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Motion of charged particles in curved planar channels: Effects of dislocations

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A simple model to discuss the motion of charged particles in curved channels, such as those around a dislocation, is presented. The curvature in the channel produced by a dislocation is approximated by an arc of constant radius R, which is determined by using the displacement equations for the case of screw dislocation. The equations of motion for the planar channeling case have been written by approximating the effects of curvature on the particle motion by an average constant centrifugal force $2E/R$, E being the average energy in the curved part of the channel. These equations are solved in the limit of small curvatures (i.e., for channels not very near to the dislocation) and an analytical expression for the change in energy loss of an initially well-channeled particle is obtained.

I. INTRODUCTION

More than a decade ago, the computer simulations[1] of charged-particle trajectories in single crystals and the range-measurement experiments[2] with heavy ions in aluminum and copper single crystals revealed for the first time[3] that the charged particles entering a crystal parallel or nearly parallel to an atomic row or plane succeed in getting their trajectories maintained along the same family of rows or planes, and thereby succeed in penetrating to much larger depths than are observed in amorphous solids or along random directions in single crystals. This directional effect, now commonly known as "channeling," and its opposite, the "blocking effect" in which the particles originating at a lattice site are blocked from traveling closely along atomic rows or planes, have since been extensively studied, both theoretically and experimentally, and have been the subject of various review articles[4] and international conferences.[5] It has been realized from the very beginning that a detailed knowledge of various aspects of these directional effects would be of great help to those concerned with technologically important subjects, such as ion implantation.[6] It has been from such technologically applied points of view, in addition to the fundamental research viewpoints, that the study of defects and lattice disorder, utilizing channeling and blocking techniques, has been motivated. Accordingly, a fair amount of work has been done in this direction, particularly with regards to the lattice location of (dopant) foreign atoms by channeling and blocking techniques on one hand (for a list of references on this subject see for example the article by Gemmell[4]) and the dechanneling effects produced by these points and extended defects[7] on the other.

As for the theoretical description of these directional effects, Lindhard's theory[8] based on the simple idea of classical steering of the ion by the continuum axial or planar potential of the channel has been found to explain with reasonably good accuracy all the existing data on heavy-ion channeling. Using this model, the effects of point defects (like substitutional or interstitial foreign atoms) have been interpreted simply by taking into account the extent of the "obstruction" effects that the passing channeled ion sees, due to the presence of these impurities. For example, if the channeled ion hits the impurity directly (i.e., if the impurity is sitting in the middle of the channel), it will get dechanneled, and if, on the other hand, the impurity is sitting on a substitutional site in the atomic row or plane, it will not have any significant effect on the motion of the channeled ion. Stacking fault[9] is an example of the obstruction being produced by a whole atomic row or plane (as against that due to a single impurity), because here whole families of atomic rows or planes in one part of the crystal are displaced with respect to corresponding atomic rows or planes in the other adjoining part of the crystal.

By contrast to these simple obstruction effects, the extended defects like dislocations produce distortion in the channels themselves. Consequently, the ion moving in an axial or planar channel is subject to additional forces due to these distortions. Depending upon the magnitude of the distortion produced, the amplitude of the oscillating particle can be changed, or may get dechanneled altogether. Quéré[10] has calculated the distance from a dislocation axis up to which an initially channeled particle will get dechanneled, and his results agree reasonably well with the computer simulations of the particle trajectories in crystals with dislocations performed by Morgan and Van Vliet.[11]

In this paper we consider the problem of motion of charged particles through a curved channel around a dislocation. Since we are only in the initial stages of developing a theory on the effects of dislocations on the motion of charged particles through crystals in general, and on the energy loss of those charged particles moving along major crystallographic directions and planes (namely the channeled particles) in particular, we confine ourselves to the simplest case of screw dislocations, and consider the case of planar channeling. However, the model proposed here is more generally applicable to the cases of edge dislocations, as well as to axial channeling. Investigations dealing with these and more general cases, where some wise simplifications and approximations (with reasonable accuracy) to the complex mathematics might be needed to get some analytical results are in progress with the ultimate aim of presenting a unified theory of these effects. The general concepts used to deal with the problem are the same as those used in the Lindhard theory[8] of channeling, namely, the treatment of the problem in the continuum approximation and the use of the corresponding continuum planar potentials. The simple model used for dislocation-affected channels in the crystal, and the relevant formalism have been discussed in Sec. II. This formalism has been used in Sec. III to discuss the changes in the energy loss of well-channeled particles due to dislocations. Finally, some concluding remarks with regard to the theory presented, and possible experiments to test it and to guide future theoretical work have been given in Sec. IV.

