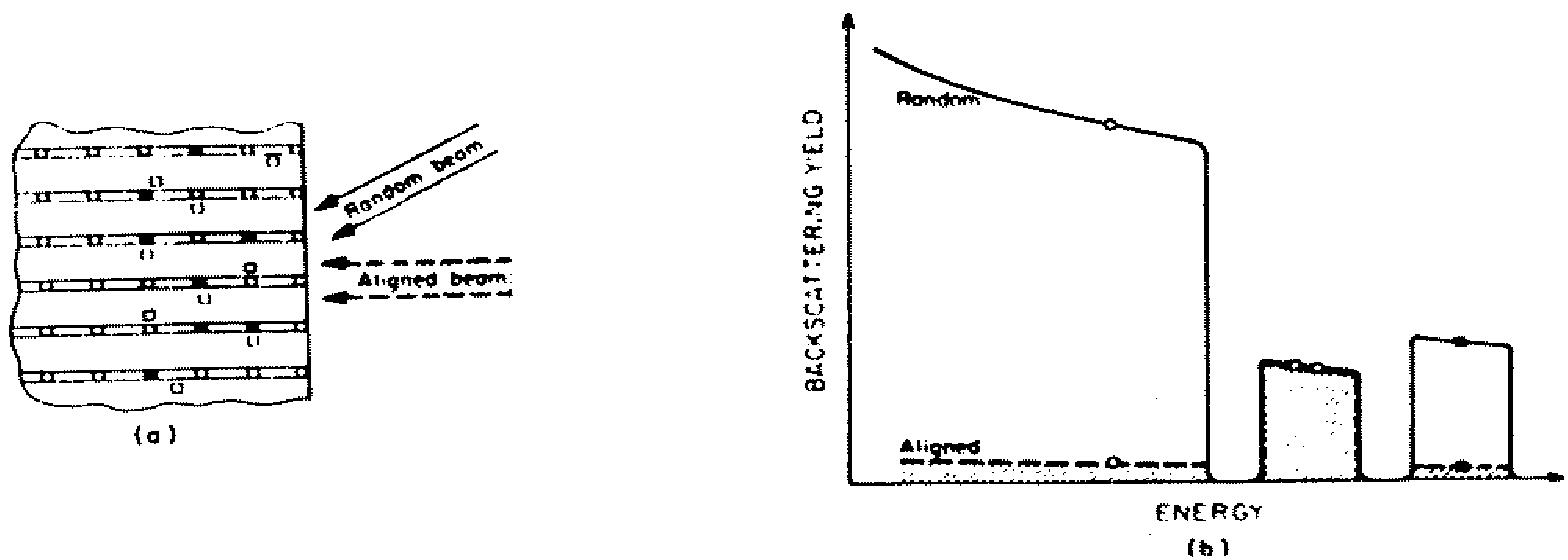
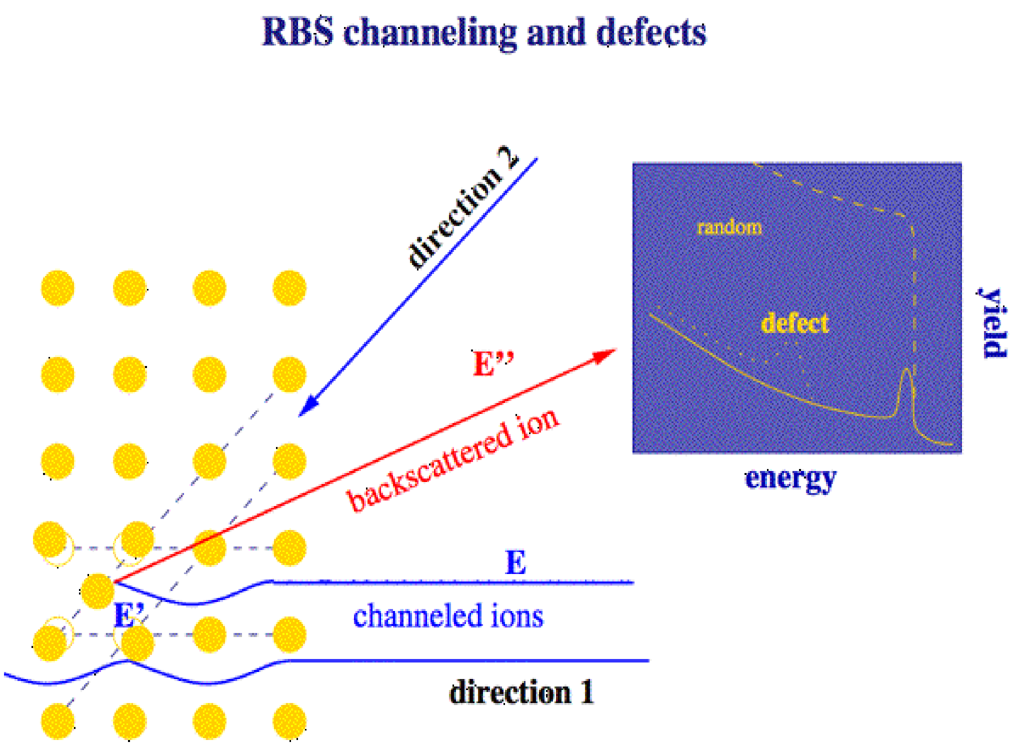


Fig. 8.1 Model of lattice atoms showing the atomic configuration in the diamond-type lattice viewed along (a) random, (b) planar, or (c) axial directions.



Backscattering spectrum



Positron planar channeling angular scans in quantum mechanical framework

- Scattering yield vs Incident angle (or occupation probability)
- Crystal structure, lattice location of host and impurity atoms, lattice strains and defects

Before entering the crystal $\Phi(x) = A\exp(ikx\sin\theta)$

Inter-atomic potential for planar channeled positron

$$V(x) \approx V_0 + \frac{1}{2}Kx^2$$

After entering into the crystal, if it is channeled

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

where coupling constant $\alpha = \sqrt{\frac{(\gamma m)\omega}{\hbar}}$

Ref: S.V.S. Nageswara Rao, Nuclear instr. and methods in phys. Res. **B** 202 (2003) 312-316

- Equating the potential energy to the max. possible K.E

$$\left(n_{\max} + \frac{1}{2}\right)\hbar\omega = \frac{1}{2} k_1 x^2{}_{\max}$$

Occupation probability of any energy level (n)

$$\pi_n = \left| \int_{\frac{-d_p}{2}}^{\frac{+d_p}{2}} \Phi(x)\psi_n(x)dx \right|^2$$

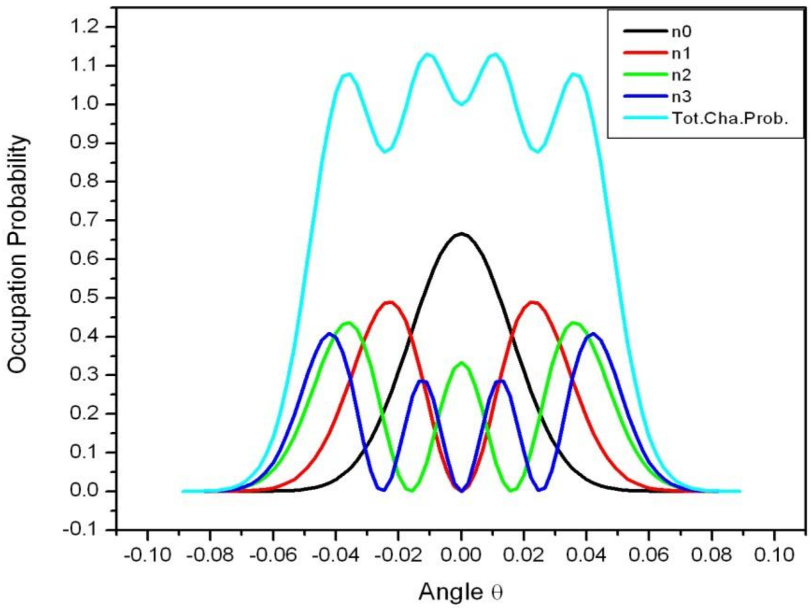
Therefore

$$\pi_n^+ = \frac{1}{M\,2^{n-1} n!} \exp\left\{\frac{-(k\sin\theta)^2}{\alpha^2}\right\} \left| H_n\left(\frac{k\sin\theta}{\alpha}\right) \right|^2$$

$$\text{where } M = \sum_{n=0}^{n_{\max}} \frac{1}{n! 2^{n-1}} \left| H_n(0) \right|^2$$

- M can be calculated by using the boundary condition

15 MeV positrons channeled along {111} planes of single crystal aluminum (n_{max}=3)

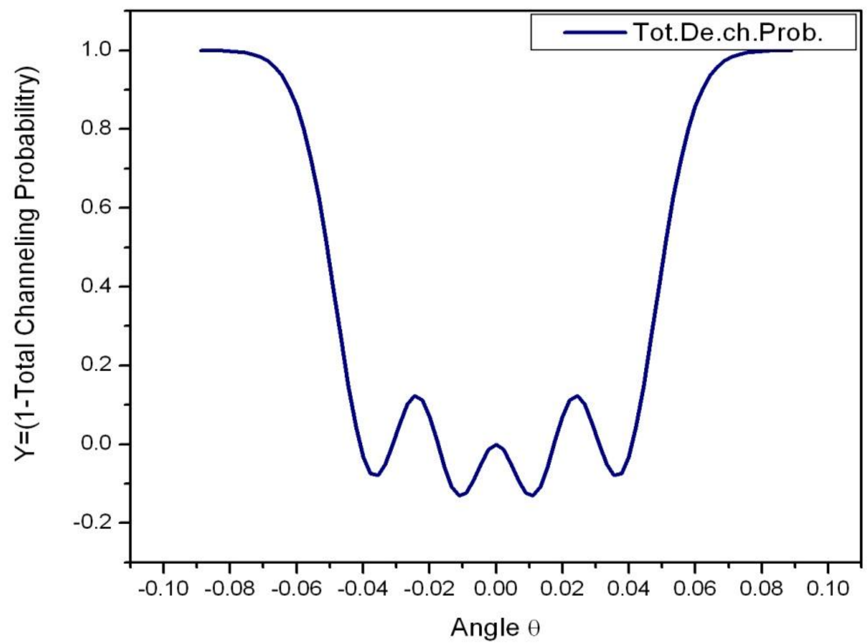


Total occupation probability

$$P_n = \sum_{n=0}^{n_{\max}} \left| < n \right\|^2$$

Dechanneling probability

$$\chi_n = 1 - P_n$$



Energy dependence

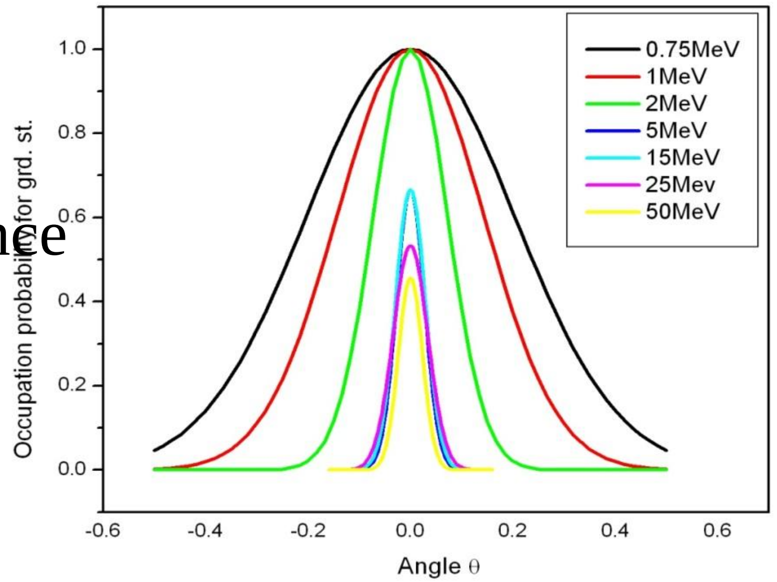
- Channeling angular scan and its FWHM determine the channeling critical angle Ψ

$$\Psi \propto E^{-1/2} \quad \{ \text{ in classical region})$$

? To verify $E^{-1/2}$ relation--- applicability for the channeling of light relativistic particles (in quantum region)

Lower energy regime (ground st.)

- Easy to understand the energy dependence
- 5 MeV positron channeled along {111} plane of Al



Ref: J.U. Andresen, et al

Occupation probability

$$\pi_0^+ = \frac{A^2\sqrt{\pi}}{\alpha 2^{0-1} 0!} \exp\left\{\frac{-(k\sin\theta)^2}{\alpha^2}\right\} \left| H_0\left(\frac{k\sin\theta}{\alpha}\right)\right|^2$$

$$\Rightarrow \frac{2A^2\sqrt{\pi}}{\alpha} \exp\left\{\frac{-(k\sin\theta)^2}{\alpha^2}\right\}$$

(compare with standard Gaussian equation)

$$w = \sqrt{2}\left(\frac{\alpha}{k}\right)$$

where w is width of the Gaussian curve

<u>Non- relativistic case</u>: $\alpha = \sqrt{\frac{(\gamma m)\omega}{\hbar}}$

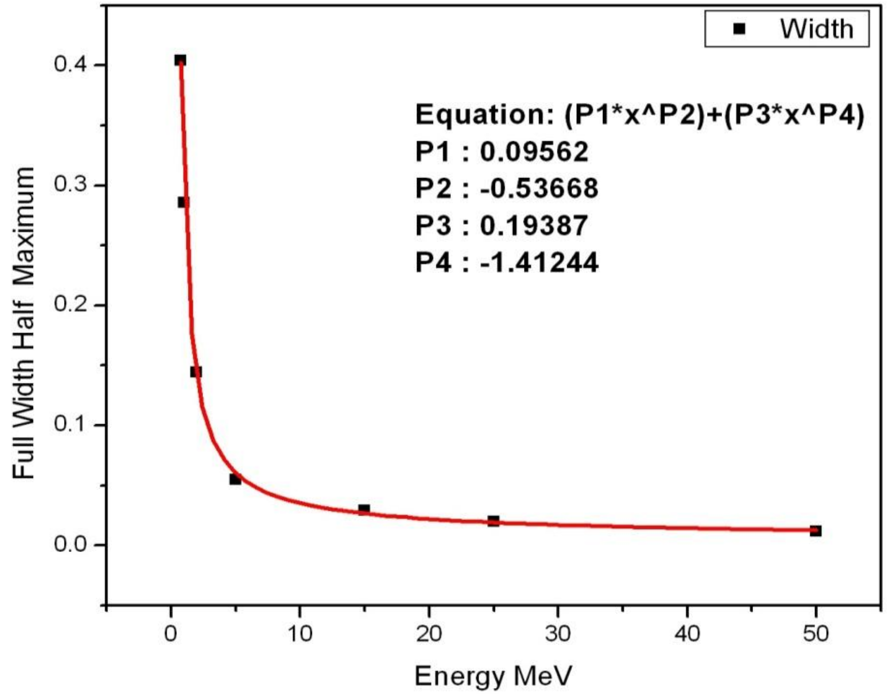
$$\gamma = 1 \qquad w \propto E^{-1/2}$$

✓Critical angle decreases with increase with incident energy

Relativistic case:

$$\gamma = 1 + \frac{E}{E_o} \qquad\qquad w = P_1 E^{-1/2} + P_2 E^{-3/2} + \ldots\ldots$$

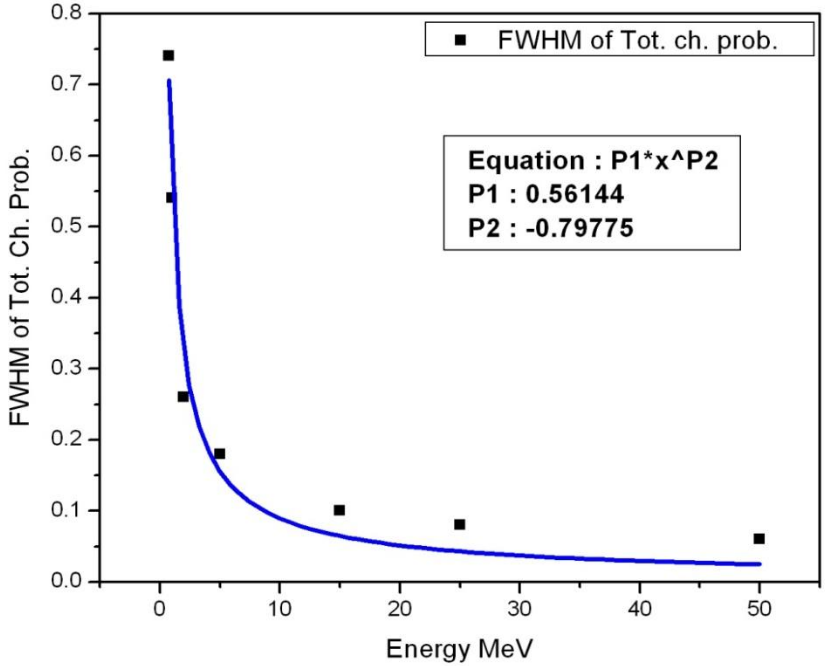
✓ Decreases with increase in energy *E* ----but not just as $E^{-1/2}$



✓The standard $E^{-1/2}$ relation is not strictly applicable for relativistic positrons

