QUANTUM MODELS FOR DECHANNELING BY POINT DEFECTS AND EXTENDED DEFECTS

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Abstract— ***A quantum mechanical description of dechanneling by point defects will be presented. The effects of electrons of heavy impurities and those of host material are treated in a double screening formulation. For extended defects like stacking faults and dislocations, a sudden approximation model is used. For positively charged channeled particles, the transition among bound states in the simple harmonic type transverse potential, induced by the sudden appearance of the extended defect (stacking fault or distortion due to dislocation) are considered. The resulting dechanneling probabilities and their energy dependences are calculated. An extension of the model to relax the sudden approximation (specially for dislocations) in a time dependent formulation has also been outlined and main results presented***.

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Keywords— **Put your keywords here, keywords are separated by comma.**

I. INTRODUCTION

The study of point defects in the crystals, their lattice location etc have been among the first applications of RBS/Channeling technique, nearly three decades back. The interaction potential between the probe projectile and the heavy impurities is appreciably modified due the presence of host crystal electrons (conduction and valence) on the one hand and the atomic electrons of the impurity, on the other. We have evaluated these effects in a double screening formulation and used the resulting double screened potential potential(1) to calculate the dechanneling cross sections and the results are given in the next section. The extended defects (stacking faults and dislocations) have been traditionally treated classically by including their obstruction and distortion effects. However, we have used quantum mechanical sudden approximation to calculate the transition probabilities on the wave functions of probe particles channeled in the perfect crystal to the dechanneling states in defective crystal. The resulting dechanneling probabilities are found to describe the phenomena accurately. The sudden approximation is relaxed for dislocations and a time dependent formulation is given which yields correct semiclassical limits.

POINT DEFECTS

The double-screened potential around a partially ionized impurity can be written as(1,2) *e-Xar* - A2e"Ar *V(r)* = *ZI r* **ë 2 - ë 2** (1) Here *Z^* = *Zð* = 1 and is omitted in the above equation and ëa is the Thomas-Fermi screening radius and is given by(4,5) 1/ëa = 0.8853ao(ZI — *Z})~1^3,* where *ao* is the Bohr radius, *ZI* is the atomic number of the impurity, *Z* is the degree of ionization of the impurity atom. ë in eq. (1) is the screening parameter which is associated with the screening of impurity by electron gas of host lattice and it is given by ë2 = *4ðe2N(EF)* with the density of final states *N(EF)*. The probability that the incident pions (or decay muons) will get trapped at impurity sites or will be diffused can be estimated applying the scattering theory; in particular the Born approximation and the double-screened potential (1,2) . Therefore the total scattering cross-section is

$$\sigma_t = \frac{32\pi Z_1^2 m^2 e^4}{\hbar^4(\lambda^2-\lambda_a^2)^2}\left[\left(\frac{\lambda^2}{2(\lambda^2+4k^2)}+\frac{\lambda_a^2}{2(\lambda_a^2+4k^2)}\right) + \frac{\lambda^2\lambda_a^2}{4k^2(\lambda^2-\lambda_a^2)} ln\left(\frac{\lambda_a^2(\lambda^2+4k^2)}{\lambda^2(\lambda_a^2+4k^2)}\right)\right] \quad (2)$$

The screened potential, in the most general form, is given by the Thomas-Fermi TF model

$$V(R) = \frac{Z_1 Z_2 e^2}{R}\phi\left(\frac{R}{a}\right) \quad (3)$$

where *Z1 and Z*$_2$ are the atomic numbers of projectile and target atoms respectively, *ö(x)* is called the Thomas-Fermi screening function. The choice of this TF function, and hence the screened potential, is not unique. This potential is related to the dielectric function *e{q)* through the Fourier transform as

$$U(q) = \frac{V(q)}{\epsilon(q)} \ where$$

$$\epsilon(q) = 1 + \frac{\Lambda^2}{q^2}\left[\frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} ln\left|\frac{2k_F + q}{2k_F - q}\right|\right] \quad (4)$$