II. THE MODEL AND THE FORMALISM

A. Channel

We know from the theory of dislocations[12] that the crystal structure is greatly distorted around a dislocation. Although in practice this distortion decreases quickly as one moves away from the dislocation axis, in principle, the effect is an asymptotic one, and the representative equations for atomic displacements predict nonzero displacement for any atom at a finite (however large) distance from the dislocation. Moreover, the curvature produced by these atomic displacements in the channels around a dislocation is, in principle, nonuniform. The movement of a charged particle in these channels is, therefore, rather complicated. One obvious way would be, of course, to simulate the trajectories on the machine. But in addition to being costly (because one has to deal with an enormously large number of atoms in the crystal that are effected by the dislocations), these machine calculations give less insight into the physics of the processes going on than one can get by even the approximate models. In an attempt to construct such an approximate model for this complicated situation, we first assume that the channel has a constant average radius, and that the length of this curved part is finite. Thus, as shown in Fig. 1, we replace an actual channel wall by an approximate channel wall QOQ' such that the parts QO and OQ' have constant radius of curvature R (with curvatures in opposite directions) which can be determined from the simple geometry using the appropriate displacement equations for atomic displacements around a dislocation axis.

For a screw dislocation, the displacement equations are fairly simple, provided one makes use of the isotropic-elastic-continuum theory. Of course it is well known that this isotropic-elastic-continuum approximation in dislocation theory breaks down near the core of the dislocation, but as we shall see later on, we are not concerned with this region around the core of the dislocation. Because the channels are completely blocked in the core region and there is no question of any channeling taking place, and as one slowly moves away from the core region, the isotropic-elastic-continuum theory starts becoming valid, and in fact has been used[7,10] to derive an average distance from the dislocation axis (the so-called radius of the "dechanneling cylinder") within which most of the particles will get dechanneled, and these theoretical results have been found to compare well with experimental results for the planar case.[9] The region of the crystal of interest in this article

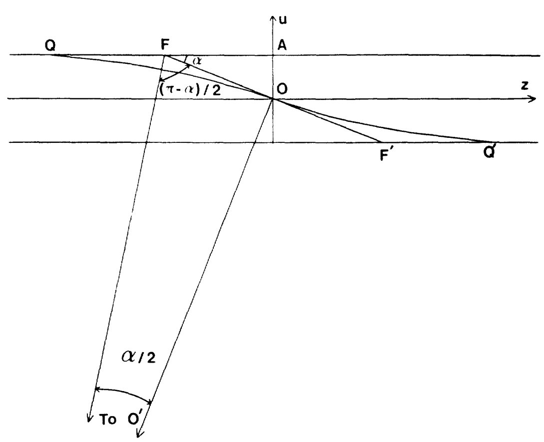

FIG. 1. Geometry used to determine the constant radius of curvature of the model channel. The actual curved plane is the one normal to the plane of the paper, and containing QOQ'. The angle α is the angle between the tangent FOF', on the curved parts QO and OQ', at the point O, and the z axis.

is outside this dechanneling cylinder, so that the isotropic-elastic-continuum theory can be safely used, and in fact its use is consistent with the approximations made later on, regarding the curvature of the channels. Thus we write the displacement equations for a screw dislocation as[12]

$$u_1 = u_2 = 0$$

and

$$u_3(\equiv u) = \frac{b}{2\pi} \cos\varphi \tan^{-1}\left(\frac{z\cos\varphi}{r_0}\right), \tag{1}$$

where r_0 is the distance measured from the dislocation axis, b is the Burger's vector, and φ is the angle between the channel and a plane perpendicular to the dislocation axis. For the planar case, the particular direction in the plane with respect to which this angle φ is measured is usually taken to be the direction of motion of the particle. Correspondingly, one has to express φ as a function of two angles,[7] θ and γ as shown in Fig. 2. Here D represents the dislocation axis and δ is the direction of motion of the particle in the plane $\bar{\omega}$ under consideration. The direction δ makes an angle θ with the projection of the dislocation axis on the plane, and $\frac{1}{2}\pi - \gamma$ is the angle between this projection and the dislocation axis itself. From simple geometry it can be shown that[7]

$$\cos\varphi = (1 - \sin^2\gamma\cos^2\theta)^{1/2} . \tag{2}$$

In order to use the displacement Eq. (1) for the planar case of Fig. 2, the Burger's vector b (along the dislocation axis D itself for the screw dislocation case) should be replaced by its component normal to the plane $\bar{\omega}$ so that

$$u = \frac{p}{2\pi} \cos\varphi \tan^{-1}\left(\frac{z\cos\varphi}{r_0}\right), \tag{3}$$

with

$$p = b\cos\gamma .$$

The radius of curvature R of the model channel of Fig. 1 can now be easily obtained. We note that $R = OO'$, O' being the point where the normal to the tangent (FOF') to the arcs QO and OQ' at point O intersects the bisector of the angle QFO. Thus,

$$R = \frac{FO}{\tan\frac{1}{2}\alpha} = \frac{FO\sin\alpha}{1-\cos\alpha} = \frac{AO}{1-\cos\alpha} . \tag{4}$$