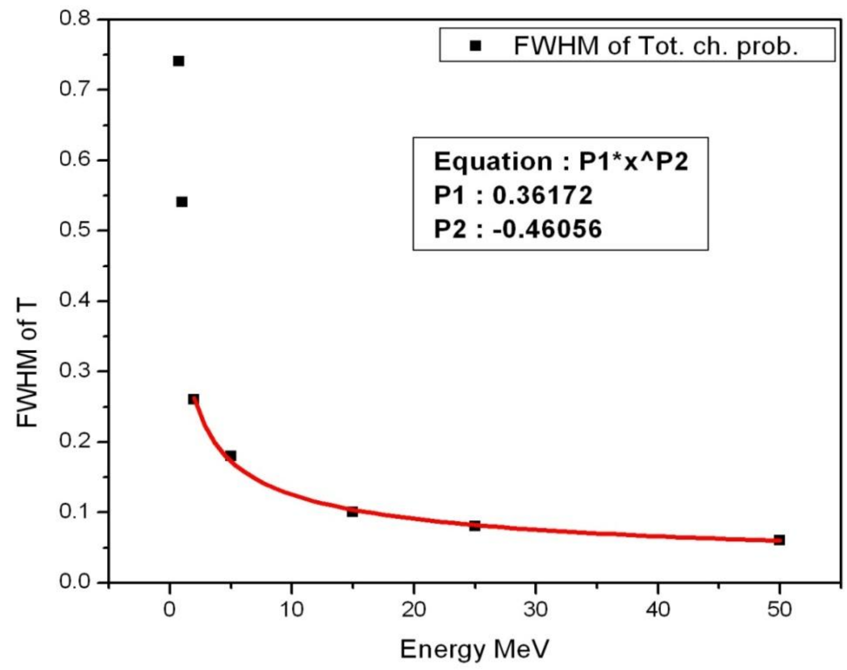
High energy regime (including all States)

- Channeling angular scan is superposition of all available states



✓It is not fitting exactly as $E^{-1/2}$

✓Fitting exactly as $E^{-1/2}$ when it enters into classical region



Anharmonic effects on positron channeling angular scans

Inter-atomic potential for planar channeled positron

$$V(x) \approx V_0 + \frac{1}{2}kx^2 + \frac{1}{4}k_1x^4$$

- Maximum number of states increase

Anharmonic oscillator wave function

$$\psi_N(x) = \psi_n(x) + KC_1^n\psi_{n-2}(x) - KC_2^n\psi_{n+2}(x) + KC_3^n\psi_{n-4}(x) - KC_4^n\psi_{n+4}(x)$$

$$C_1^n = (2n-1)\sqrt{n(n-1)}$$

$$C_2^n = (2n+3)\sqrt{(n+1)(n+2)}$$

$$C_3^n = \frac{1}{4}\sqrt{n(n-1)(n-2)(n-3)}$$

$$C_4^n = \frac{1}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)}$$

$$K = \frac{\lambda}{4\hbar\omega\alpha^4}$$ momentum of the incident particle

Ref: M.K. Abu- Assy, Physica Scripta

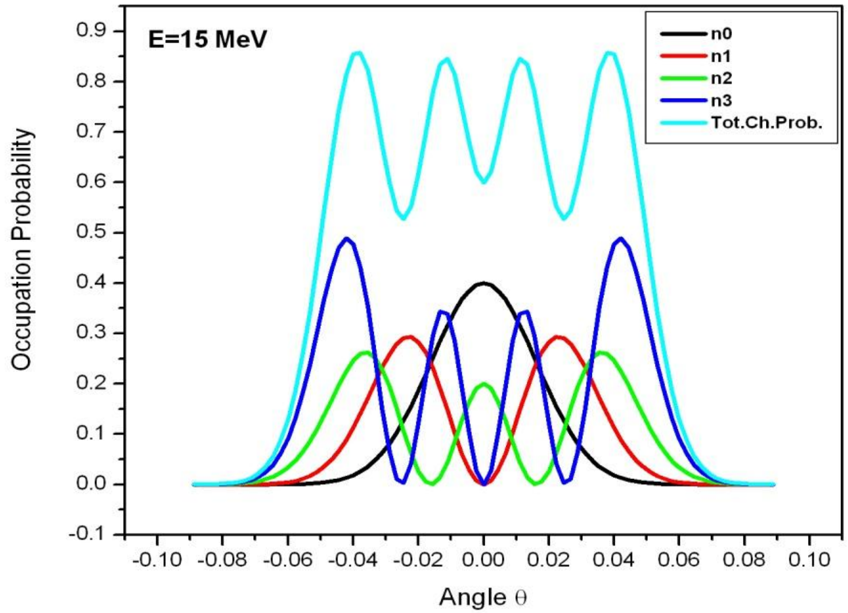
Occupation probability of any energy level (N)

$$\pi_N^+ = \int_{-\infty}^{+\infty} \Phi(x)\ \psi_N(x)\ dx$$

Therefore

$$\pi_N^+ = \frac{1}{T\,2^{n-1}\,n!}\exp\left(\frac{-(k\sin\theta)^2}{\alpha^2}\right)\left\{\left|H_n\left(\frac{k\sin\theta}{\alpha}\right)\right|^2 + \frac{4K^2(2n-1)^2}{(n-2)(n+1)}\left|H_{n-2}\left(\frac{k\sin\theta}{\alpha}\right)\right|^2 - \frac{K^2(2n+3)^2}{4}\left|H_{n+2}\left(\frac{k\sin\theta}{\alpha}\right)\right|^2 + \frac{K^2}{(n-4)(n+1)}\left|H_{n-4}\left(\frac{k\sin\theta}{\alpha}\right)\right|^2 - \frac{K^2}{256}\left|H_{n+4}\left(\frac{k\sin\theta}{\alpha}\right)\right|^2\right\}$$

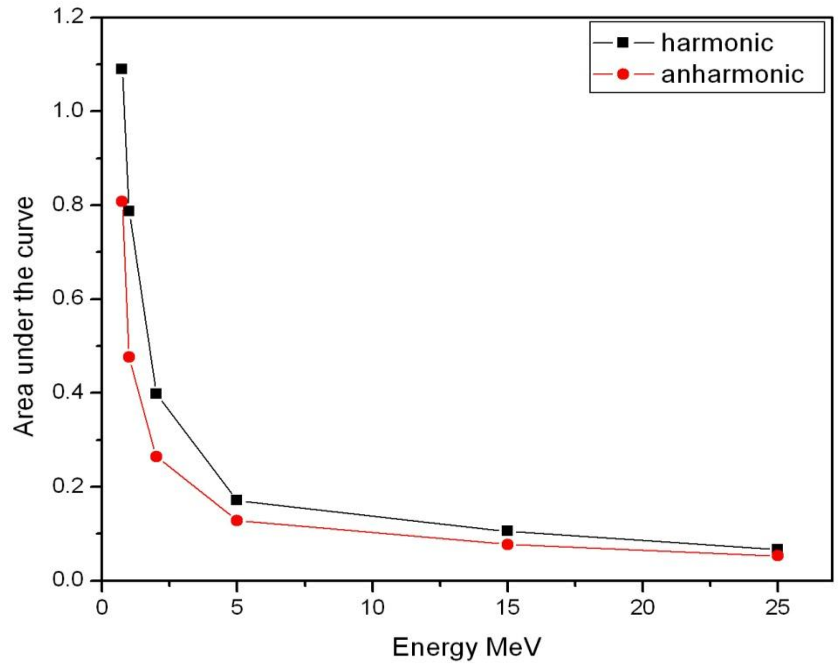
15 MeV positrons channeled along {111} planes of single crystal aluminum ($n_{max}=3$)



Total occupation probability

$$P_N = \sum_{N=0}^{n_{\max}} |< N \|^2$$

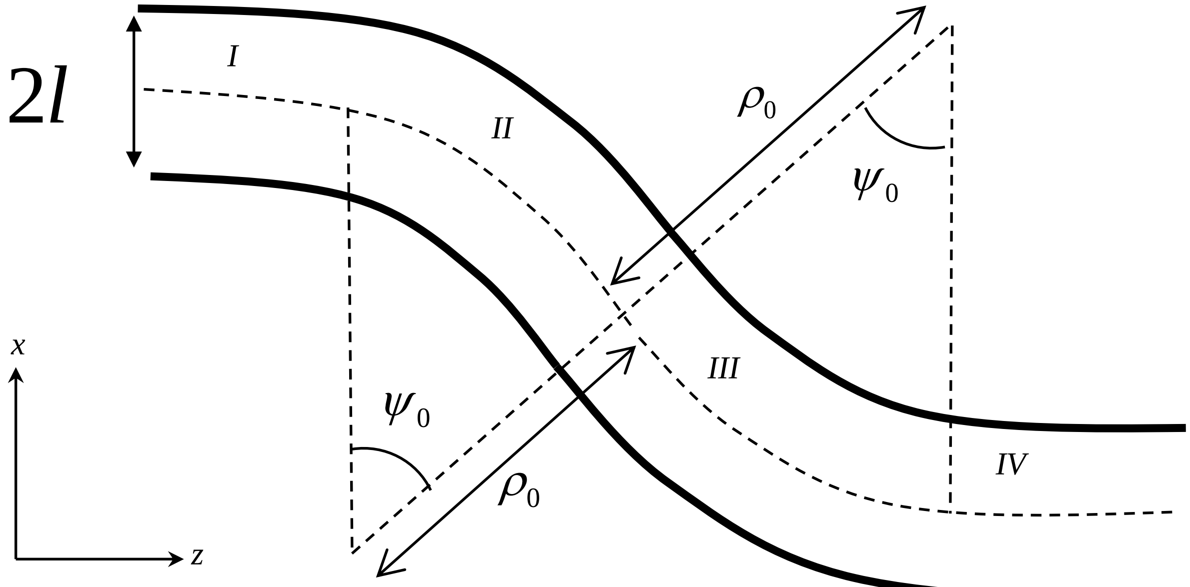
❖ The area under the curve of tot.ch.prob. for anharmonic case resembles with harmonic case , with increase in energy



Types of defects

- Zero dimension – vacancy, substitutional, interstitial
- One dimension – dislocation, slip
- Two dimension– stacking fault, twins, Grain boundary
- Three dimension - voids

The Model



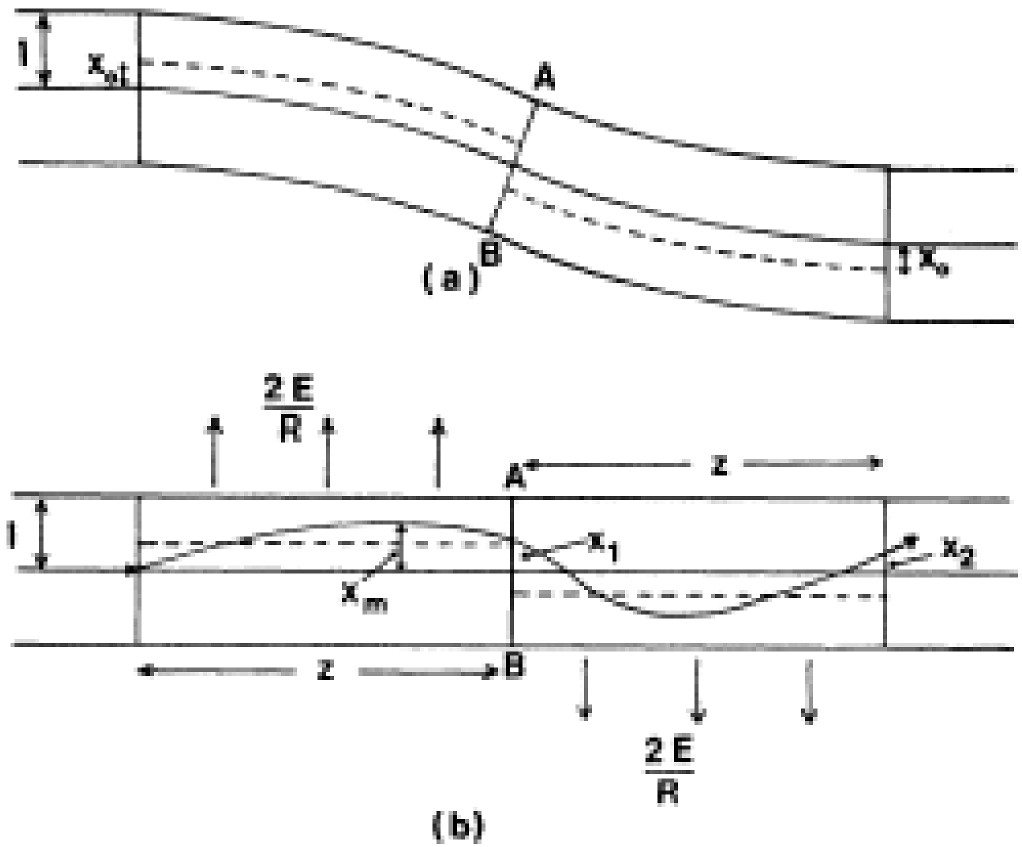


FIG. 3. (a) Typical channel at some finite distance from a dislocation. (b) Straight model channel replacing the channel of part (a) and showing the coordinates used in the text. Here, l is the half-width of the channel, x_m is the amplitude in the first part of the channel, x_0 is the equilibrium position about which the particle will oscillate, and x_1 and x_2 are the positions at which the particle arrives after having traversed the first and second parts of the channel, respectively.

Region I

The Schrödinger Equation for planar channeling

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

Equations for the transverse and longitudinal motion,

$$-\frac{\hbar^2}{2m}X^{I''}(x)+\frac{1}{2}m\omega^2x^2X^I(x)=E_T^IX^I(x)$$

$$-\frac{\hbar^2}{2m}Z^{I''}(z)=E_L^IZ^I(z)$$

solutions

$$X_n^I(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}(2^n n!)^{-1/2}H_n(ax)e^{-a^2x^2/2}$$

$$Z^I(z)=Ae^{ikz}+Be^{-ikz}$$ *where* $$a=(m\omega/\hbar)^{1/2}$$

If x_0 is the initial amplitude of the channelon

$$\Psi^I(x,z)=X^I(x-x_0)Z^I(z)$$

After including the effects of several transverse states

$$\Psi^I(x,z)=A_0X_0^I\,e^{ik_0z}+\sum_{n=0}B_n\,X_n^I\,e^{-ik_nz}$$

Region II

The Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2_{\rho,\varphi}\Psi^{II}(\rho,\varphi)+V(\rho)\Psi^{II}(\rho,\varphi)=E^{II}\Psi^{II}(\rho,\varphi)$$

The transverse potential due to the curved atomic planes is also assumed as harmonic around the central region

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

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

Separation of variables gives the azimuthal equation

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

with solution

$$F^{II}(\varphi)=Ce^{i\mu\varphi}+De^{-i\mu\varphi}$$

and radial equation.

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

Effective potential

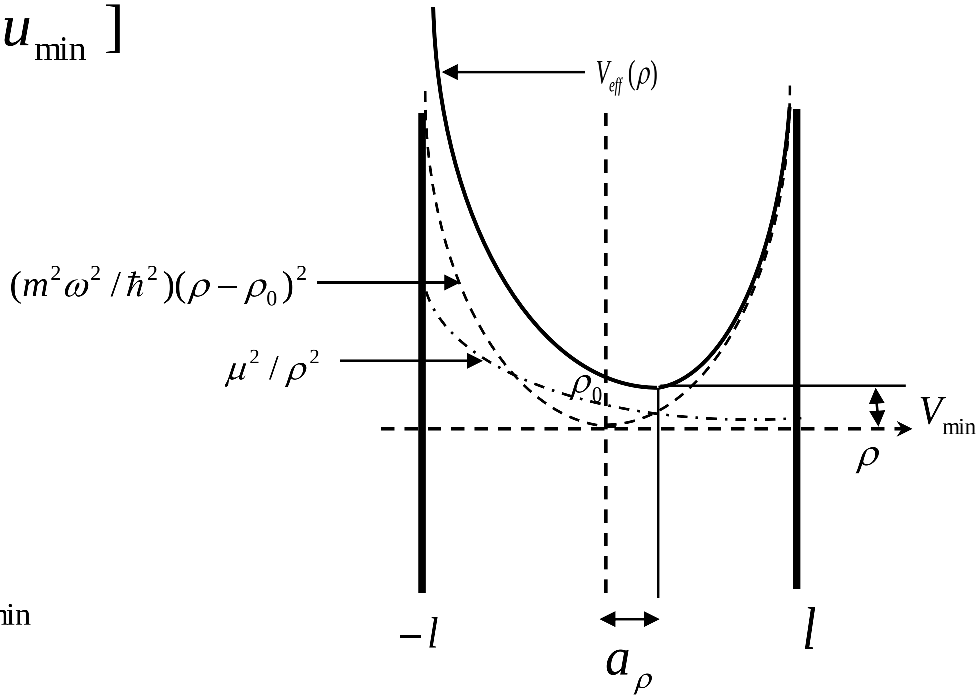
$$V_{eff}(\xi) \approx \frac{\hbar^2}{2m}[\ (\lambda/\rho_0^4)(\xi - a_p)^2 + u_{\min}\ ]$$

with $\xi = \rho - \rho_0$

$$\lambda = a^4\rho_0^4 + 3\mu^2$$

$$a_p = \mu^2\rho_0/\lambda$$

$$u_{\min} = \frac{\mu^2(\lambda - \mu^2)}{\rho_0^2\lambda} = (2m/\hbar^2)V_{\min}$$



The frequency in the second region

$$\omega' = (\hbar/m)(\lambda/\rho_0^4)^{1/2}$$

After including the effects of several transverse states

$$\Psi^{II}(x,z) = \sum_{m=0} R_m^{II}[C_m e^{i\mu\varphi} + D_m e^{-i\mu\varphi}]$$

Region III

The Schrödinger Equation

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

Separation of variables gives the azimuthal eqn.

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

with solution

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

and radial eqn.

