this generalization. The ratio of ionic radii Yb^{3+}/Ca^{2+} is 0.95. The $R_{\parallel}$ coefficient for Yb^{3+} in $CaWO_4$ is much smaller than any of the other electric shift parameters observed in this series of experiments and is within a factor of 2 of the value calculated for the electronic effect.

[14]The crystal field terms V_K^Q are often expressed as $A_K^Q Y_K^Q(\theta, \varphi)$, where $Y_K^Q(\theta, \varphi)$ are the conventional normalized spherical harmonics. In recent years, many papers on this subject use the related harmonic

$$C_K^Q(\theta, \varphi) = [(2K+1)/4\pi]^{1/2} Y_K^Q(\theta, \varphi),$$

hence

$$V_K^Q = B_K^Q C_K^Q(\theta, \varphi) = [4\pi/(2K+1)]^{1/2} A_K^Q C_K^Q(\theta, \varphi).$$

We shall use the C_K^Q harmonic in this paper. When B_K^Q is a term induced by the applied electric field, we will use the lower-case symbol b_K^Q to conform to Ref. 1.

[15]It is still essential, however, that the undisplaced ion should be at a site which lacks inversion symmetry. If this is not so, the new even-field terms will be quadratic in the displacement u.

[16]In the case of a linear chain, if the force constant is k, the restoring force is proportional to $2k$. (In Ref. 1, we set $\beta = 2k$.) This duplicity of notation seems to be extravagant and we will define k as the *restoring force* throughout this paper.

[17]Other parameters of less importance here are "ρ," the hardness parameter, and β_{+-}, a charge distribution parameter, as presented in the treatment of the Born model by Mario Tosi, in *Solid State Physics*, Vol. 1b, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1965), p. 1.

[18]Charles Kittel, *Introduction to Solid State Physics*, 2nd ed. (Wiley, New York, 1956), p. 167.

[19]We use moduli $|B_K^Q C_K^Q|$ instead of the actual combinations $B_K^Q C_K^Q + B_K^{-Q} C_K^{-Q}$, etc., in order to obtain estimates of the magnitudes $R_{\parallel}$ and $R_{\perp}$. The phases of the spherical harmonics determine $\phi_{\parallel}$ and $\phi_{\perp}$.

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[22]It is important to note that interaction assumed in perturbation A [Fig. (a)] is intended primarily to be representative of the types of perturbations leading to the D term in $Mn^{2+}:SrWO_4$. Another sequence of matrix elements, which is particularly appropriate to nearly cubic crystals, is described in R. R. Sharma, T. P. Das, and R. Orbach, Phys. Rev. 149, 257 (1966). The exact form is immaterial, however, since we use the observed $\chi = D/B_2^0$ [see discussion leading to Eq. (5)], which should be independent of which perturbation term dominates.

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Brehmsstrahlung Spectrum of Energetic β Particles Traversing Single Crystals in Lattice-Directed Trajectories

Hans C. H. Nip and J. C. Kelly

Materials Irradiation Group, Department of Physics, University of New South Wales, Sydney, Australia 2033

(Received 29 June 1970)

For lattice-directed trajectories, the Fourier spectrum of the interaction between an energetic ($\gtrsim 10^5$eV) β particle and the lattice atoms is different from the Fourier spectrum of the interaction with randomly distributed target atoms by significant terms of frequencies near $(sv/2a)$. Here s is an integer, v is the velocity of the β particle parallel to the low-index crystallographic direction, and $2a$ is the interatomic spacing in this low-index direction in the reference frame of the β particle. It is suggested that these frequencies will dominate the brehmsstrahlung spectrum of an energetic β particle traversing a single crystal in a lattice-directed trajectory. This effect is considered in terms of the quantal time-dependent perturbation theory. Its magnitude is estimated using the classical theory of radiation.