Using Eq. (3),

$$AO = u(\text{at } z=\infty) = \tfrac{1}{4}p\cos\varphi ,$$

and

$$\tan\alpha = \frac{du}{dz}(\text{at } z=0) = \frac{p\cos^2\varphi}{2\pi r_0} ,$$

so that Eq. (4) gives

$$R = \frac{p}{4}\cos\varphi \frac{(1+p^2\cos^4\varphi/4\pi^2 r_0^2)^{1/2}}{(1+p^2\cos^4\varphi/4\pi^2 r_0^2)^{1/2} - 1} . \tag{5}$$

If we neglect $p^2\cos^4\varphi/4\pi^2 r_0^2$ compared to unity in the binomial expansion of numerator and its second and higher powers in the binomial expansion in denominator, we get a simple expression for R as

$$R = 2\pi^2 r_0^2/p\cos^3\varphi , \tag{6a}$$

and in the same approximation, the arc length QO is found to be identical to

$$z = \pi r_0/\cos\varphi . \tag{6b}$$

The approximation used above can be seen to introduce a negligibly small error. For example, if we calculate the maximum value of $p^2\cos^4\varphi/4\pi^2 r_0^2$ (i.e., corresponding to $\cos\varphi = 1$ and for the minimum possible value of r_0, i.e., for $r_0 = p$), we get $1/4\pi^2$ which is about 0.0253. Therefore, the approximation introduces a maximum possible error of 2.53% in the extreme case. Since we

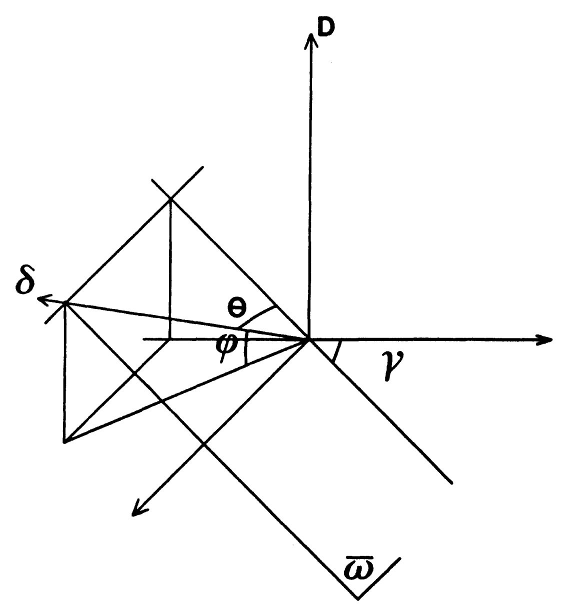

FIG. 2. Geometry showing different angles for a planar channel $\bar{\omega}$ near a screw dislocation of Burger's vector b lying along the dislocation axis D. Here δ is the actual direction of motion of the particle in the plane $\bar{\omega}$. In order to illustrate other angles clearly in this figure, it has not been possible to show the curvature of the plane, but actually this plane is curved and a projection of the curvature along the direction δ is that shown in Fig. 1.

shall be concerned only with the channels outside the dechanneling cylinder,[10] r_0 will usually be several times p. Moreover, because $\cos\varphi$ enters with a fourth power, the expressions (6) for R and z tend to be fairly accurate.

B. Equation of motion and the planar potential

Thus, having replaced the actual channel affected by dislocation by a model channel of constant radius R, the next step is to consider the effects that this curvature will have on the motion of an initially channeled particle. In order to keep the treatment simple and to get analytical results, we shall deal only with those particles which enter this curved channel with zero transverse energy, i.e., the well-channeled particles. The model used to discuss these effects is shown in Fig. 3, where both parts of the curved channel shown in Fig. 3(a) (i.e., to the left and to the right of the line AB, hereafter called the first and second part, respectively), are replaced by straight channels and the effect of curvature is included by applying a force $2E/R$ (the centrifugal force) to the channeled ion of energy E, normal to the channel axis, and in the opposite directions in the two parts as shown in Fig. 3(b). The coordinates used in the analysis are also shown in this figure, the distance x is measured from the halfway point between two planes (i.e., channel axis), $2l$ is the distance between two planes surrounding the channel, and x_m is the amplitude of oscillation of the particle.

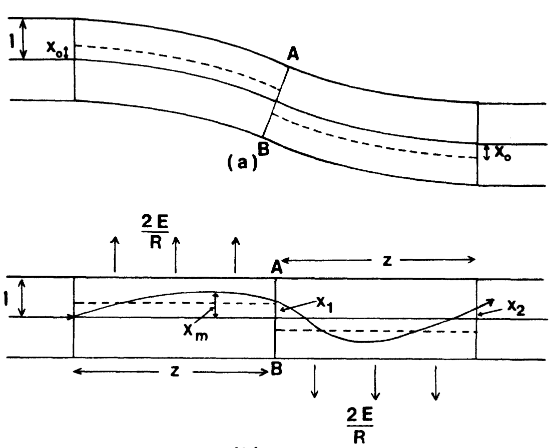

FIG. 3. (a) Typical channel at some finite distance from a dislocation. (b) Straight model channel replacing the channel of part (a) and showing the coordinates used in the text. Here, l is the half-width of the channel, x_m is the amplitude in the first part of the channel, x_0 is the equilibrium position 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.