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

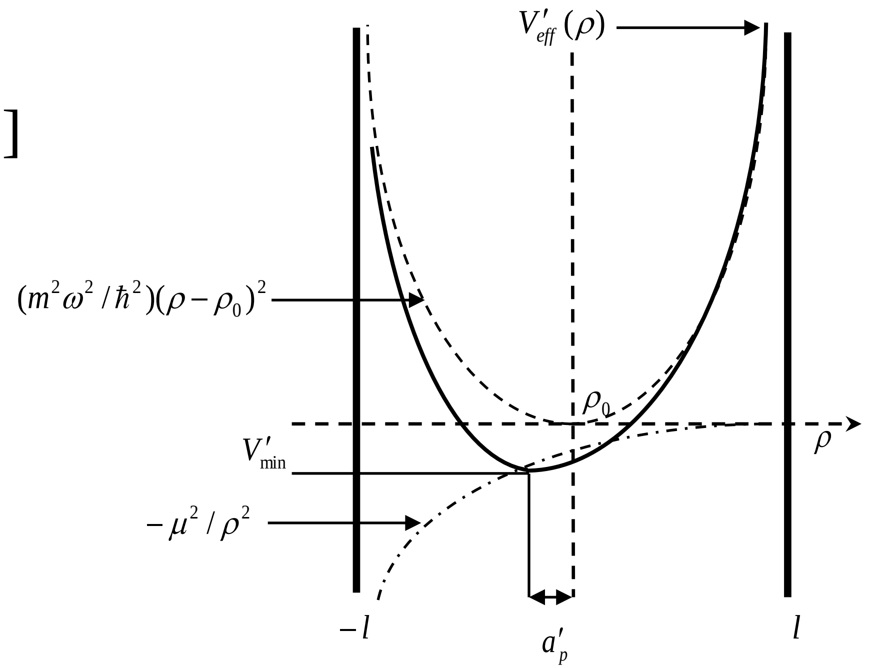
Effective potential

$$V'_{eff}(\xi) \approx \frac{\hbar^2}{2m}[\,(\lambda'/\rho_0^4)(\xi + a'_p)^2 + u'_{\min}\,]$$

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

$$a'_p = \mu^2\rho_0/\lambda'$$

$$u'_{\min} = -\frac{\mu^2(\lambda' + \mu^2)}{\rho_0^2\,\lambda'} = -(2m/\hbar^2)V'_{\min}$$



The frequency in the second region

$$\omega'' = (\hbar/m)(\lambda'/\rho_0^4)^{1/2}$$

After including the effects of several transverse states

$$\Psi^{III}(x,z) = \sum_{m=0} R_m^{III}[G_m e^{i\mu\varphi} + H_m e^{-i\mu\varphi}]$$

Region IV

Region 4 is a perfect channel, wavefunction of positron in this region is of the same form as in the 1st region

$$\Psi^{IV}(x,z) = X_n^{IV} I_n e^{ik_n z}$$

Boundary Conditions

Boundary I

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

$$AX^{I} + BX^{I} = R^{II}[C + D]$$

$$\frac{\partial \Psi^{I}}{\partial z}\Bigg|_{z=0} = \frac{1}{\rho_0}\frac{\partial \Psi^{II}}{\partial \varphi}\Bigg|_{\varphi=0}$$

$$ikAX^{I} - ikB\,X^{I} = \frac{i\mu}{\rho_0}R^{II}[C - D]$$

Boundary II

$$\Psi^{II}\Big|_{\varphi=\varphi_0} = \Psi^{III}\Big|_{\varphi=0}$$

$$R^{II}[Ce^{i\mu\varphi} + De^{-i\mu\varphi}] = R^{II}[G + H]$$

$$\frac{\partial \Psi^{II}}{\partial \varphi}\Bigg|_{\varphi=\varphi_0} = \frac{\partial \Psi^{III}}{\partial \varphi}\Bigg|_{\varphi=0}$$

$$R^{II}[Ce^{i\mu\varphi} - De^{-i\mu\varphi}] = R^{II}[G - H]$$

Boundary III

$$\Psi^{III}\Big|_{\varphi=\varphi_0} = \Psi^{IV}\Big|_{z=t}$$

$$R^{III}[Ge^{i\mu\varphi} + He^{-i\mu\varphi}] = IX^{IV}e^{ikt}$$

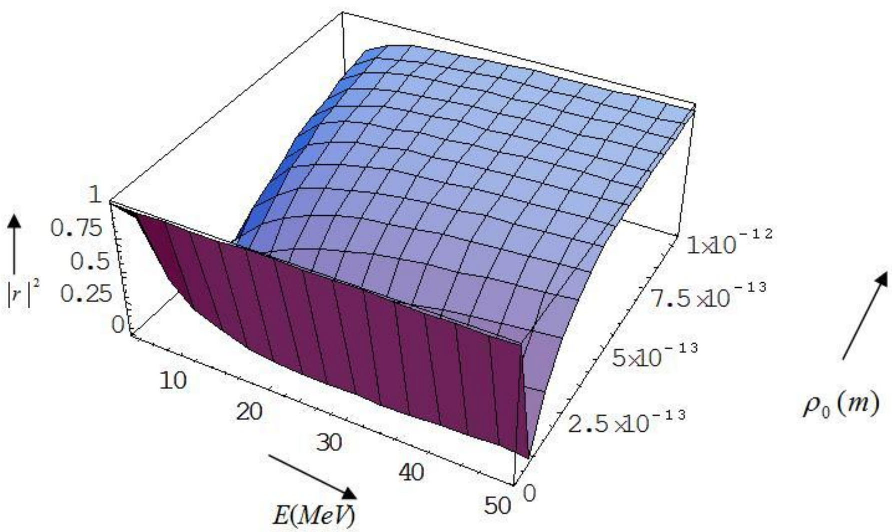
$$\frac{1}{\rho_0}\frac{\partial \Psi^{III}}{\partial \varphi}\Bigg|_{\varphi=\varphi_0} = \frac{\partial \Psi^{IV}}{\partial z}\Bigg|_{z=t}$$

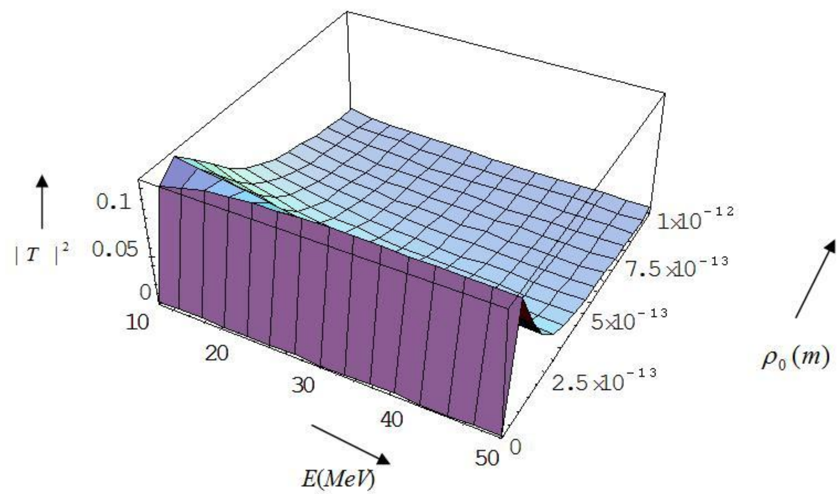
$$\frac{i\mu}{\rho_0}R^{III}[Ge^{i\mu\varphi} + He^{-i\mu\varphi}] = ikIX^{IV}e^{ikt}$$

*The **Reflection and Transmission co-efficient** in terms of the various parameters of the dislocation affected channel*

$$|r|^2 = \frac{|B|^2}{|A|^2} = \frac{(-\mu^2 + k^2\rho_0^2)^2 Sin^2(2\mu\varphi_0)}{4k^2\mu^2\rho_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + k^2\rho_0^2)^2 Sin^2(2\mu\varphi_0)}$$

$$|T|^2 = 1 - |r|^2 = \frac{4k^2\rho_0^2\mu^2}{4k^2\mu^2\rho_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + k^2\rho_0^2)^2 Sin^2(2\mu\varphi_0)}$$





Effects of dislocation and anharmonic interaction on channeling radiation

Region I

The periodic potential of a positron including the anharmonic term is

$$V(x) = V_0 x^2 + V_1 x^4$$

where

$$V_0 = \frac{4\pi Z_1 Z_2 e^2 C a^2 N_p}{(l+a)^3}$$

$$V_1 = \frac{4\pi Z_1 Z_2 e^2 C a^2 N_p}{(l+a)^5}$$

In the region I the total transverse energy can be written as

$$E_T^I = \left(n + \frac{1}{2}\right)\hbar\omega + \frac{3}{4} V_1 \alpha^4 (2n^2 + 2n + 1)$$

The wavefunction in this region is given by

$$\Psi^I(x,z) = A_0 X_0^I e^{ik_0 z} + \sum_{n=0} B_n X_n^I e^{-ik_n z}$$

Region II

The Schrodinger equation for the region,

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

where

$$U(\rho)=V_0(\rho-\rho_0)^2+V_1(\rho-\rho_0)^4$$

Separating variables, the azimuthal and radial equations,

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

$$R''^{II}(\rho)+\frac{2m}{\hbar^2}\left[E^{II}-V_0(\rho-\rho_0)^2-V_1(\rho-\rho_0)^4-\frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}\right]R^{II}(\rho)=0$$

The effective potential after including the centrifugal term is given by,

$$V_{eff}=V_0(\rho-\rho_0)^2+V_1(\rho-\rho_0)^4+\frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}$$

The effective potential,

$$V_{eff}(\xi) = \frac{\hbar^2}{2m}\left\{\frac{\lambda_1}{\rho_0^4}(\xi - a_{p_1})^2 + \frac{\lambda_1'}{\rho_0^6}(\xi - a_{p_1}')^4 - \frac{6\mu^2\rho_0^2}{\lambda_1'^2}\left(\xi - \frac{a_{p_1}'}{3}\right)^2 + U_{min}\right\}$$

Where

$$\lambda_1 = a^4\rho_0^4 + 3\mu^2$$

$$a_{p_1} = \frac{\mu^2\rho_0}{\lambda_1}$$

$$\lambda_1' = \frac{2mV_1\rho_0^6}{\hbar^2} + 5\mu^2$$

$$a_{p_1}' = \frac{\mu^2\rho_0}{\lambda_1'}$$

$$U_{min} = \frac{\mu^2\rho_0^4}{\lambda_1'^4}\left[\frac{(\lambda_1 - \mu^2)\lambda_1'^3}{\lambda_1} - \frac{\mu^6}{3}\right]$$

and wavefunction in this region

$$\Psi^{II}(\rho,\varphi) = \sum_{m=0} R_m^{II}\left[C_m e^{i\mu\varphi} + D_m e^{-i\mu\varphi}\right]$$

Region III

The effective potential

$$V_{eff} = V_0(\rho - \rho_0)^2 + V_1(\rho - \rho_0)^4 - \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}$$

After simplification,

$$V_{eff}(\xi) = \frac{\hbar^2}{2m}\left\{\frac{\lambda_2}{\rho_0^4}(\xi + a_{p_2})^2 + \frac{\lambda_2'}{\rho_0^6}(\xi + a_{p_2}')^4 - \frac{6\mu^2\rho_0^2}{\lambda_2'^2}\left(\xi + \frac{a_{p_2}'}{3}\right)^2 - U_{min}'\right\}$$

where

$$\lambda_2 = a^4\rho_0^4 - 3\mu^2$$

$$a_{p_2} = \frac{\mu^2\rho_0}{\lambda_2}$$

$$\lambda_2' = \frac{2mV_1\rho_0^6}{\hbar^2} - 5\mu^2$$

$$a_{p_2}' = \frac{\mu^2\rho_0}{\lambda_2'}$$

$$U_{min}' = \frac{\mu^2\rho_0^4}{\lambda_2'^4}\left[\frac{(\lambda_2 + \mu^2)\lambda_2'^3}{\lambda_2} + \frac{5\mu^6}{3}\right]$$

Wavefunction in region III

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

<u>Region IV</u>

Wavefunction in the region (straight channel) where there are only transmitted waves

$$\Psi^{IV}(x,z) = X_n^{IV} I_n e^{ik_n z}$$

The Schrödinger Equation for **electron** planar channeling

Region I

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)\Psi^I(x,z)+U(x)\Psi^I(x,z)=E^I\ \Psi^I(x,z) \qquad E^I=\frac{mV_0^2}{2\hbar^2 n^2}+\frac{\hbar^2 k^2}{2m}$$

$$U(x)=-\frac{V_0}{x+a_T} \qquad V_0=2Z_1Z_2e^2Nd_pCa^2$$

Equations for the transverse and longitudinal motion,

$$-\frac{\hbar^2}{2m}X^{I''}(x)+\frac{V_0}{x+a_T}X^I(x)=E_T^I X^I(x)$$

$$-\frac{\hbar^2}{2m}Z^{I''}(z)=E_L^I Z^I(z)$$

If x_0 *is the initial amplitude of the channelon*

$$\Psi^I(x,z)=X^I(x-x_0)Z^I(z)$$

After including the effects of several transverse states, we can write

$$\Psi^I(x,z)=A_0X_0^I e^{ik_0z}+\sum_{n=0}B_n X_n^I e^{-ik_nz}$$

Region II

The Schrödinger Equation

$$-\frac{\hbar^2}{2m}\nabla^2_{\rho,\varphi}\Psi^{II}(\rho,\varphi)+V(\rho)\Psi^{II}(\rho,\varphi)=E^{II}\Psi^{II}(\rho,\varphi)$$

The transverse potential due to the curved atomic planes is assumed to shift with respect to lattice plane, due to curvature;

$$V(\rho)=-\frac{V_0}{(\rho-\rho_0)+a_T}$$

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

Separation of variables gives the azimuthal equation

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

with solution

$$F^{II}(\varphi)=Ce^{i\mu\varphi}+De^{-i\mu\varphi}$$

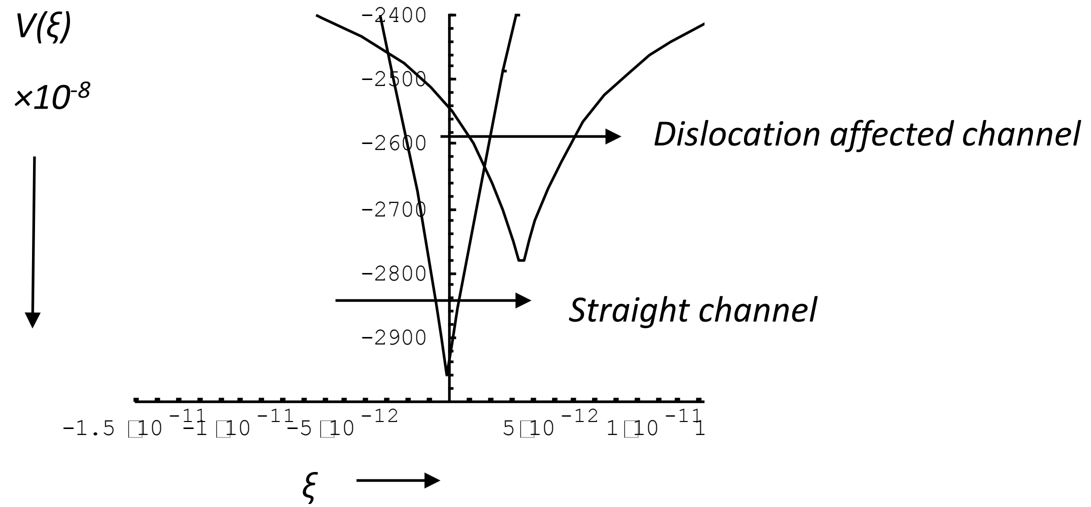
and radial equation

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

Effective potential for electron case

$$V_{eff}(\xi) = \frac{\hbar}{2m}\left\{\frac{\lambda_1'^3}{\lambda_1^2 \rho_0^4 a_{TF}^3 [2\xi + \frac{\lambda_1'}{\lambda_1}]} - \frac{\lambda_1'^2}{\lambda_1 \rho_0^4 a_{TF}^3} + \frac{\lambda_1''}{\rho_0^4 a_{TF}^3}\right\}$$

$$\begin{aligned}
\lambda_1 &= -2a^4\rho_0^4 + 3\mu^2 a_{TF}^3 \\
\lambda_1' &= -a^4\rho_0^4 a_{TF} + \mu^2 a_{TF}^3 \rho_0 \\
\lambda_1'' &= -2a^4\rho_0^4 a_{TF}^2 + \mu^2 a_{TF}^3 \rho_0^2
\end{aligned}$$



After including the effects of several transverse states

$$\Psi^{II}(x,z) = \sum_{m=0} R_m^{II}[C_m e^{i\mu\varphi} + D_m e^{-i\mu\varphi}]$$

Region III

Effective potential is given by

$$V_{eff}(\xi) = \frac{\hbar}{2m}\left\{\frac{\lambda_2'^3}{\lambda_2^2\rho_0^4 a_{TF}^3[2\xi + \frac{\lambda_2'}{\lambda_2}]} - \frac{\lambda_2'^2}{\lambda_2\rho_0^4 a_{TF}^3} + \frac{\lambda_2''}{\rho_0^4 a_{TF}^3}\right\}$$

$$\begin{aligned} \lambda_2 &= -2a^4\rho_0^4 - 3\mu^2 a_{TF}^3 \\ \lambda_2' &= -a^4\rho_0^4 a_{TF} - \mu^2 a_{TF}^3\rho_0 \\ \lambda_2'' &= -2a^4\rho_0^4 a_{TF}^2 - \mu^2 a_{TF}^3\rho_0^2 \end{aligned}$$