Neglecting the higher order terms of 'q' and realizing the fact that the screened potential is further modified due to the presence of interstitial impurities, the potential thus derived in the long wavelength limit has been used for scattering amplitudes(2). *e{q)* has a singularity at *q = 2Kf* which is not analytic at that point. As a result of this singularity, the potential contains the well known Friedel oscillations of wave-number *2kF*. Expanding the log terms in the parenthesis, we get *e(q)* = 1—7$_2$—*â$_2$q$_2$* + *(ë/q)$_2$*, where *â$_2$ = 2me$_2$/ll5h$_2$irk$_F$*, ã$_2$ = *me$_2$/3h$_2$irkF* and the potential, which is modified due to the presence of impurities, is given by

$$U(r) = \frac{Z_1 Z_2 e^2}{r}\left[\frac{1}{\beta^2}\left(\frac{x^2\cos xr}{z(x^2+\lambda_a^2)} - \frac{y^2 e^{-yr}}{2z(\lambda_a^2 - y^2)} + \frac{\lambda_a^2 e^{-\lambda_a r}}{(\lambda_a^2+x^2)(\lambda_a^2-y^2)}\right)\right] \quad (5)$$

where ëa and ë are the screening parameters which are described by the relevant dielectric function and *z = (a2 + b) a* = (1 - ã2)/2â2 , *b = ë2/â2 and x,y =* The above formulation highlights the fact that the conduction electrons of the host lattice and the atomic electrons of the impurity play an important role in such an interaction(6). The weakly decaying nature of this screened potential shows its signature here which is otherwise not observed elsewhere(7). Treating the work of Chylinski et al(1) as a prototype, we can write the dechanneling crosssectionfor the potential as

$$\sigma(E) = KE^{-1/2}\left[\frac{1}{\beta^2}\left(\frac{\lambda_a}{(\lambda_a^2+x^2)(\lambda_a^2-y^2)} - \frac{y}{2z(\lambda_a^2-y^2)}\right)\right], \quad (6)$$

where $K = \frac{Z_1 Z_I \pi e^2}{x_c}\sqrt{\frac{Y(Y^2-x_c^2)}{A}}$,

$A = 6\pi Z_2 e^2 N_p a_T^2$,

$Y = d + \frac{a_T}{2}$, and $x_c = \left(\frac{d_p}{2}\right) - a_T$.

EXTENDED DEFECTS

The channeling phenomena, for the case of extended defects which is basically a transition from one harmonic potential to the other, is governed by the transition probability evaluated in terms of matrix element of the wave functions corresponding to various portions of obstruction distortion. These effects can be suitably incorporated by calculating the number of quantum states supported by the planar channel. Under the sudden approximation the general expression for overlap integral < *ipi\ipf* > is obtained as(8)

$$\langle n|m\rangle = \frac{exp(-\alpha^2 a_s^2/4)}{\sqrt{2^{m+n}m!n!}}\left(\sum_{r=max(0,m-n)}^{m}(-1)^{n-m+r}\right.$$
$$\left. x2^{m-r}m_{C_r}\frac{n!}{(n-m+r)!}(\alpha a_s)^{n-m+2r}\right) \qquad (7)$$

Here 'n' and 'm' represent harmonic oscillator states corresponding to initial state (left part of the channel before the fault) and final state(after fault) respectively and a_s is stacking shift. Dislocation is an example of distortion in the channel, the amount of the distortion decreasing with increasing distance from the dislocation core. The distortion effects on channeling are incorporated by introducing a transverse potential energy term, to be added to continuum potential(4). Channeling/dechanneling phenomena under this situation is governed by the overlap integrals of the appropriate wave functions in various regions. Here we consider 12.25 Mev positrons channeled along the distorted channel. The motion of the positrons described in the rest frame of the particle where the particle "sees" a modified continuum potential *ãV*$_e$*ff(x)* (i.e., due to channel distortion in the transverse direction *(x))* and this curvature will not affect the motion of the particle along the propagation *(z)*. The expression for *V*$_e$*ff* is obtained as(9)

$$\gamma V_{eff} = \gamma V(x) - \gamma^2 m v_Z^2\left\{\frac{b}{\pi}.\frac{r_0(\gamma Z)}{(r_0^2+\gamma^2 Z^2)^2}\right\}x \qquad (8)$$

Here *V(x)* is planar potential in undistorted channel. As before we apply the harmonic approximation to above effective planar potential and this analysis is appropriate for the channels that are situated far away from the dislocation (concentrations typically 10_6 to 10_8 per cm_2).