The equations of motion for transverse and longitudinal motion in the first part are

$$m\ddot{x}+\frac{dV}{dx}-\frac{2E}{R}=0 \tag{7}$$

and

$$m\ddot{z}+S(x,E)=0\ , \tag{8}$$

respectively, where V is the planar potential (due to both planes) and $S(x,E)$ is the stopping power function.[13] Following Robinson,[13] we have neglected the inelastic term in Eq. (7) for the transverse motion, because the direction of motion of the channeled ion always remains within ~0.5° of the channel plane, and correspondingly the longitudinal component of $S(x,E)$ is replaced by $S(x,E)$ itself in Eq. (8). Here it should be remembered that in principle the centrifugal force term in Eq. (7) is not constant throughout the length of the channel because as the particle moves, its total energy decreases, as does the centrifugal force. But if the length of the curved part is less than one wavelength of the particle oscillation (which is the case for energetic particles and a typical channel not too far away from the dechanneling cylinder), one can assume this force to be constant and, if needed, replace E by an average energy, as discussed in Sec. III. Now writing Eq. (7) as

$$\frac{d}{dx}\left(\tfrac{1}{2}m\dot{x}^2+V(x)-\frac{2E}{R}x\right)=0\ ,$$

so that

$$\tfrac{1}{2}m\dot{x}^2+V(x)-(2E/R)x=\text{const}=V(x_m)-(2E/R)x_m\ ,$$

and we get:

$$\dot{x}=(2/m)^{1/2}[V(x_m)-V(x)+(2E/R)(x-x_m)]^{1/2}\ . \tag{9}$$

For an initially well-channeled particle, the initial conditions are $x(t=0)=0$, $\dot{x}(t=0)=0$, so that Eq. (9) gives

$$V(x_m)-(2E/R)x_m=V(0) \tag{10}$$

and

$$\dot{x}=(2/m)^{1/2}[V(0)-V(x)+(2E/R)x]^{1/2}\ . \tag{11}$$

Equation (10) can be used to find the amplitude with which the initially well-channeled particle starts oscillating in the curved channels. The equilibrium position x_0 about which the particle will oscillate is determined from the condition

$$\frac{2E}{R}-\frac{dV}{dx}\bigg|_{x=x_0}=0\ . \tag{12}$$

The corresponding equations for the second part are easily obtained by changing the sign of $2E/R$, and the initial conditions for the second part are obtained by solving the above equations for the first parts of position and transverse velocity of the particle after it has traversed the first part.

To solve the above equations of motion, we need a suitable planar potential. We shall apply a simple mathematical approximation[14,15] to the Lindhard's planar potential,

$$V(x)=2V_0a\left(\frac{1}{l+a-x}+\frac{1}{l+a+x}\right)=\frac{4V_0La}{L^2-x^2}\ , \tag{13}$$

with

$$V_0=\pi Z_1Z_2e^2N_pCa\ ,$$

and

$$L=l+a\ ,$$

where Z_1 and Z_2 are the atomic numbers of the incident ion and target atom, respectively, e is the electronic charge, N_p ($=2lN$) is the atomic density in the plane under consideration (N being the atomic concentration per unit volume in the crystal), a is the Thomas-Fermi screening radius given by

$$a=0.8853a_0(Z_1^{2/3}+Z_2^{2/3})^{-1/2}\ ,$$

with a_0 the Bohr radius and C is the constant appearing in the Lindhards standard interatomic potential[8] ($C=\sqrt{3}$). This potential (13) originally used by Mory[14] and Quéré[15] has been shown to differ from Lindhard's planar potential by not more than 2%. More recently,[16] it has been shown that this potential gives a stopping function $S(x,E)$ whose magnitude as well as variation with x is very close to that obtained with Molière and Lindhard's potentials. The interatomic potential to which this planar potential (13) corresponds has been shown to be[16]

$$V_{\text{int}}(r)=\frac{Z_1Z_2e^2}{r}\frac{Ca^2}{(r+a)^2}\ , \tag{14}$$

whose variation with r agrees quite well with Molière and Lindhard's standard potential down to the interatomic distance $r=a$, and in fact can be made to agree even for $r<a$ by taking the constant C smaller than $\sqrt{3}$ for $r<a$ (and $C=1$ for $r=0$) as suggested previously.[8,16] However, since in most of the problems related to channeling, one is not concerned with these smallest interatomic distances and can keep $C=\sqrt{3}$, and use the simple forms (13) and (14). It is worth pointing out that the dependence of this potential (14) on the interatomic distance is very close to what one would derive[17] from the planar channeling experiments (since $r^{-7/2}$ dependence suggested by Robinson[17] is subject to 10% uncertainties). Thus we see that although originally purely a mathematical approximation to the Lindhard's planar potential, the planar potential (13) corresponds to a physically reasonable interatomic potential, and gives most of the physical quantities in reasonable agreement with those obtained from other standard potentials.