After including the effects of several transverse states

$$\Psi^{III}(x,z) = \sum_{m=0} R_m^{III}[G_m e^{i\mu\varphi} + H_m e^{-i\mu\varphi}]$$

Region IV

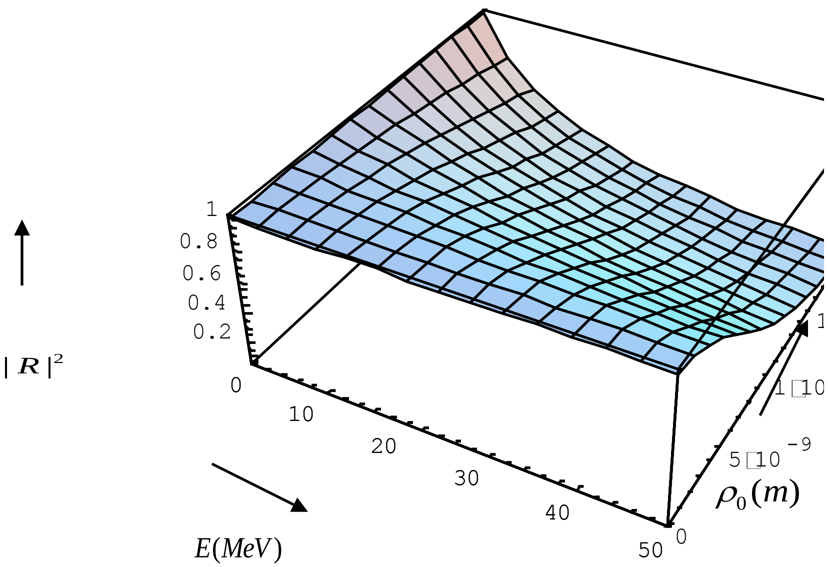
Region 4 is a perfect channel, wavefunction of electron in this region is of the same form as in the 1st region

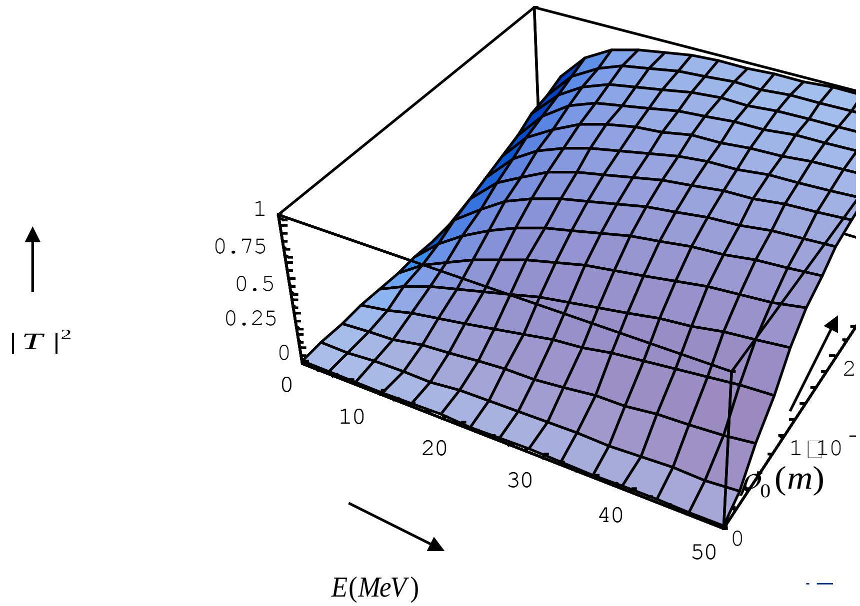
$$\Psi^{IV}(x,z) = X_n^{IV} I_n e^{ik_n z}$$

The *__Reflection and Transmission co-efficients__* *in terms of the various parameters of the dislocation affected channel*

$$|R|^2 = \frac{|B|^2}{|A|^2} = \frac{(-\mu^2 + 2mE\rho_0^2)^2 Sin^2(2\mu\varphi_0)}{8mE\mu^2\rho_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + 2mE\rho_0^2)^2 Sin^2(2\mu\varphi_0)}$$

$$|T|^2 = 1 - |R|^2 = \frac{8mE\rho_0^2\mu^2}{8mE\mu^2\rho_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + 2mE\rho_0^2)^2 Sin^2(2\mu\varphi_0)}$$





- *For a relativistic particle, the emission process is considered in the rest frame of the particle moving through the crystal.*

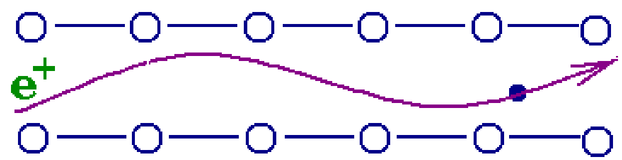
- *Since the crystal is rushing back at a speed –v, it appears Lorentz-contracted*

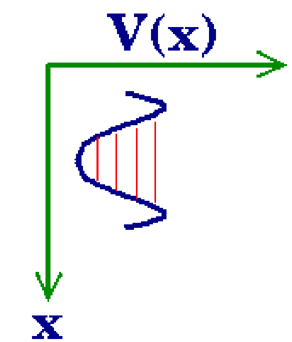
$$d^R = \frac{d}{\gamma}$$

$$E_\perp^R = \gamma E_\perp$$

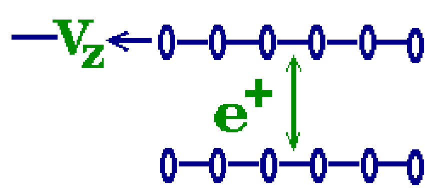
$$V^R = \gamma \, \mathrm{V}$$

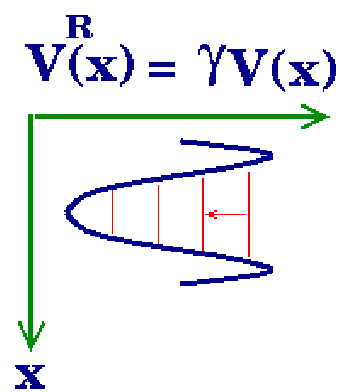
Lab Frame



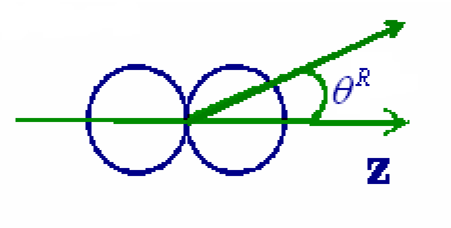


Rest Frame



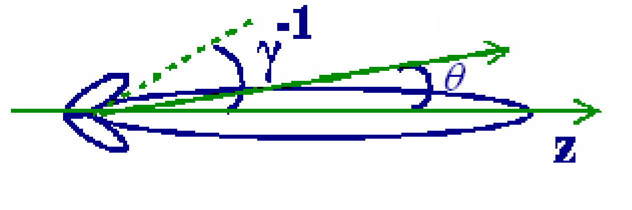


The frequency in the rest frame



$$\omega^R = \gamma\omega_0$$

The emission in the rest frame is observed in the lab frame



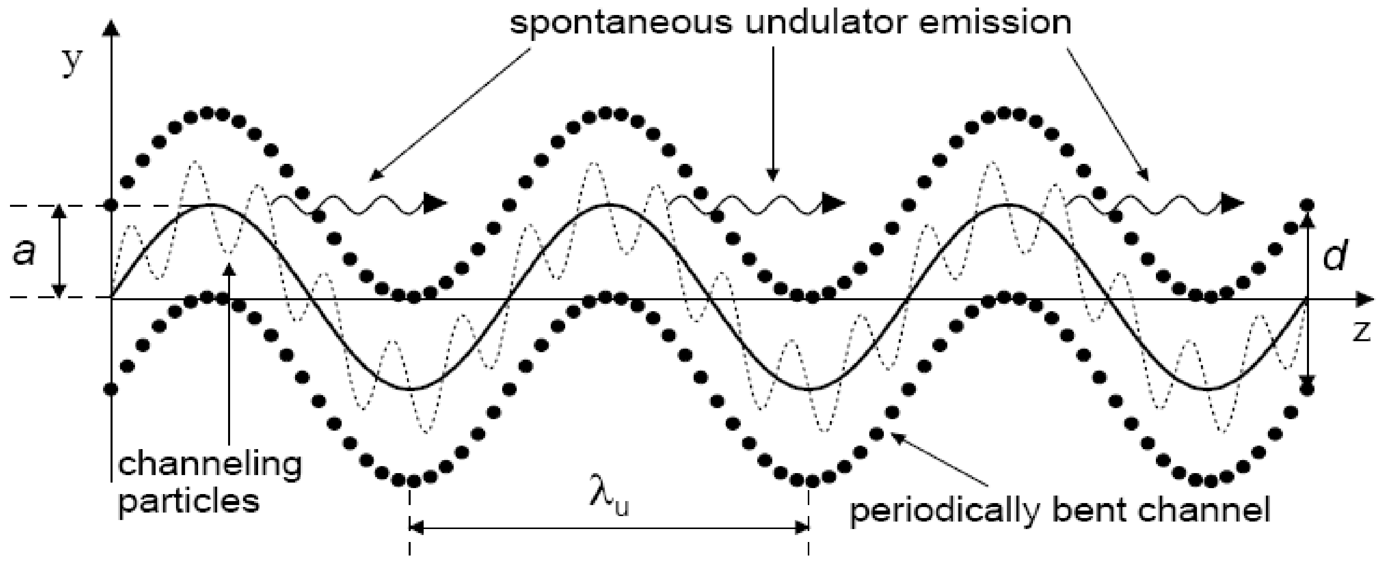
$$\omega^L = \frac{\omega_0}{1-\beta\cos\theta}$$

The maximum frequency is in the forward direction,

i.e., at $\theta = 0$ ($\beta = 1$)

$$\omega_m = 2\gamma^2\omega_0$$

Crystalline Undulator



A crystalline Undulator consist of

- *A channel which is periodically bent*
- *Channeling of ultra relativistic positively charged particles*

Channeling takes place if the maximum centrifugal force due to the bending is less than the maximal force due to the interplanar field.

We consider a crystal whose planes are periodically bent following a perfect harmonic shape

$$x(z) = a\ sin(k_u z)$$

The transverse and longitudinal coordinates of a channeled particle in such a periodically bent crystal

$$\tilde{x} = x - a\ sin(k_u z)$$

Where a is the amplitude of bending of the channel and

$$k_u = \frac{2\pi}{\lambda_u}$$

Region I & IV

The Schrödinger Equation for planar channeling

$$-\frac{\hbar^2}{2m}\left(\frac{\delta^2}{\delta x^2}+\frac{\delta^2}{\delta z^2}\right)\ \Psi^I(x,z)+U(x)\ \Psi^I(x,z)=E^I\ \Psi^I(x,z)$$

Region II & III

Centrifugal force proportional to μ^2/ρ_0^2 is responsible for the curved regions of the channel.

$\mu^2=l(l+1)$ with l as the orbital angular momentum quantum number and ρ_0 is the radius of curvature of the channel.

Assume that a finite number of undulator periods are there in a length of the dislocation affected region of the channel.

If λ_d is the wavelength of the dislocation affected region and x_d is the corresponding a $\lambda_d = n\,\lambda_u$ *f the waves*

$$
\begin{aligned}
r_1 &= a\ sin(nk_d z) \\
r_2 &= x_d\ sin(k_d z)
\end{aligned}
$$

Both these waves can be written in the form

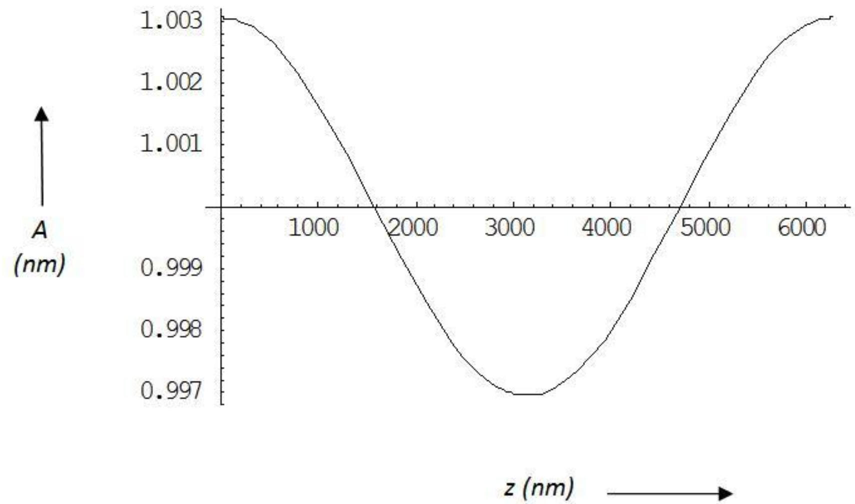
$$r = A\ sin(k_d z + \Phi)$$

Addition of the waves gives

$$
\begin{aligned}
A^2 &= a^2 + x_d^2 + 2ax_d\ cos[(n-1)k_d z - \phi] \\
tan\ \Phi &= \frac{a\ \ sin[(n-1)k_d z] + x_d\ sin\phi}{a\ cos[(n-1)k_d z] + x_d\ cos\phi}
\end{aligned}
$$

the final wave.

Amplitude is no longer constant but varies periodically with respect to the depth



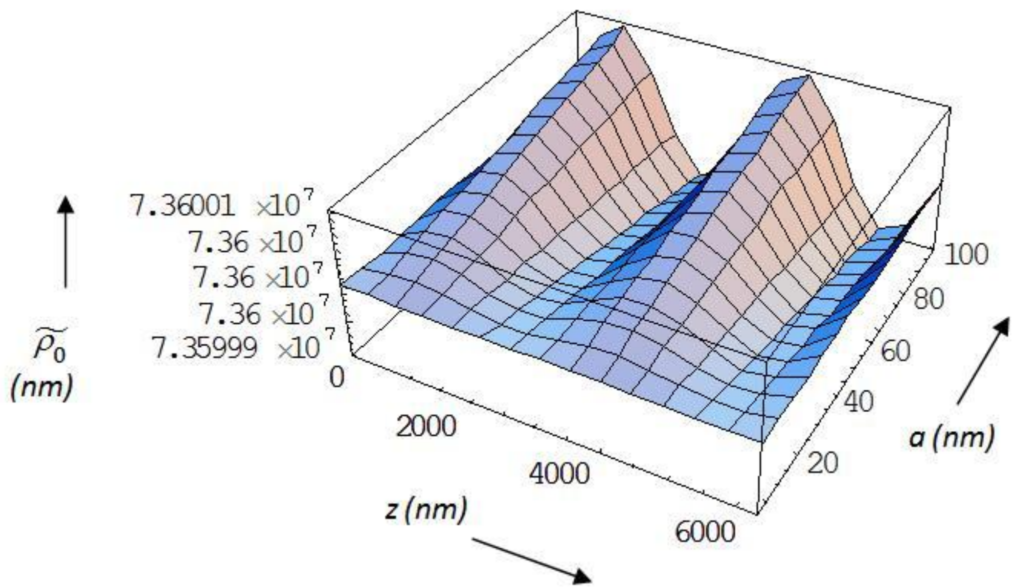
$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right]\Psi^{II}(\rho,\varphi)+U(\rho)\Psi^{II}(\rho,\varphi)=E^{II}\ \Psi^{II}(\rho,\varphi)$$

With the channel periodically bent, the radius of curvature of the dislocated affected region,

$$V(\rho)=-\ \frac{V_0}{(\rho-\tilde{\rho}_0)+a_T}$$

$$\tilde{\rho}_0=\rho_0-x_d\ sin(k_d z)+A\ sin(k_u z)$$

Larger the value of a, larger is the variation of $\tilde{\rho}_0$ with z.