During the passage through the distorted channel, the particle has to cross three boundaries (before distortion which is straight-+ ve curvature— -ve curvature— un-distorted) to find itself again in straight channel. The wavefunction of the particle in different regions may be denoted as *<fi(ax), <p(c/x + a'a$_r$), (p(a'x — a'a$_r$), <pf(ax)* respectively, where *<p(x)* represents the eigen function of the harmonic oscillator and *á, a'* are the coupling terms in straight and distorted portion respectively. The channeling probability of the particle with initial state |*i* > to cross interface (I) and to *Jrnax* be in state |*j* > in distorted part, is defined as *Pi^j* = | < *ip~ \ipi* > | $_2$; *pIi* = J 3 | < *j \i* > | *2j=0* where subscript T on the state denotes the relevant wave function corresponds to distorted channel after I interface. The equivalent expressions in other regions as described above, are obtained with similar procedure. The general expression for the total channeling probability of the particle with a specific initial state |*i* > so that the particle feels itself again in the straight channel with final state |*f* > (after passing through the various portions of distortion) is given by

$$p_{i\longrightarrow f} = \sum_{k^{(2)}=0}^{k^{(2)}_{max}}\left(p_{k^{(2)}\longrightarrow f}\left[\sum_{j^{(1)}=0}^{j^{(1)}_{max}} p_{i\longrightarrow j^{(1)}} \times p_{j^{(1)}\longrightarrow k^{(2)}}\right]\right)$$
$$= p_{f\longrightarrow i} \qquad (9)$$

The summation over all final states, to find itself again in the straight channel leads to the total dechanneling probability. The variation of the perturbed hamiltonian in the above approach is assumed to be sudden and the the description is given with the assumption that the curvature is nearly constant. The non-uniformity effects in curvature mentioned above are taken in terms of a time-dependent force term which cause transition from bound state to scattering state .The dechanneling phenomena under this situation is governed by the transition of the particle from a bound state (harmonic oscillator) to a scattering state (plane wave). The time dependent centrifugal energy term in
relativistic case is obtained by replacing *Z* by $v_z t$ in eqn. (9). Unlike previous case, here we consider bound - scattering (continuum) transitions and corresponding transitions

manifest the dechanneling process. The expression for total dechanneling probability of a particle with initial bound state |*i* > (due to channel distortion) to continuum is obtained by integration over T *r* ,> *i* T *i* T _ / N_ *i* — (*mub* \ 2 (*2ur* density of final states, and it is obtained as ÷*n* = *(2n+1)* ÷*0*; *with* ÷ 0 =— *exp \2V2haJ* Here *UJ = (Eb— Ei)/h, Eb* is energy background in which the particle propagates after getting dechanneled and ÷0 is obtained with specific reference to initially well channeled particles. The dechanneling probability is maximum for those channels which are situated below the dechanneling radius (i.e. critical distance of the channel from the dislocation below which the particle completely gets dechanneled). This happens for *Co = ãvz/r0*. Thus one can make a qualitative estimate for dechanneling radius and hence for the dechanneling width for initially well channeled particles is obtained as Classically, the transverse energy *E*± : 0.13b *JjE/E±;* A = *f* ÷*0(r)dr* = *2r0* respectively. *Eøp2*, where *øp* is planar critical angle. By replacing *E*± by equivalent classical expression, one gets ë = *(0A4:)\QuereZ2 Vb* where *b* is in A. The dechanneling widths *ën* are estimated for positrons along Al(111) for various initial states *(*|*i* >). The dechanneling width for *He* ions has also been estimated and compared with existing theory and experimental data(10). These details are given below, showing reasonable agreement.

Particulars of the crystal	Dechanneling widths$^{(a)}$ in μm			
	$\bar{\lambda}_o$	$\bar{\lambda}_1$	$\bar{\lambda}_2$	$\bar{\lambda}_3$
$Al(111), b = 2.86\AA$	47.12	141.38	235.6	329.8

Particulars of the crystal	Dechanneling widths$^{(b)}$		
	Exptl[10]	Quere	Present
$Al(111), b = 2.86\AA$	$85\sqrt{E}$	$79\sqrt{E}$	$90\sqrt{E}$

(a): corresponds to positrons of 12.25 Mev

(b): corresponds to *He* of given energy *E*

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