Now using (13) in Eqs. (10) and (11), we get

$$x_m-\frac{2BL}{L^2-x_m^2}+\frac{2B}{L}=0 \tag{15}$$

and

$$\dot{x}=\left(\frac{4E}{mR}\right)^{1/2}\left(x-\frac{2BL}{L^2-x^2}+\frac{2B}{L}\right)^{1/2}\ , \tag{16}$$

and Eq. (12) yields a fourth-degree equation for the equilibrium position x_0:

$$x_0^4-2x_0^2L^2-4xBL+L^4=0\ . \tag{17}$$

In Eqs. (15)–(17), the abbreviation $B=RV_0\,a/E$ has been introduced, and will hereafter be used.

C. Approximate solutions

Equations (15)–(17), along with Eq. (8), describe the motion of the particle completely, but in their present form they give little information unless solved numerically. In order to get some analytical results giving some insight into the problem, we make another approximation, namely, neglect fourth and higher powers of x/L. This amounts to being restricted to small amplitudes of oscillation, which in turn means that we are dealing with those channels which do not have large curvatures, i.e., which are not very close to the dislocation axis. To get some feeling about the accuracy of this approximation, we note for example, that for amplitude $x_m=\frac{1}{2}L$, the approximation introduces a maximum percentage error of about 6%. In this approximation the Eqs. (15)–(17) can be shown to give

$$x_m=L^3/2B\ , \tag{18}$$

$$\dot{x}=\left(\frac{4E}{mR}\right)^{1/2}\left(x-\frac{2B}{L^3}x^2\right)^{1/2}\ , \tag{19}$$

and

$$x_0=(B^2/L^2+\tfrac{1}{2}L^2)^{1/2}-B/L\ . \tag{20}$$

Thus, having known x_0 and x_m, we can now calculate different quantities of interest. From Eq. (19), we get the period of oscillation as

$$T=4\left(\frac{mR}{4E}\right)^{1/2}\int_{x_0}^{x_m}\frac{dx}{[x-(2B/L^3)x^2]^{1/2}}$$
$$=\left(\frac{2mRL^3}{BE}\right)^{1/2}\left(\frac{\pi}{2}-\sin^{-1}\frac{x_0-L^3/4B}{L^3/4B}\right), \quad (21)$$

and using Eq. (20), one can show that

$$T=\left(\frac{2mRL^3}{BE}\right)^{1/2}\sin^{-1}\left\{\frac{4B}{L^3}\left[\frac{L^4+4B^2}{2BL}\left(\frac{L^4+2B^2}{2L^2}\right)^{1/2} - \left(\frac{L^4+2B^2}{L^2}\right)\right]^{1/2}\right\}. \quad (22)$$

If the time taken by the particle to cross the first part of the channel is t_1, we can find the corresponding position x_1 of the particle by integrating Eq. (19):

$$\int_0^{t_1}dt=\left(\frac{mR}{4E}\right)^{1/2}\int_0^{x_1}\frac{dx}{[x-(2B/L^3)x^2]^{1/2}},$$

or

$$t_1=\frac{1}{2}\left(\frac{mRL^3}{2BE}\right)^{1/2}\left(\sin^{-1}\frac{x_1-L^3/4B}{L^3/4B}+\sin^{-1}1\right),$$

which gives

$$x_1=\frac{L^3E}{2RV_0a}\cos^2\left[\frac{t_1}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right]. \quad (23)$$

The corresponding transverse velocity at point x_1 is easily obtained either by differentiating Eq. (23) or by substituting this value of x_1 into Eq. (19) to get

$$v(x_1)=-\frac{L^{3/2}E}{R(2V_0am)^{1/2}}\sin\left[\frac{2t_1}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right]. \quad (24)$$

For the second part of the curved channel, the initial conditions are $x=x_1$ and $\dot{x}=v(x_1)$. Using these initial conditions in the equation of motion,

$$m\ddot{x}+\frac{dV}{dx}+\frac{2E}{R}=0, \quad (25)$$

we get

$$\dot{x}^2-v^2(x_1)=(2/m)[V(x_1)-V(x) + (2E/R)(x_1-x)], \quad (26)$$

and the equation giving the amplitude x_m' as:

$$v^2(x_1)=(2/m)[V(x_m')-V(x_1) + (2E/R)(x_m'-x_1)]. \quad (27)$$

The term $2E/R$ in Eq. (25) has a sign opposite to that in Eq. (7) because as shown in Fig. 3, the centrifugal forces act in opposite directions in the two parts of the channel. The magnitude of this force, as stated previously, will be an average foce over the whole curved part so that E again represents an average energy corresponding to the particular channel in question. We need not write the corresponding equation for the position x_0' of the equilibrium axis in the second part, because from symmetry it is clear that $x_0'=-x_0$.