Assume a finite number of undulator periods in a length of the dislocation affected region of the channel (low or medium dislocation concentration). If λ_d is the wavelength of the dislocation affected region and x_d is the corresponding amplitude of the waves

$$\lambda_d = n\,\lambda_u$$

The equation of motion of both the waves

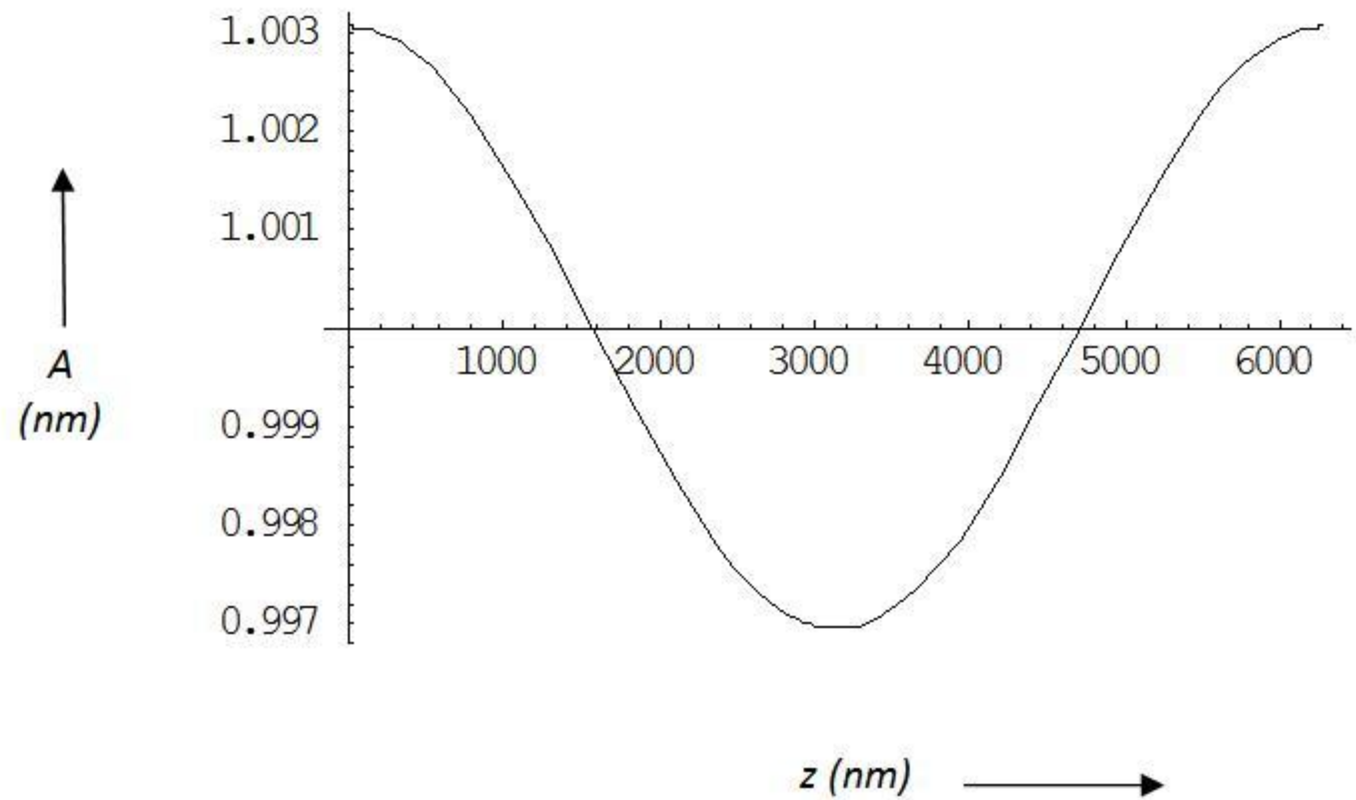
$$r_1 = a\ sin(nk_d z)$$
$$r_2 = x_d\ sin(k_d z)$$

Superposition of the two waves gives

$$r = A\ sin(k_d z + \varepsilon)$$

Where A and ε are the effective amplitude and phase of the final wave.

$$A^2 = a^2 + x_d^2 + 2ax_d\ cos[(n-1)k_d z - \phi]$$
$$tan\ \varepsilon = \frac{a\ sin[(n-1)k_d z] + x_d\ sin\phi}{a\ cos[(n-1)k_d z] + x_d\ cos\phi}$$

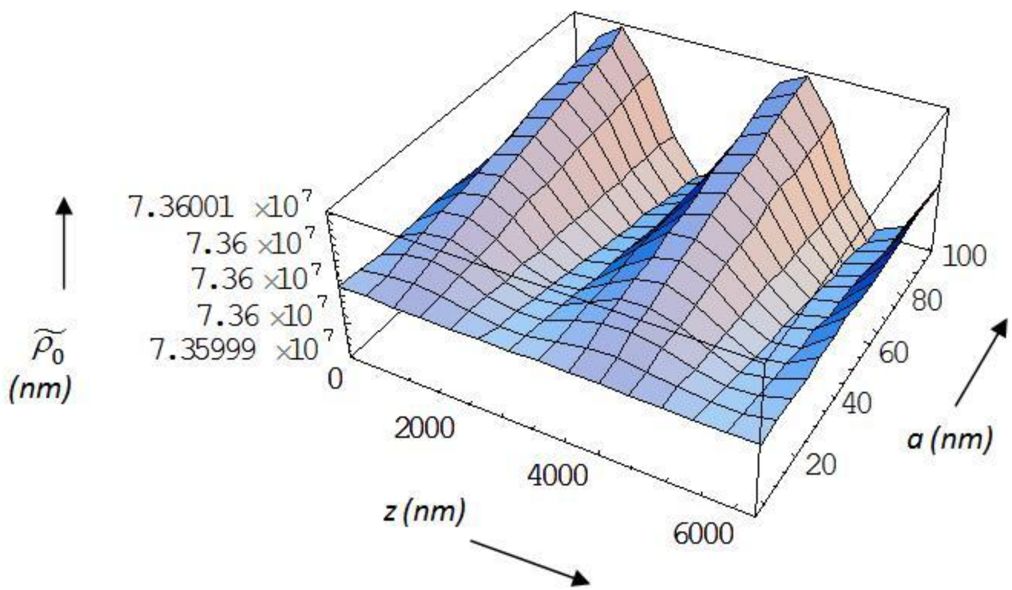

1.003
1.002
1.001
0.999
0.998
0.997
1000
2000
3000
4000
5000
6000
A
(nm)
z (nm)

The Schrödinger Equation

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

With the channel periodically bent, the radius of curvature of the dislocated affected region,

$$\tilde{\rho_0}=\rho_0-x_d\ sin(k_d z)+A\ sin(k_u z)$$



The variation of parameters of the dislocation affected region with dislocation density,

Dislocation density	r_0	Radius of Curvature	2z (Length of the curved part)
$10^{10}/cm^2$	$0.5\times\ 10^2$ nm	$10.28\ \times\ 10^5$ nm	$6.28\ \times\ 10^2$ nm
$10^9/cm^2$	$1.58\ \times\ 10^2$ nm	$10.26\ 6\times\ 10^6$ nm	$9.92\ \times\ 10^2$ nm
$10^8/cm^2$	$0.5\ \times\ 10^3$ nm	$10.28\ \times\ 10^7$ nm	$6.28\ \times\ 10^3$ nm

Range of various parameters of the periodically bent channel affected with dislocation corresponding to a dislocation density of $10^8/cm^2$,

a (cm)	λ_u (cm)	R_u (cm)	E (Mev)	x_d amplitude of the dislocation wave
$1\ \times\ 10^{-7}$	$3.14\times\ 10^{-4}$	$2.5\ \times\ 10^{-2}$	142.363	$2.198\ \times\ 10^{-3}$
$10\ \times\ 10^{-7}$	$3.14\times\ 10^{-4}$	$2.5\ 6\times\ 10^{-3}$	14.236	$2.198\ \times\ 10^{-4}$
$100\ \times\ 10^{-7}$	$3.14\ \times\ 10^{-4}$	$2.5\times\ 10^{14}$	1.412	$2.198\ \times\ 10^{15}$

When $\lambda_d < \lambda_u$

Range of various parameters of the periodically bent channel affected with dislocation at $\lambda_u = 2\,\lambda_d$

Dislocation density	λ_d (cm)	λ_u (cm)	a (cm)	R_u (cm)	E (MeV)
$1.5\times 10^9/cm^2$	1.66×10^{-4}	3.32×10^{-4}	1×10^{-7}	2.8×10^{-2}	150
			10×10^{-7}	2.8×10^{-3}	15
			100×10^{-7}	2.8×10^{-4}	1.5

Equation of motion,

$$\tilde{x} = x - a\ sin(k_u v t)$$

$$\ddot{\tilde{x}} = \ddot{x} + a k_u^2 v^2\ sin(k_u v t)$$

$$\frac{1}{R} = a k_u^2\ sin(k_u v t)$$

$$\ddot{\tilde{x}} + \frac{qe}{m\gamma}U(\tilde{x}) - \frac{\gamma v^2}{R}\tilde{x} = 0$$

The maximum amplitude of oscillation

$$\tilde{x}_m = \frac{m\gamma^2 v^2}{qeV_0 R}$$

And the equilibrium axis shifts to,

$$\tilde{x}_0 = \frac{m\gamma^2 v^2}{2qeV_0 R}$$

The period of oscillation of the particle in the channel,

$$T = \left(\frac{m\gamma}{2qeV_0}\right)^{1/2} Sin^{-1}\left\{1 - \frac{2qeV_0 R}{m\gamma^2 v^2} cos(k_u z)\right\}$$

The reflection and transmission coefficients FOR ELECTRONS case

$$|R|^2 = \frac{(-\mu^2 + 2mE\tilde{\rho}_0^2)^2 Sin^2(2\mu\varphi_0)}{8mE\mu^2\tilde{\rho}_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + 2mE\tilde{\rho}_0^2)^2 Sin^2(2\mu\varphi_0)}$$

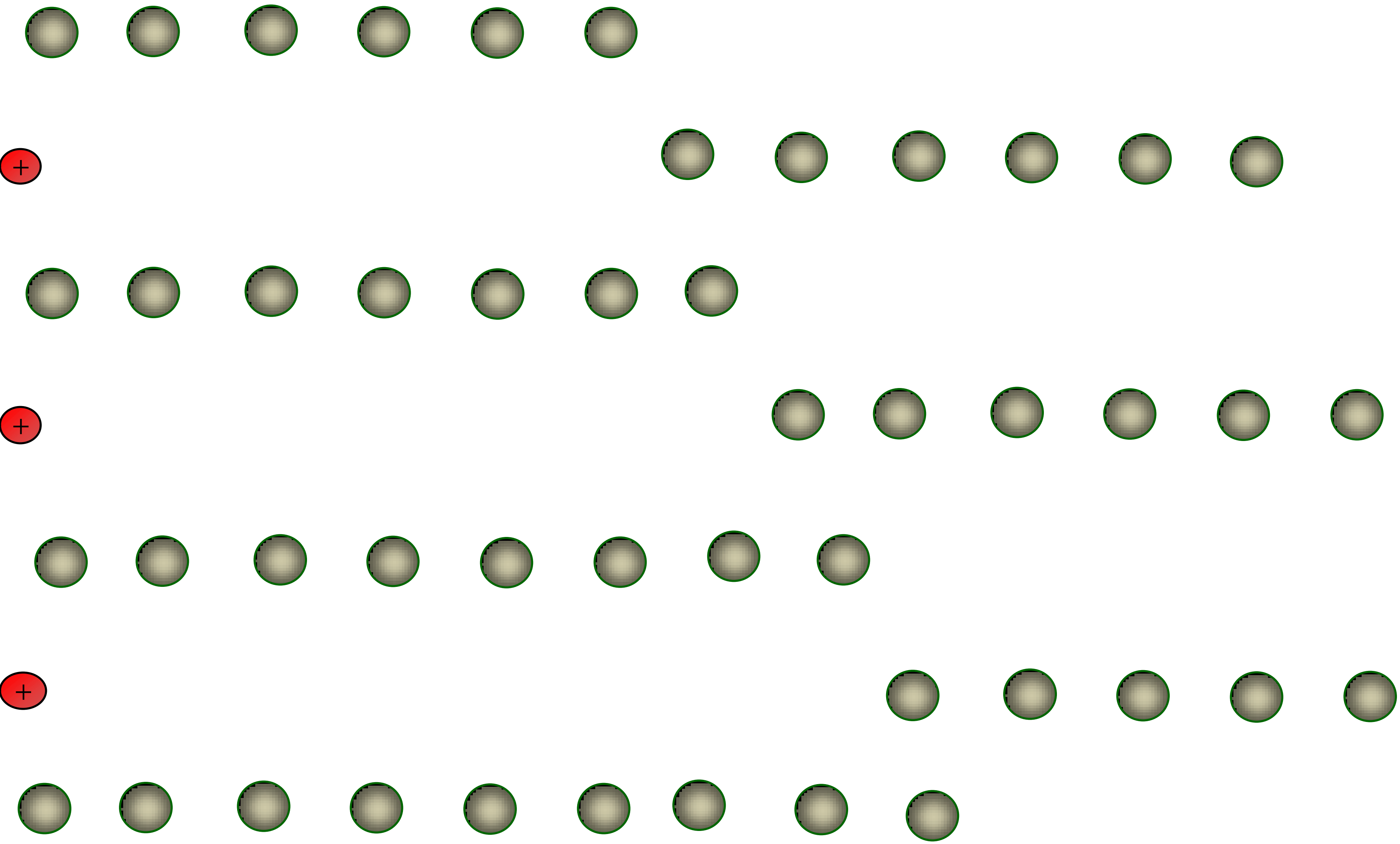
$$|T|^2 = \frac{8mE\tilde{\rho}_0^2\mu^2}{8mE\mu^2\tilde{\rho}_0^2 Cos^2(2\mu\varphi_0) + (\mu^2 + 2mE\tilde{\rho}_0^2)^2 Sin^2(2\mu\varphi_0)}$$

Dislocations in a periodically bent crystal changes the channeling and dechanneling coefficients by the parameters of the crystalline undulator.

For low dislocation density, $\lambda_d > \lambda_u$, the channelled particle SEES the effects of dislocations because several undulations of crystalline undulator are within one period of dislocation affected channel.

In the opposite case of $\lambda_d < \lambda_u$, (High dislocation density) the undulator effects are largely UNEFFECTED by dislocations, because dislocation affected regions are like point defects on the scale of undulator affected regions

Channelons in Stacking Faults



Positron channeling in Stacking Faults

- Quantum model[1]

- Energy dependence[2]

[1] *L. N. S. Prakash Goteti, Anand P. Pathak, J. Phys.* ***C 9 (1997) 1709.***

[2] V.S. Vendamani, S.V.S. Nageswara Rao, Nucl. Instr. Meth. Phys. Res. ***B 268 (2010)*** *2312–2317.*

Effects of stacking fault on positron planar channeling – energy dependence (Harmonic potential)

Dechanneling probability varies as (in classical region)

- point defects $E^{-1/2}$

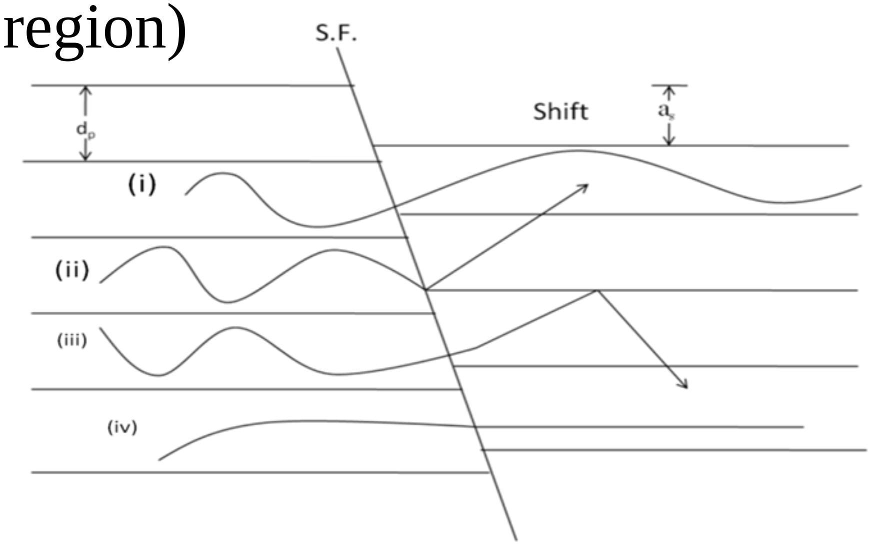
- dislocations E

- stacking fault E^0 (independent of incident energy)

? To verify whether this relation is applicable for light relativistic particles (in quantum region)

Channeling on stacking faults

- Mismatched stacking sequence



Ref: A.P. Pathak, Rad. Eff. 61, 1 (1982); J.J. Quillico and J.C. Jousset, Phys. Rev. **B** 11, 1791 (1975)

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

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

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

$$<n|m> = \frac{\exp\left(\frac{-b^2}{4} \right)}{\sqrt{2^{m+n} m! n!}} \left(\sum_{r=\max(0,m-n)}^{m} (-1)^{n-m+r} 2^{m-r} m_{c_r} \frac{n!}{(n-m+r)!} (b)^{n-m+2r} \right)$$

Channeling probability $$P_n = \sum_{m=0}^{n_{\max}} |<n|m>|^2,$$

Dechanneling probability $$\chi_n = 1 - P_n$$

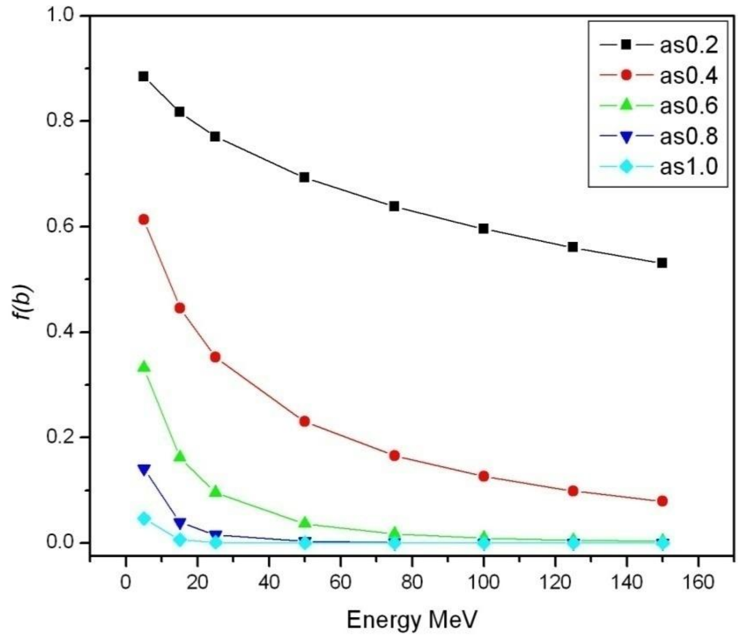
Ref: L.N.S. Prakash Goteti, J. Phys.: Condens. Matter **9**, 1709 (1997)