We solve these equations using again the planar potential (13) in similar approximation as used previously. Equation (27) gives

$$x_m'=-\frac{L^3}{4B}\pm\frac{L^3}{4B}\left\{1+8\cos^2\left[\frac{t_1}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right]\right\}^{1/2}, \quad (28)$$

and Eq. (26) gives after integration:

$$t-t_1=\left(\frac{mRL^3}{8BE}\right)^{1/2}\left(\sin^{-1}\frac{x+L^3/4B}{(x_1L^3/B+L^6/16B^2)^{1/2}} - \sin^{-1}\frac{x_1+L^3/4B}{(x_1L^3/B+L^6/16B^2)^{1/2}}\right),$$

which gives, after some algebra,

$$x=-\frac{L^3}{4B}+x_1^{1/2}\left(\frac{L^3}{2B}-x_1\right)^{1/2}\sin\left[\frac{2t'}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right] \pm\left(x_1+\frac{L^3}{4B}\right)\cos\left[\frac{2t'}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right], \quad (29)$$

where t' $(=t-t_1)$ is the time measured within the second part. Expression (29), along with Eq. (23) for x_1, gives the position of the particle at any time. The complete equation for the particle trajectory is obtained by integrating Eq. (8) for the longitudinal motion, and combining these solutions with Eqs. (23) and (29), similar to the case of perfect crystals.[13] In order to be consistent with our previous procedure of using a constant average centrifugal force, we take the time needed to cross the second part of the channel t_2 as equal to t_1 and again, as discussed in Sec. III, we shall use an average value. Thus using Eq. (29) with $x=x_2$ for $t'=t_2$ $(=t_1)$ we get, after some algebra,

$$x_2=\frac{L^3E}{2RV_0a}\cos\left[\frac{2t_1}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right], \quad (30)$$

and the corresponding velocity as:

$$v(x_2)=-\frac{2L^{3/2}E}{R(2V_0am)^{1/2}}\sin\left[\frac{2t_1}{L}\left(\frac{2V_0a}{mL}\right)^{1/2}\right], \quad (31)$$

which is twice the value of $v(x_1)$, in this approximation.

III. ELECTRONIC ENERGY LOSS

After the particle has crossed the curved parts of the channel, it again finds itself in a perfect straight channel and oscillates with an amplitude given by the equation

$$V(x_{\text{amp}}) = \tfrac{1}{2} m v^2(x_2) + V(x_2) , \tag{32}$$

which gives, within the approximations used previously,

$$x^2_{\text{amp}} = [\tfrac{1}{2} m v^2(x_2) L^3 + 4V_0 a x_2^2]/4V_0 a , \tag{33}$$

and using Eqs. (30) and (31) we get a simple expression,

$$x_{\text{amp}} = L^3 E/2RV_0 a . \tag{34a}$$

Expression (34a) tells us that an initially well-channeled particle, after passing through two curved channels of equal length with radii of curvature R in opposite directions, will start oscillating with an amplitude which is directly proportional to the particle energy and the cruvature $(1/R)$ of the channels.

Before proceeding further, we must discuss the choice of the energy E and time t_1 used in Sec. II. If the initial energy of the particle is E_0 and the length $2z$ of the curved channel is not large compared to the oscillation wavelength of the particle, we can use the initial stopping power $\overline{S}(E_0)$ $[=(dE/dz)|_{E=E_0}]$ to find $E_f = E_0 - 2z\overline{S}(E_0)$, and choose the E appearing in the centrifugal-force term as $E=\frac{1}{2}(E_0+E_f) = E_0 - z\overline{S}(E_0)$. Correspondingly, we can determine the approximate time t_1 (where $2t_1$ is time taken to cross both parts of curved channel) as

$$t_1 = z(m/2E)^{1/2} = zm^{1/2}/[2E_0 - 2z\overline{S}(E_0)]^{1/2} .$$

The $\overline{S}(E_0)$ in these expressions for E and t_1 is to be taken as an average over the period of oscillation in the channel. To get some feeling about the range of validity and accuracy of this procedure, we note that for MeV α particles the oscillation wavelength in planar channeling is typically of the order of 10^3 Å,[9,17] whereas the corresponding radius of the dechanneling cylinder is less than 10^2 Å [e.g., for 5-MeV α particles in (111) planes of Al, the diameter of this dechanneling cylinder is 175 Å theoretically, and 140 ± 40 Å experimentally[9]]. Therefore, if one is about a distance of the order of 10^2 Å away from the dislocation axis (i.e., outside the dechanneling cylinder), $2z$ would be, on the average, less than or of the order of 10^3 Å, i.e., of the order of an oscillation wavelength. Thus, the present procedure to estimate E and t_1 will be a reasonable approximation for those planes which are within a distance of few tens of angstroms outside the dechanneling cylinder. However, for the planes much farther from the dislocation axis (and typically, say, several hundreds of angstroms away from the dechanneling cylinder), so that the length of the curved part of the channel becomes large compared to one oscillation wavelength, one can make corresponding corrections by using $\overline{S}(E)$ instead of the initial stopping power $\overline{S}(E_0)$, and using a self-consistent procedure to determine E and t_1, to be used in the expressions of the Sec. II.