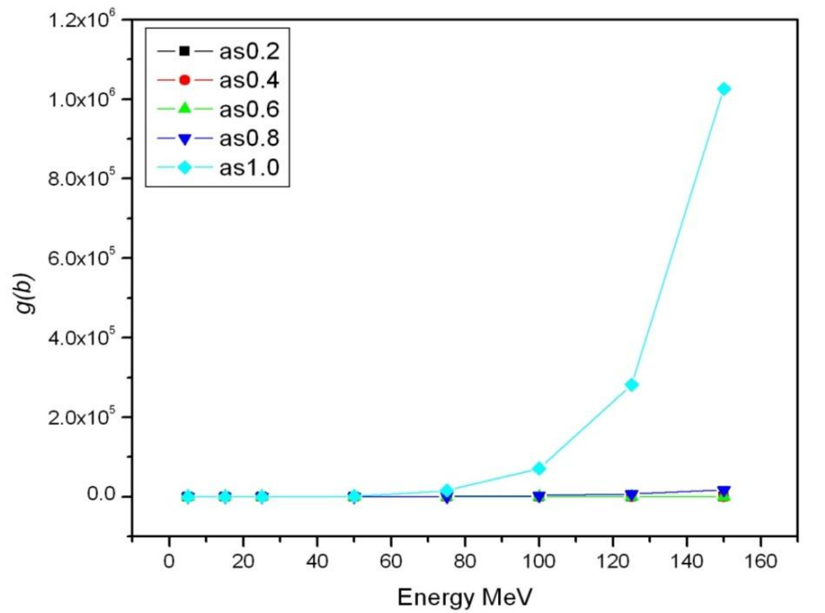
Energy dependence

- Characterize the nature of defects present in crystals
- Well channeled configuration (all particles are in grd. St.)

$$<0/m>_= \left|\exp\left(\frac{-b^2}{4}\right)\right|^2 \sum_{i=0}^{n_{\max}} \left|\frac{b^i}{\sqrt{2^i i!}}\right|^2_= f(b).g(b)$$

where $f(b) = \left|\exp\left(\frac{-b^2}{4}\right)\right|^2$ and $g(b) = \sum_{i=0}^{n_{\max}} \left|\frac{b^i}{\sqrt{2^i i!}}\right|^2$, where $b = \alpha . a_s$

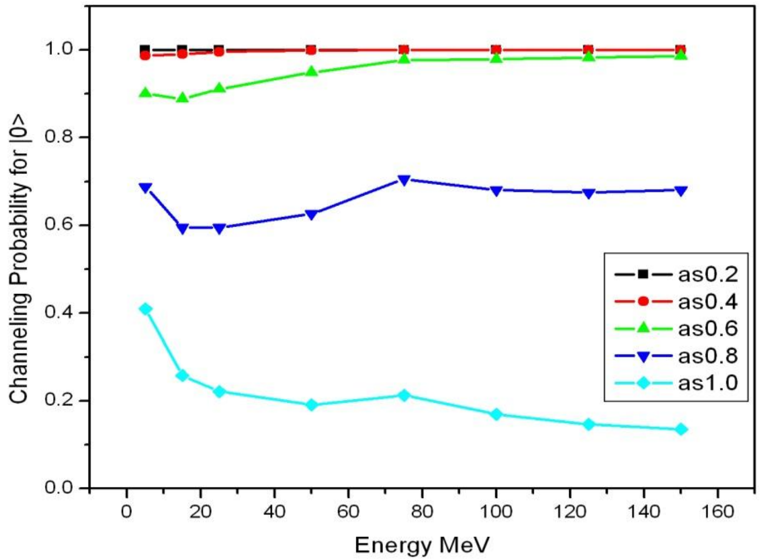


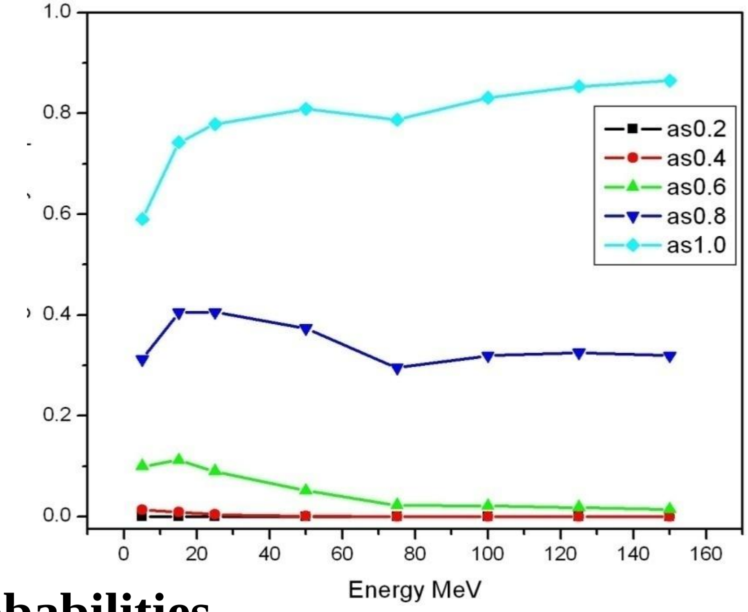


✓Decrease with increase in energy

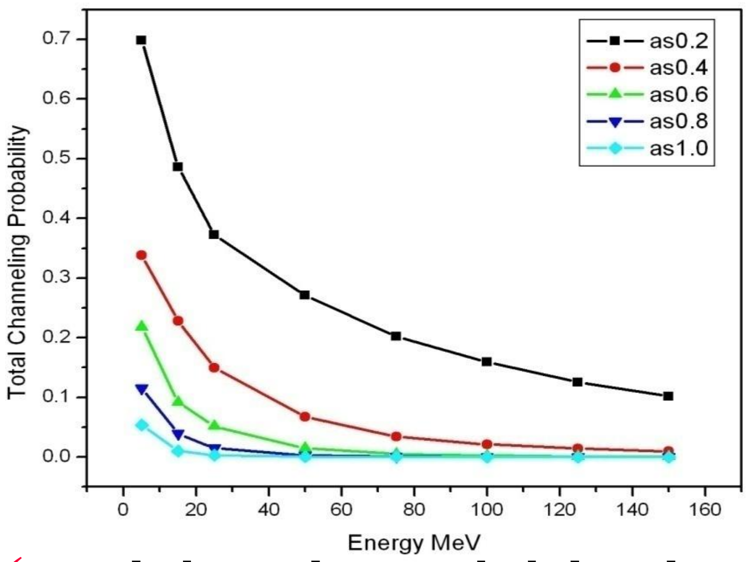
✓Increase with increase in energy

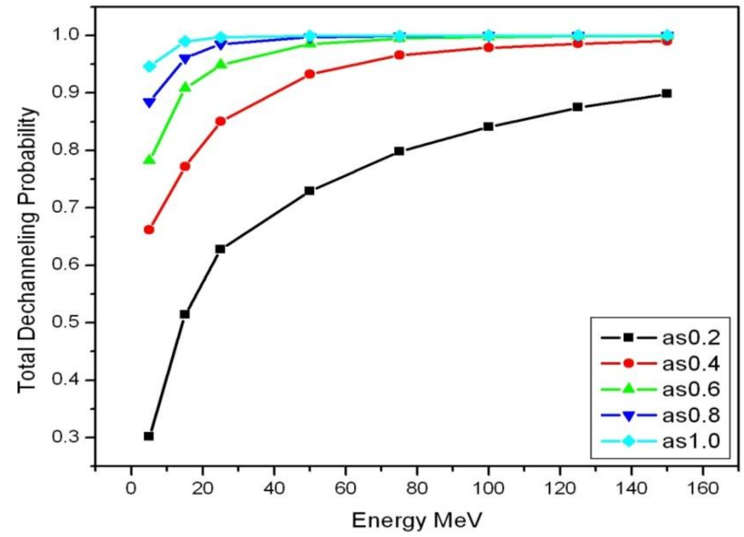
Channeling and dechanneling probabilities for ground state





Total channeling and dechanneling probabilities





- ✓ Total channeling probability decreases with increase in energy.
- ✓ Decreasing for increasing staking shift.

Effects of stacking fault on positron planar channeling – energy dependence (Anharmonic potential)

- Matrix element across the stacking faults

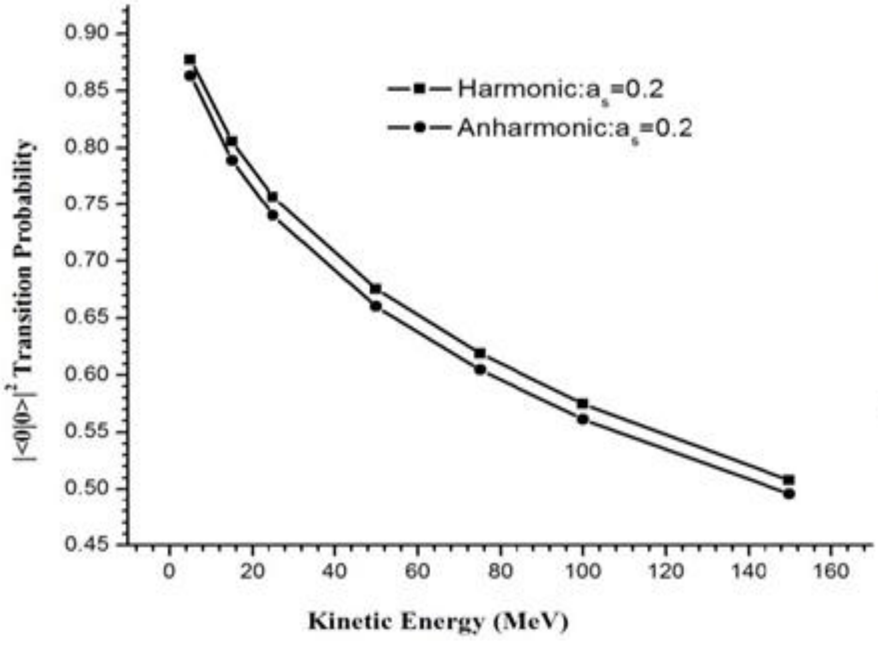
$$
\begin{aligned}
\left\langle m^{(1)} \middle| n^{(1)} \right\rangle = {} & \left\langle m^{(0)} \middle| n^{(0)} \right\rangle + kC_1^n \left\langle m^{(0)} \middle| n-2^{(0)} \right\rangle - kC_2^n \left\langle m^{(0)} \middle| n+2^{(0)} \right\rangle + kC_3^n \left\langle m^{(0)} \middle| n-4^{(0)} \right\rangle - kC_4^n \left\langle m^{(0)} \middle| n+4^{(0)} \right\rangle \\
& + kC_1^m \left\langle m-2^{(0)} \middle| n^{(0)} \right\rangle + k^2 C_1^m C_1^n \left\langle m-2^{(0)} \middle| n-2^{(0)} \right\rangle - k^2 C_1^m C_2^n \left\langle m-2^{(0)} \middle| n+2^{(0)} \right\rangle + k^2 C_1^m C_3^n \left\langle m-2^{(0)} \middle| n-4^{(0)} \right\rangle \\
& - k^2 C_2^m C_1^n \left\langle m+2^{(0)} \middle| n-2^{(0)} \right\rangle + k^2 C_2^m C_2^n \left\langle m+2^{(0)} \middle| n+2^{(0)} \right\rangle - k^2 C_2^m C_3^n \left\langle m+2^{(0)} \middle| n-4^{(0)} \right\rangle + k^2 C_2^m C_4^n \left\langle m+2^{(0)} \middle| n+4^{(0)} \right\rangle \\
& + kC_3^m \left\langle m-4^{(0)} \middle| n^{(0)} \right\rangle + k^2 C_3^m C_1^n \left\langle m-4^{(0)} \middle| n-2^{(0)} \right\rangle - k^2 C_3^m C_2^n \left\langle m-4^{(0)} \middle| n+2^{(0)} \right\rangle + k^2 C_3^m C_3^n \left\langle m-4^{(0)} \middle| n-4^{(0)} \right\rangle - k^2 C_3^m C_4^n \left\langle m-4^{(0)} \middle| n+4^{(0)} \right\rangle \\
& - kC_4^m \left\langle m+4^{(0)} \middle| n^{(0)} \right\rangle - k^2 C_4^m C_1^n \left\langle m+4^{(0)} \middle| n-2^{(0)} \right\rangle + k^2 C_4^m C_2^n \left\langle m+4^{(0)} \middle| n+2^{(0)} \right\rangle - k^2 C_4^m C_3^n \left\langle m+4^{(0)} \middle| n-4^{(0)} \right\rangle + k^2 C_4^m C_4^n \left\langle m+4^{(0)} \middle| n+4^{(0)} \right\rangle
\end{aligned}
$$

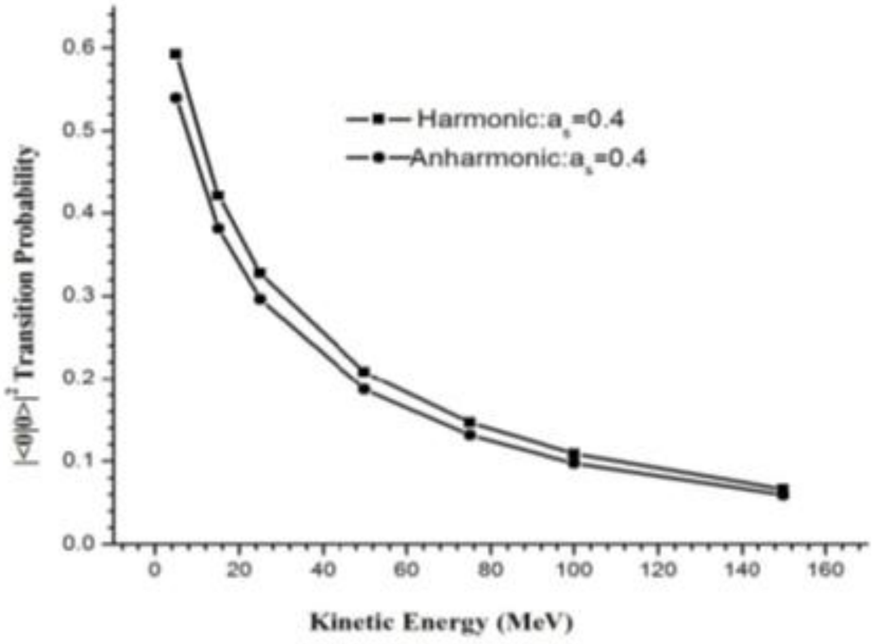
Channeling probability $$P_n = \sum_{m=0}^{n_{\max}} \left| < n \,|\, m > \right|^2 ,$$

Dechanneling probability $$\chi_n = 1 - P_n$$

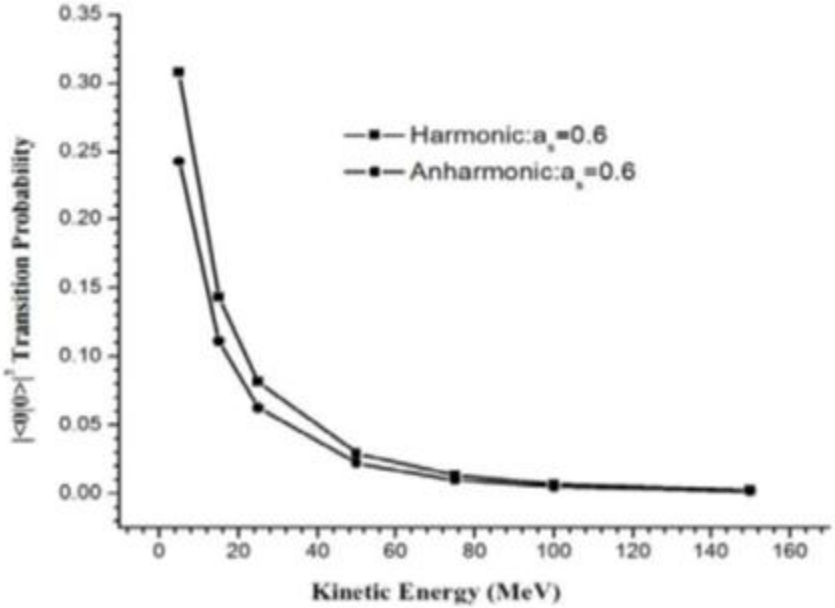
• **Well channeled configuration**

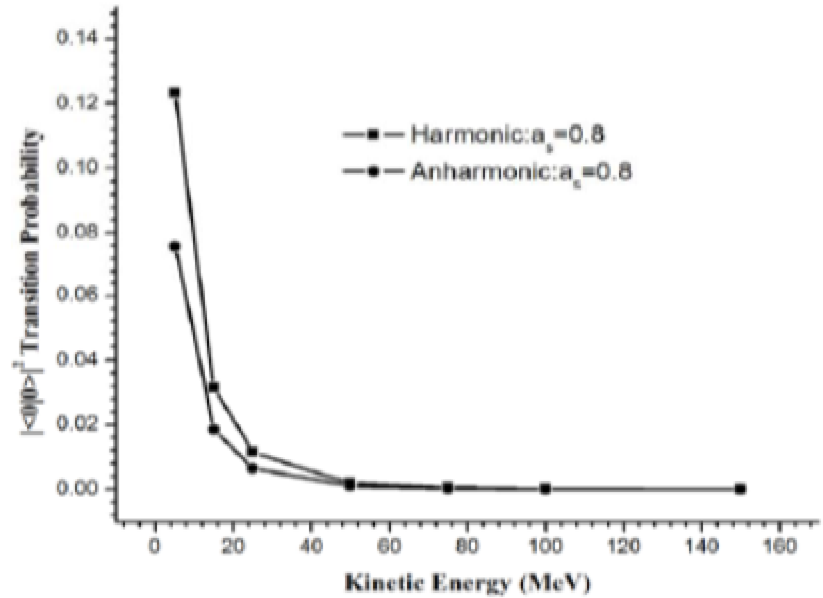
$$\langle 0^{(1)}|0^{(1)}\rangle = \langle 0^{(0)}|0^{(0)}\rangle - 3\sqrt{2}k\langle 0^{(0)}|2^{(0)}\rangle - \frac{\sqrt{6}}{2}k\langle 0^{(0)}|4^{(0)}\rangle - 3\sqrt{2}k\langle 2^{(0)}|0^{(0)}\rangle$$
$$+18k^2\langle 2^{(0)}|0^{(0)}\rangle + 3\sqrt{3}k^2\langle 2^{(0)}|4^{(0)}\rangle - \frac{\sqrt{6}}{2}k\langle 4^{(0)}|0^{(0)}\rangle + 3\sqrt{3}k^2\langle 4^{(0)}|2^{(0)}\rangle + \frac{3}{2}k^2\langle 4^{(0)}|4^{(0)}\rangle$$





✓ Decreases with increase in energy and saturates as the system approaches to classical regime.

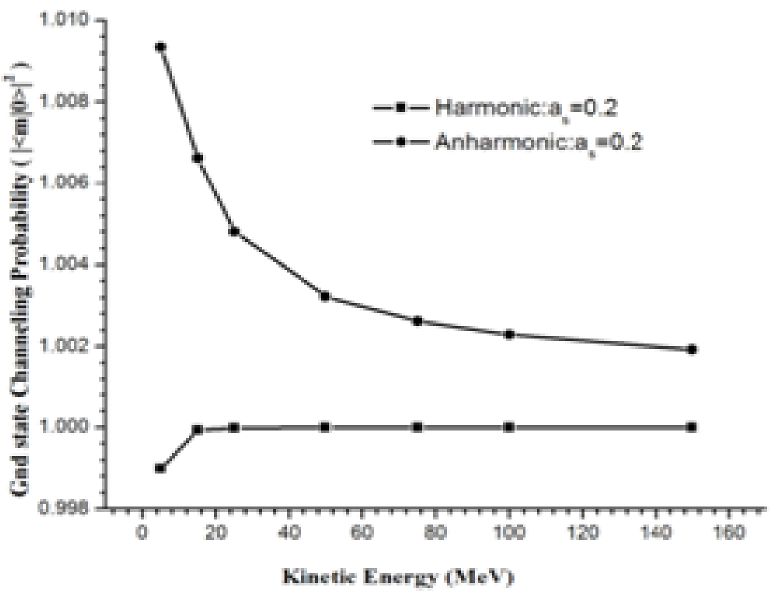


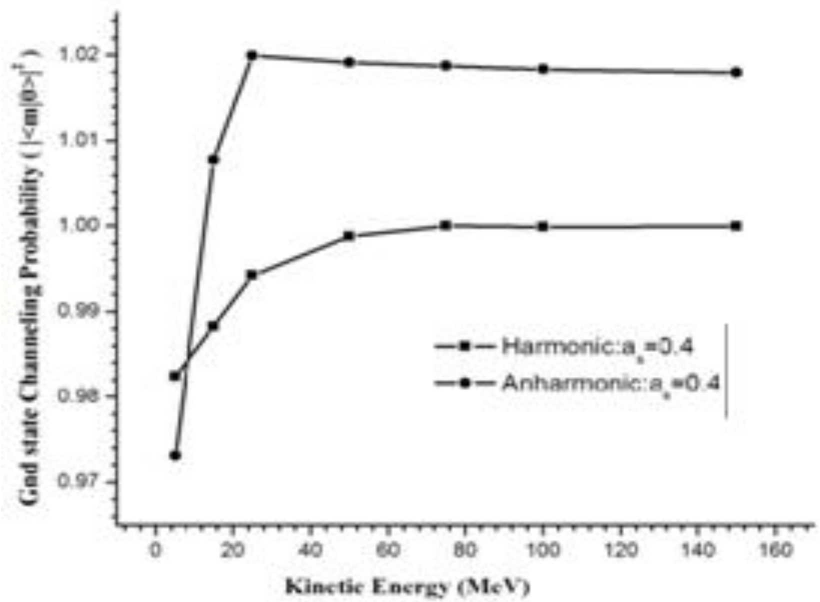


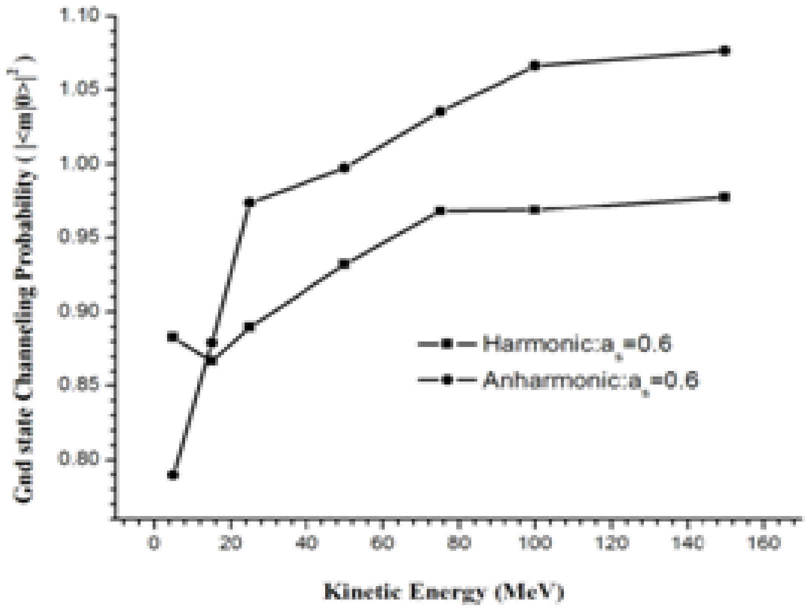
- ✓Dechanneling probability follows similar trend in both anharmonic and harmonic cases.
- ✓ Anharmonic approximation is found to be less when compared to harmonic approximation.

• Initially well channeled configuration

$$
\begin{aligned}
\left\langle m^{(1)} \middle| 0^{(1)} \right\rangle = {} & \left\langle m^{(0)} \middle| 0^{(0)} \right\rangle - kC_2^n \left\langle m^{(0)} \middle| 2^{(0)} \right\rangle - kC_4^n \left\langle m^{(0)} \middle| 4^{(0)} \right\rangle + kC_1^m \left\langle m-2^{(0)} \middle| 0^{(0)} \right\rangle \\
& - k^2 C_1^m C_2^n \left\langle m-2^{(0)} \middle| 2^{(0)} \right\rangle - k^2 C_1^m C_4^n \left\langle m-2^{(0)} \middle| 4^{(0)} \right\rangle - kC_2^m \left\langle m+2^{(0)} \middle| 0^{(0)} \right\rangle \\
& + k^2 C_2^m C_2^n \left\langle m+2^{(0)} \middle| 2^{(0)} \right\rangle + k^2 C_2^m C_4^n \left\langle m+2^{(0)} \middle| 4^{(0)} \right\rangle + kC_3^m \left\langle m-4^{(0)} \middle| 0^{(0)} \right\rangle \\
& - k^2 C_3^m C_2^n \left\langle m-4^{(0)} \middle| 2^{(0)} \right\rangle - k^2 C_3^m C_4^n \left\langle m-4^{(0)} \middle| 4^{(0)} \right\rangle - kC_4^m \left\langle m+4^{(0)} \middle| 0^{(0)} \right\rangle \\
& + k^2 C_4^m C_4^n \left\langle m+4^{(0)} \middle| 4^{(0)} \right\rangle
\end{aligned}
$$







✓Saturation of energy dependence occurs for lower energies in anharmonic approximation.

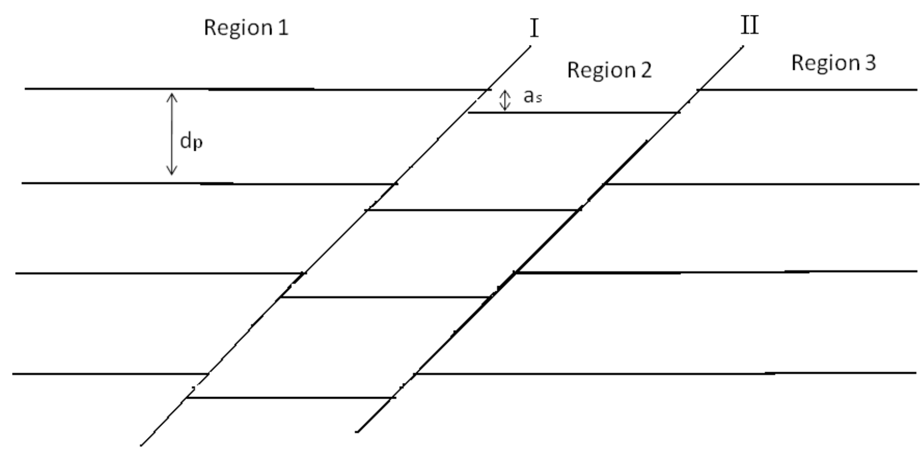
Energy dependence of positron dechanneling –Platelets

- Transition probability

$$p_{i\to k}=\sum_{k=0}^{k_{\max}}\left[\sum_{j=0}^{j_{\max}}\left(p_{i\to j}\times p_{j\to k}\right)\right]$$

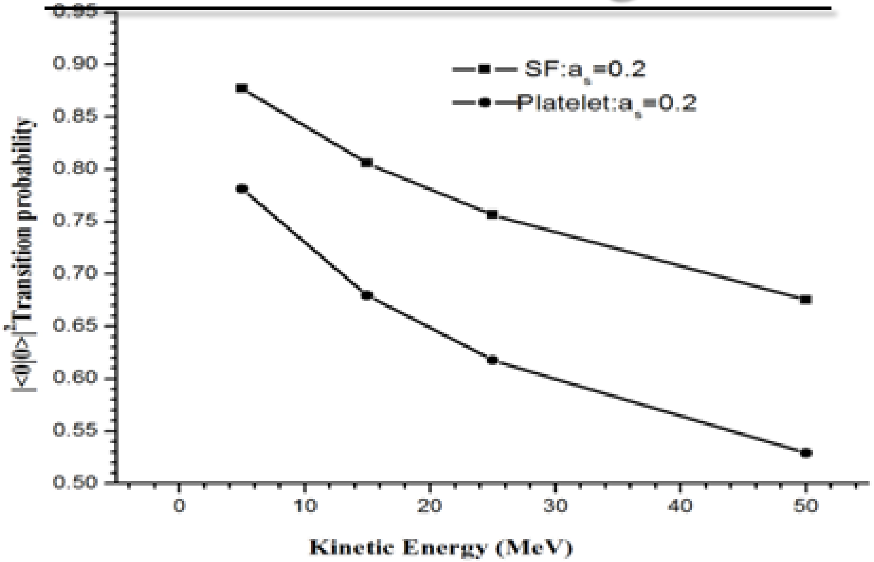
- Dechanneling probability

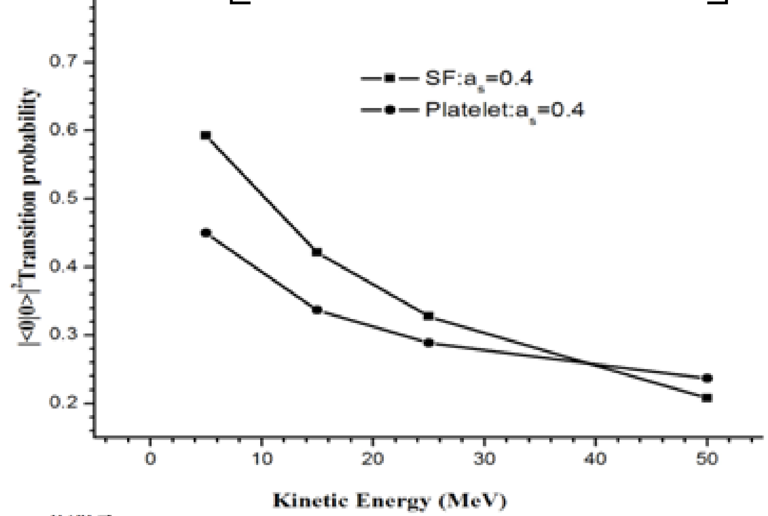
$$\chi_i = 1 - p_{i\to k}$$

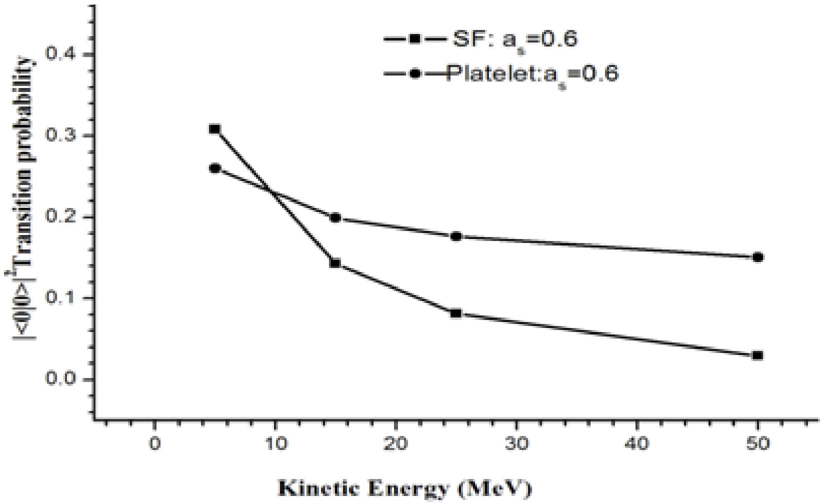


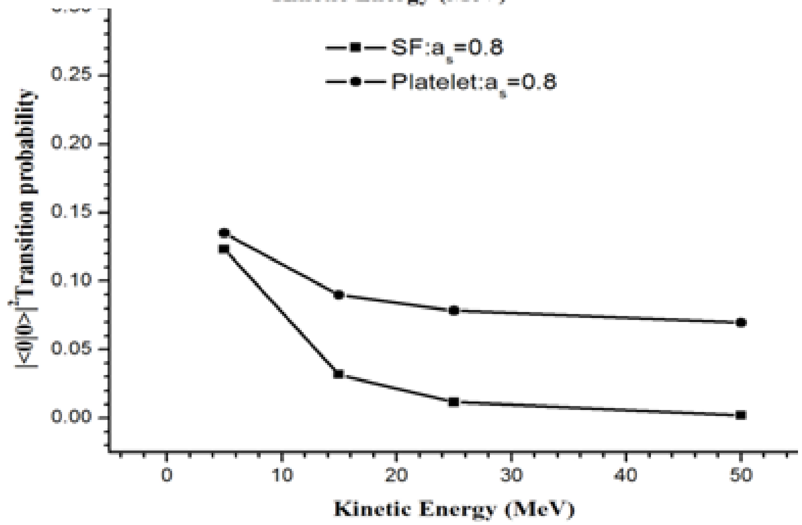
•Well channeled configuration

$$p_{i=0\rightarrow k=0} = \sum_{k=0}^{0}\left[\sum_{j=0}^{j_{\max}}\left(p_{i=0\rightarrow j} \times p_{j\rightarrow k=0}\right)\right]$$





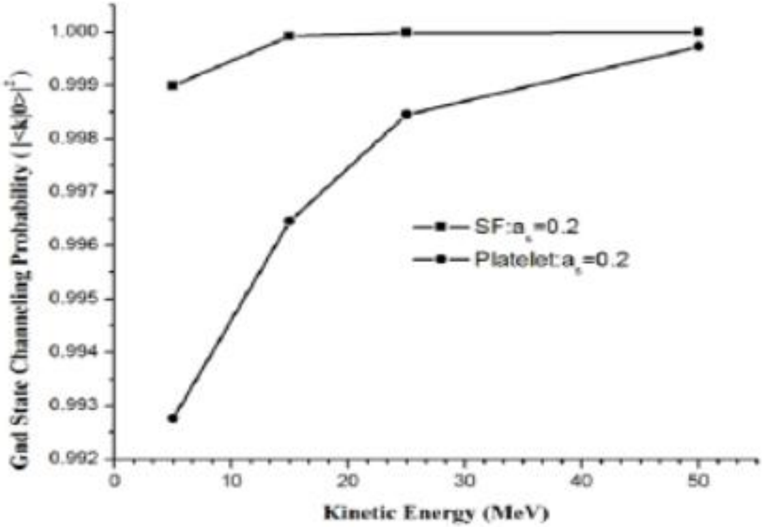


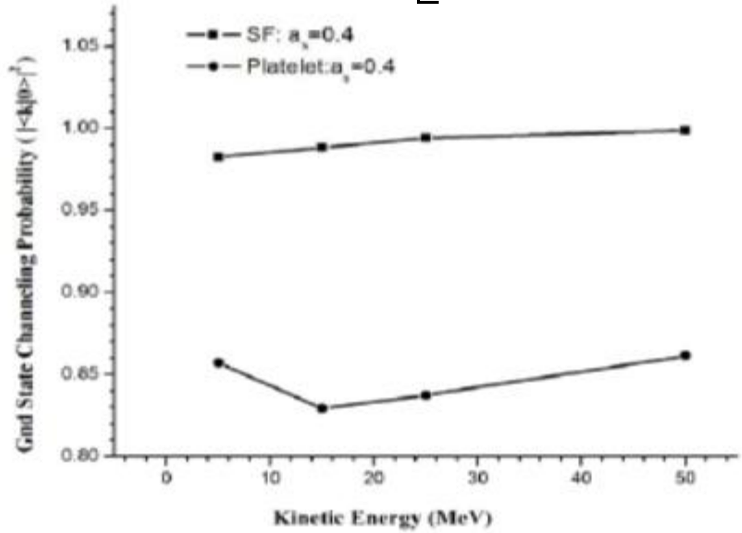


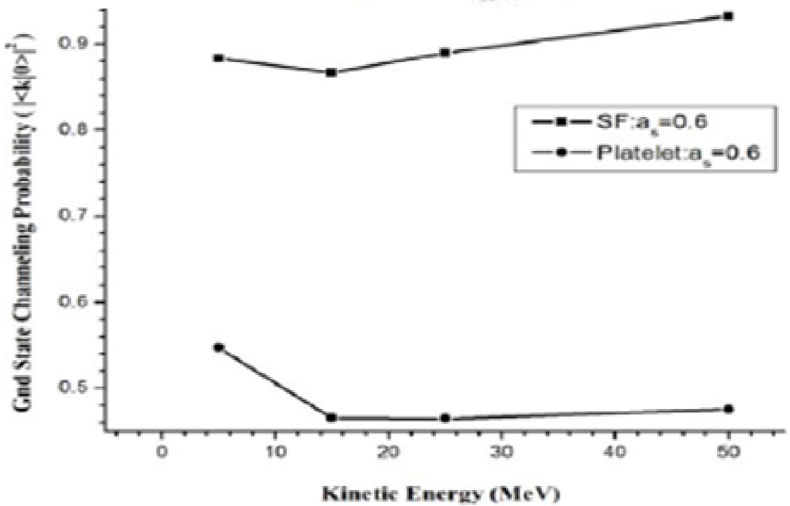
- ✓Transition probability decreases with increase in energy and saturates at higher energies.
- ✓ Transition probability in platelet is less as compared to stacking fault case.