Now using equation (6a) in equation (34a) we get

$$x_{\text{amp}} = \frac{L^3 E}{2V_0 a} \frac{p\cos^3\varphi}{2\pi^2 r_0^2} . \tag{34b}$$

In a recent preliminary report[18] we found an average value of $\bar{x}_{\text{amp}}$ simply by substituting $\cos^3\varphi$ by its average value $4/3\pi$ which would thus correspond to a special case in which the direction δ of the particle's motion is along the projection of the dislocation axis on the plane. For a general case, from Eqs. (34), (2), and (3), we get

$$\bar{x}_{\text{amp}} = L^3 E b q/4V_0 a \pi^2 r_0^2 , \tag{35}$$

where the constant q is given by

$$q = \frac{4}{\pi^2}\int_0^{\pi/2} \cos\gamma\, d\gamma \int_0^{\pi/2} (1-\sin^2\gamma\cos^2\theta)^{3/2} d\theta$$
$$\cong 0.49 , \tag{36}$$

which is not very different from the approximate value $4/3\pi$ taken previously.[18] Once the amplitude of oscillation of the particle motion is known, the energy loss can be easily found. If one prefers to use some experimental information from the planar channeling experiments with thin crystals, the procedure of Robinson[13,17] can be used to write

$$S(x,E) = s_0 + s_1[\sigma(x) - 1] , \tag{37}$$

where s_0 and s_1 are the energy-dependent quantities and are to be determined from the experiment, and the position dependent function is given[16,17] as

$$\sigma(x) = \frac{d}{dx}\left(\frac{2}{V''(0)}[V(x)-V(0)]^{1/2}\right)$$
$$= L^3/(L^2 - x^2)^{3/2} . \tag{38}$$

In this procedure, one has to calculate an average value of $\sigma(x)$ over the period of oscillation, i.e.,

$$\langle\sigma(x)\rangle = \left(\int_0^{x_{\text{amp}}} \sigma(x)\frac{dx}{\dot{x}}\right) \Big/ \int_0^{x_{\text{amp}}} \frac{dx}{\dot{x}} , \tag{39}$$

where, for a straight dislocation free channel,

$$\dot{x} = (2/m)^{1/2}[V(x_{\text{amp}}) - V(x)]^{1/2} ,$$

so that the period of oscillation for potential (13) is given by:

$$T = 4\int_0^{x_{\rm amp}} \frac{dx}{\dot{x}}$$

$$= 4\left(\frac{m}{2}\right)^{1/2} \int_0^{x_{\rm amp}} \frac{dx}{[V(x_{\rm amp}) - V(x)]^{1/2}}$$

$$= \left[\frac{2mL(L^2 - x^2_{\rm amp})}{V_0 a}\right]^{1/2} F\left(\frac{x_{\rm amp}}{L}\right), \qquad (40)$$

where F is the complete elliptic integral of second kind. Using Eqs. (38) and (40) in (39), and calculating the numerator, we get the following simple expression

$$\langle\sigma(x)\rangle = \frac{\pi L}{2(L^2 - x^2_{\rm amp})^{1/2}} \frac{1}{F(x_{\rm amp}/L)} \ . \qquad (41)$$

Thus, the change in the energy loss of well channeled particles due to their passage through a single channel affected by dislocation is easily found through the expression:

$$\Delta S = S(x,E) - s_0 = s_1(\langle\sigma(x)\rangle - 1) \ .$$

An alternative procedure, purely theoretical and not utilizing any experimental informations like the s_0 and s_1 needed in the above procedure, would be to utilize the relevant theoretical expressions for the energy loss. Such expressions have recently been shown to give the position dependence of the stopping power in the channel, which agrees with that obtained by the above procedure of Robinson, as long as one is not too close to the channel wall (i.e., as long as the oscillation amplitude is not so large as to be close to the channel width), in both the low-velocity[19] and high-velocity[20] cases. In these expressions, the position dependence comes from the *effective* channel-electron density responsible for stopping and this, for the planar case, was obtained by making a planar average of the spherically averaged electron density due to the individual contributing target shells. Thus one gets

$$n(x) = \rho(l - x) + \rho(l + x) \ , \qquad (42)$$

with

$$\rho(y) = Nl \sum_j \frac{(2\xi_j)^{2n_j}}{2n_j} \omega_j e^{-2\xi_j y} \times \sum_{k=0}^{2n_j-1} \frac{y^{2n_j-1-k}}{(2\xi_j)^k (2n_j - 1 - k)!} \ , \qquad (43)$$

where n_j, ω_j, and ξ_j are the principal quantum number, the occupation number, and the radial orbital exponent for the jth shell, respectively, and $y = l - x$ is the distance from the plane.