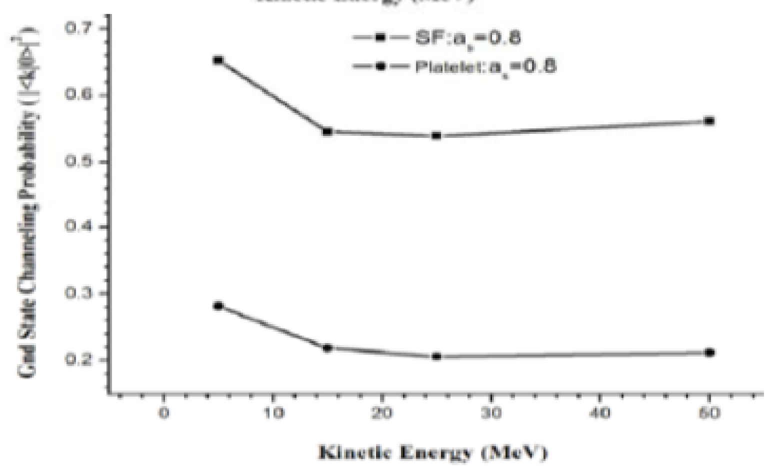
Initially well channeled configuration

$$p_{i=0\to k}=\sum_{k=0}^{k_{\max}}\left[\sum_{j=0}^{j_{\max}}\left(p_{i=0\to j}\times p_{j\to k}\right)\right]$$









- ✓Dechanneling probability is independent of energy in case on classical regime.
- ✓ At high energies platelet behave as stacking fault.

Conclusions

- ✓ The standard critical angle Ψ ($E^{-1/2}$) relation is not strictly valid for light relativistic particles (positrons).
- ✓ The area under the curve of total channeling probability for anharmonic case resembles with harmonic case for **increasing energy**.
- ✓ Total channeling and dechanneling probability are not independent of energy in the presence of stacking fault.
- ✓ Dechanneling probability follows similar trend in both anharmonic and harmonic cases.
- ✓ Saturation of energy dependence of dechanneling probability occurs for lower energies in anharmonic approximation.
- ✓ Dechanneling probability due to platelets is also independent of energy in classical regime as known for simple stacking faults.

India

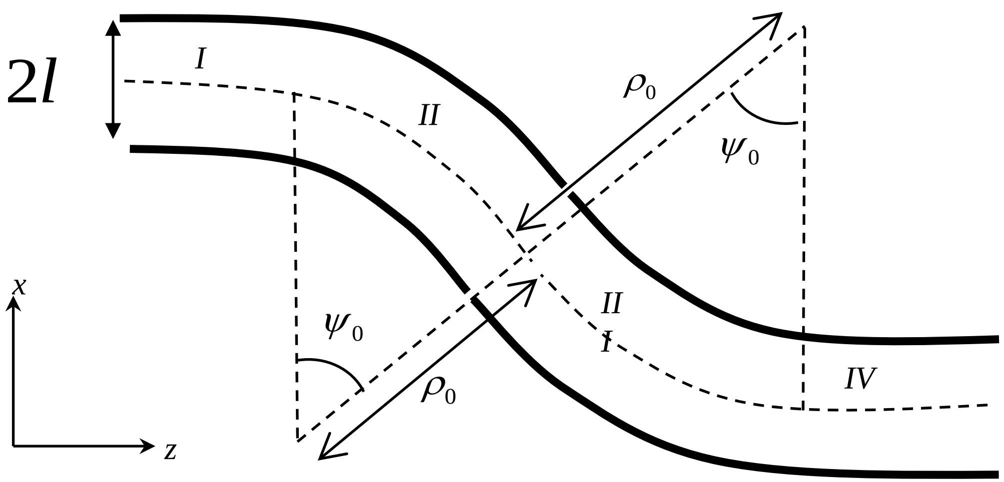
Equation of motion of a crystalline undulator

$$\tilde{x} = x - a\ sin(k_u z)$$

Where a is the amplitude of bending of the channel and

$$k_u = \frac{2\pi}{\lambda_u}$$

The dislocation affected region,



Region I

The Schrödinger Equation for planar channeling

$$-\frac{\hbar^2}{2m}\left(\frac{\delta^2}{\delta x^2}+\frac{\delta^2}{\delta z^2}\right)\ \Psi^I(x,z)+U(x)\ \Psi^I(x,z)=E^I\ \Psi^I(x,z)$$

$$\begin{aligned} U(x) &= V_0\tilde{x}^2 \\ &= V_0(x-a\ sin(k_u z))^2 \end{aligned}$$

Region II

Centrifugal force proportional to μ^2/ρ_0^2 is responsible for the curved regions of the channel.

$\mu^2=l(l+1)$ with l as the orbital angular momentum quantum number and ρ_0 is the radius of curvature of the channel.

Assume a finite number of undulator periods in a length of the dislocation affected region of the channel (low or medium dislocation concentration). If λ_d is the wavelength of the dislocation affected region and x_d is the corresponding amplitude of the waves

The equation of motion of both the waves

$$\lambda_d = n\,\lambda_u$$

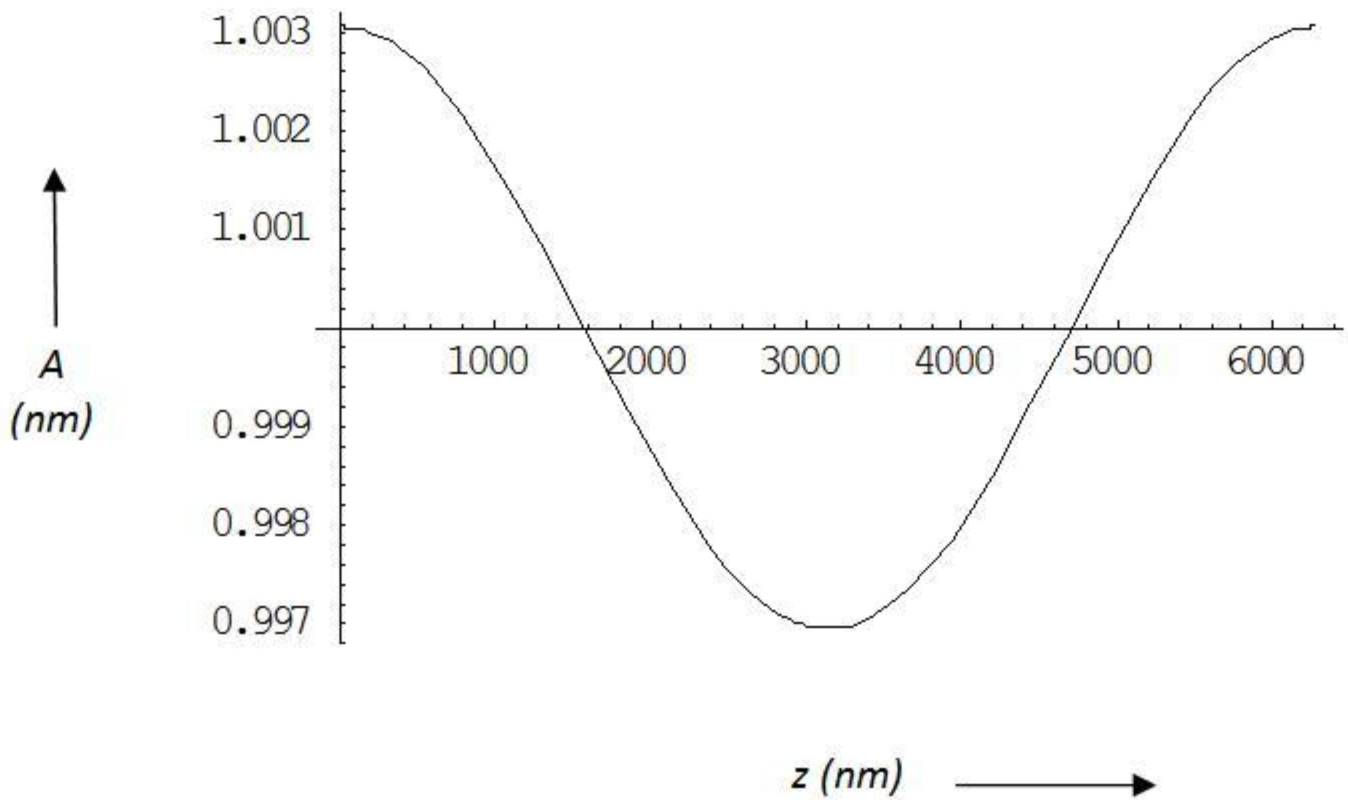
$$r_1 = a\ sin(nk_d z)$$
$$r_2 = x_d\ sin(k_d z)$$

Superposition of the two waves gives

$$r = A\ sin(k_d z + \varepsilon)$$

Where A and ε are the effective amplitude and phase of the final wave.

$$A^2 = a^2 + x_d^2 + 2ax_d\ cos[(n-1)k_d z - \phi]$$
$$tan\ \varepsilon = \frac{a\ sin[(n-1)k_d z] + x_d\ sin\phi}{a\ cos[(n-1)k_d z] + x_d\ cos\phi}$$

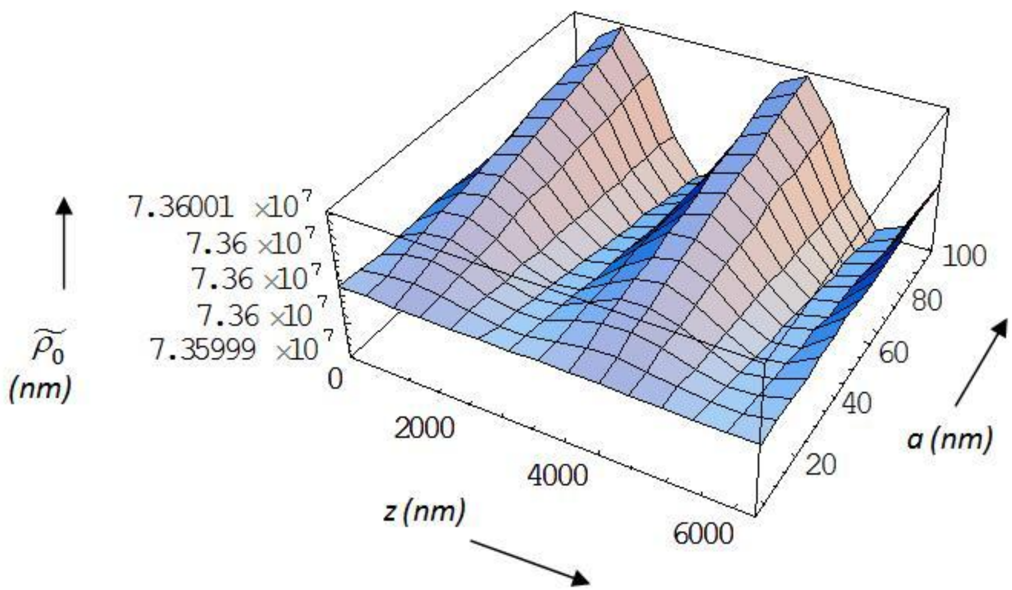

1.003
1.002
1.001
0.999
0.998
0.997
1000
2000
3000
4000
5000
6000
A
(nm)
z (nm)

The Schrödinger Equation

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

With the channel periodically bent, the radius of curvature of the dislocated affected region,

$$\tilde{\rho_0}=\rho_0-x_d\ sin(k_d z)+A\ sin(k_u z)$$



The variation of parameters of the dislocation affected region with dislocation density,

Dislocation density	r_0	Radius of Curvature	2z (Length of the curved part)
$10^{10}/cm^2$	$0.5\times\ 10^2$ nm	10.28×10^5 nm	6.28×10^2 nm
$10^9/cm^2$	1.58×10^2 nm	$10.26\ 6\times\ 10^6$ nm	9.92×10^2 nm
$10^8/cm^2$	0.5×10^3 nm	10.28×10^7 nm	6.28×10^3 nm

Range of various parameters of the periodically bent channel affected with dislocation corresponding to a dislocation density of $10^8/cm^2$,

a (cm)	λ_u (cm)	R_u (cm)	E (Mev)	x_d amplitude of the dislocation wave
1×10^{-7}	$3.14\times\ 10^{-4}$	2.5×10^{-2}	142.363	2.198×10^{-3}
10×10^{-7}	$3.14\times\ 10^{-4}$	$2.5\ 6\times\ 10^{-3}$	14.236	2.198×10^{-4}
100×10^{-7}	3.14×10^{-4}	$2.5\times\ 10^{14}$	1.412	2.198×10^{15}

The effective potential

$$V_{eff} = V_0(\rho - \tilde{\rho}_0)^2 + \frac{\hbar^2}{2m}\frac{\mu^2}{\rho^2}$$

$$V_{eff}(\xi) = \frac{\hbar^2}{2m}\left[\frac{\lambda}{\tilde{\rho}_0{}^4}(\xi - \tilde{a_p})^2 + U_{min}\right]$$

$$\xi = \rho - \tilde{\rho}_0$$

$$\lambda = 3\mu^2 + b^4\tilde{\rho}_0{}^4$$

$$\tilde{a_p} = \frac{\tilde{\rho}_0\mu^2}{\lambda}$$

$$U_{min} = \frac{\mu^2}{\lambda\tilde{\rho}_0{}^2}(\lambda - \mu^2)$$

$$b = \left(\frac{m\omega}{\hbar}\right)^{1/2}$$

The frequency of oscillation in the region,

$$\omega' = \left(\frac{\hbar}{m}\right)\sqrt{\frac{\lambda}{\tilde{\rho}_0{}^4}}$$

With the effective wavefunction

$$\Psi^{II}(\rho,\varphi) = \sum_{m=0} R_m^{II}\left[C_m e^{i\mu\varphi} + D_m e^{-i\mu\varphi}\right]$$

Region III

The effective potential

$$V_{eff}(\xi) = \frac{\hbar^2}{2m}\left[\frac{\lambda'}{\tilde{\rho_0}^4}(\xi + \tilde{a_p'})^2 + U'_{min}\right]$$

$$\lambda' = -3\mu^2 + b^4\tilde{\rho_0}^4$$

$$\tilde{a_p'} = \frac{\tilde{\rho_0}\mu^2}{\lambda'}$$

$$U'_{min} = -\frac{\mu^2}{\lambda'\tilde{\rho_0}^2}(\lambda' + \mu^2)$$

The frequency of oscillation in the region,

$$\omega'' = \left(\frac{\hbar}{m}\right)\sqrt{\frac{\lambda'}{\tilde{\rho_0}^4}}$$

The wavefunction in region III

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

Region IV

$$\Psi^{IV}(x,z) = X_n^{IV} I_n e^{ik_n z}$$

The reflection and transmission coeffcients

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

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

When $\lambda_d < \lambda_u$

Range of various parameters of the periodically bent channel affected with dislocation at $\lambda_u = 2\lambda_d$

Dislocation density	λ_d (cm)	λ_u (cm)	a (cm)	R_u (cm)	E (MeV)
$1.5\times10^9/cm^2$	1.66×10^{-4}	3.32×10^{-4}	1×10^{-7}	2.8×10^{-2}	150
			10×10^{-7}	2.8×10^{-3}	15
			100×10^{-7}	2.8×10^{-4}	1.5

Equation of motion,

$$\tilde{x} = x - a\ sin(k_u vt)$$

$$\ddot{\tilde{x}} = \ddot{x} + ak_u^2 v^2\ sin(k_u vt)$$

$$\frac{1}{R} = ak_u^2\ sin(k_u vt)$$

$$\ddot{\tilde{x}} + \frac{qe}{m\gamma}U(\tilde{x}) - \frac{\gamma v^2}{R}\tilde{x} = 0$$

The maximum amplitude of oscillation

$$\tilde{x}_m = \frac{m\gamma^2 v^2}{qeV_0R}$$

And the equilibrium axis shifts to,

$$\tilde{x}_0 = \frac{m\gamma^2 v^2}{2qeV_0R}$$

$$T = \left(\frac{m\gamma}{2qeV_0}\right)^{1/2} Sin^{-1}\left\{1 - \frac{2qeV_0R}{m\gamma^2 v^2}cos(k_u z)\right\}$$

The period of oscillation of the particle in the channel,