Here, the energy loss of well-channeled particles is obtained by using $n(0) = 2\rho(l)$ in the relevant expressions,[19,20] and the quantitative values thus found are in good agreement with experiments. The energy loss of a particle oscillating with an amplitude $x_{\rm amp}$ is obtained by using the effective average-electron density sampled by the particle during its motion, i.e.,

$$\bar{n} = \frac{1}{2x_{\rm amp}} \int_{-x_{\rm amp}}^{x_{\rm amp}} [\rho(l - x) + \rho(l + x)]\, dx \ ,$$

which gives

$$\bar{n} = \frac{Nl}{x_{\rm amp}} \sum_j \sum_{k=0}^{2n_j-1} \sum_{m=0}^{2n_j-1-k} \frac{\omega_j}{2n_j} [(l - x_{\rm amp})^{2n_j-1-k-m} e^{-2\xi_j(l - x_{\rm amp})} - (l + x_{\rm amp})^{2n_j-1-k-m} e^{-2\xi_j(l + x_{\rm amp})}] \times [(2\xi_j)^{m+1+k-2n_j}(2n_j - 1 - k - m)!]^{-1} , \qquad (44)$$

where the summation over j runs over all significantly contributing target shells. This procedure of taking a planar average of the effective electron density has recently been used to predict[21] the changes in energy loss of well-channeled particles due to introduction of a low concentration (α-phase) of hydrogen in palladium.

IV. CONCLUSIONS

In this article, an attempt has been made to deal with the rather complicated problem of charged-particle motion in single crystals having a small concentration of dislocations. As is quite well known,[7,9-11] as far as channeling is concerned, there exists a so-called "dechanneling cylinder" around a dislocation axis such that the majority of the initially channeled particles passing through this region will get dechanneled. The region immediately outside this dechanneling cylinder affects the motion of most of the channeled particles to a lesser extent. The channeled particles entering this outer region generally will not get dechanneled, but because of the finite curvature of the channels, their state of motion is modified and their oscillation amplitude changes appreciably. In this preliminary theoretical study, we have tried to develop a simple model which can then be used to calculate the relevant physical quantities, such as energy loss. It was felt from the very beginning that a knowledge of the nature of the experimental information which can possibly be obtained through current channeling experiments would be a useful guide to direct theoretical work.

In the absence of any experimental information about channel stopping power in the presence of dislocations, we have concentrated on the simplest problem, namely to calculate the effect of channel distortion due to a screw dislocation on the energy-loss rate of the well-channeled particles. This has been done in the framework of a simple model for curved channels in which the curvature is assumed to be constant, and a constant average centrifugal force $2E/R$ is included to represent the effects of this curvature on the particle motion. It is also assumed that the overall length of the curved part is not more than a wavelength of the particle oscillation. Under these simplifying assumptions we calculate the amplitude with which an initially well-channeled particle will start oscillating after passing through such a channel, so that the change in energy-loss rate for such a particle can be calculated for individual curved channels. If an experiment along these lines can be performed to find the difference in the minimum energy-loss rates (i.e., corresponding to the edge of the energy-loss spectra), without and with a very low concentration of screw dislocations introduced as a very thin layer of known thickness in the target crystal, then this minimum energy loss should, on the average, correspond to those particles which have passed through the channels situated farthest from a dislocation axis. This farthest $r_0^{\max}$ is, on the average, given by $r_0^{\max}=(3/4\pi n)^{1/3}$, where n is the concentration of dislocations. Using this $r_0^{\max}$ and the known thickness of the dislocation-affected region, we can calculate the change in minimum energy-loss rate by using Eqs. (34)–(43), and compare the calculated and experimental values. It must be emphasized, however, that the accuracy of such an experiment must be high in order to detect the difference in the edge of the energy-loss spectra, because the number of well-channeled particles is small and out of these one has to look for those which pass through the channels of smallest curvatures.

From the theoretical point of view, it is quite obvious from the discussion given in Secs. II and III that much more detailed calculations are needed. For example, a more generalized theory for the motion of any particle (and not just the well-channeled ones) is needed so that suitable statistical averages corresponding to fluxes of particles for a given initial amplitude can be made to calculate a spectrum of the outgoing particles. Similarly, a detailed study of particle motion in long curved channels such that the change in centrifugal force due to energy loss in the curved channel itself is properly taken into account, would be useful.

In conclusion, it can be said that detailed experimental work in this field is needed to guide the theoretical work in a useful direction. It is also being felt that for preliminary order-of-magnitude estimates of the experimentally useful quantities, like energy-loss rates, even a simpler model, like solving the harmonic-oscillator problem could be a useful guide for detailed theoretical as well as experimental work.

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