I. INTRODUCTION

During the last decade, appreciable interest has been focused on the lattice-directed trajectories of energetic positive[1-4] and negative[3-5] particles. In a lattice-directed trajectory, the direction of motion of the projectile particle is aligned with the lattice atoms in a simple crystallographic direction. Therefore, the Fourier spectrum of the interaction between the lattice atoms and the projectile particle will contain significant terms of frequencies around integral multiples of the interaction frequency. These terms have to be considered in the derivation of the transition probabilities between the various quantum states of the energetic projectile particle.[6-10] If we consider the projectile particle free except for the periodic perturbation of the interaction with the lattice atoms, we can apply quantal time-dependent perturbation theory to obtain these transition probabilities. As is well known,[11] we will obtain a strongly increased transition probability to states which differ in energy from the initial state by an amount $sh\gamma$, where s is an integer, h is Planck's constant, and γ is the frequency of the interaction.

For channelled or blocked heavy ions, these energies $sh\gamma$ will be of the same order of magnitude as the energy differences between electronic excited states of the heavy ion. When two such excited states differ in energy by a multiple of $h\gamma$, large differences can be expected in the distributions over the various excited states of the channelled and the randomized heavy ions. For energetic ($\gtrsim 10^5$ eV) positrons and electrons in lattice-directed trajectories, these frequencies lie in the brehmsstrahlung range and we expect that these frequencies will dominate the brehmsstrahlung spectrum.

We will derive an expression for the experimentally measured wavelengths of these lattice-enhanced radiations and make an estimate of the magnitude of the effect for β particles in lattice-directed trajectories.

II. WAVELENGTHS OF LATTICE-ENHANCED RADIATIONS

In considering the motion of a sufficiently localized energetic β particle parallel to a low-index row, we can treat the interaction with the lattice atoms as a perturbation. Moreover, the total time spent in the crystal travelling along the row is much larger than the time between successive interactions from neighboring lattice sites. Hence we may apply quantal time-dependent perturbation theory.

If d is the interatomic spacing of the row under consideration in the laboratory system and $2a$ is the interatomic spacing in the reference frame initially at rest with respect to the β particle, we have

$$2a = d(1-\beta^2)^{1/2}, \quad (1)$$

where $\beta = v/c$ and c is the velocity of light *in vacuo*. Hence the interaction frequency $(v/2a)$ in the reference frame initially at rest with respect to the β particle is given by

$$\gamma = \beta c/d(1-\beta^2)^{1/2}. \quad (2)$$

We can write the interaction potential between the β particle and the lattice atoms in the row as

$$W(t) = \sum_{s=1}^{\infty} (A_s e^{2\pi i\gamma s t} + A_s^* e^{-2\pi i\gamma s t}). \quad (3)$$

Let the β particle at the time $t=0$ be in a wave state $|k_1\rangle$ with energy $E=0$, and let the β particle be in a wave state $|k_2\rangle$ with energy E' after absorption of a virtual photon[6] of energy $h\gamma_e$. The probability of a transition from $|k_1\rangle$ to $|k_2\rangle$ during the time t is, to the first order, given by[11]

$$h^{-2}\left|\sum_{s=1}^{\infty}\left(\langle k_2|A_s|k_1\rangle \int_0^t e^{2\pi i(\gamma_e+\gamma s)t'}dt' + \langle k_2|A_s^*|k_1\rangle \int_0^t e^{-2\pi i(\gamma_e-\gamma s)t'}dt'\right)\right|^2. \quad (4)$$

This transition probability will be very small except for transitions with

$$\gamma_e \simeq \gamma s. \quad (5)$$

Next, the β particle will recoil after emission of a photon γ'. As is well known from the Compton effect,

$$\gamma' < \gamma_e, \quad (6)$$

but for the energies considered we can safely approximate $\gamma' = \gamma_e$. Hence, the radiative transitions with frequencies around γs will dominate the radiation spectrum of the β particle.

To obtain the values γ_l of these frequencies γ_e in the laboratory system, we transfer from the reference frame initially at rest with respect to the β particle to the laboratory system. Because the atomic row is moving with a velocity $(-\beta c)$ with respect to the former reference frame, we have[12]

$$\gamma_l = \gamma_e[(1+\beta\cos\theta_e)/(1-\beta^2)^{1/2}]. \quad (7)$$

Here, the subscript l refers to the value of the parameter in the laboratory system, and the subscript e refers to the value of the parameter in the reference frame initially at rest with respect to the β particle. The angle between the direction of motion of the row and the photon in the latter reference system is denoted by θ_e. We have[12]

$$\cos\theta_e = (\cos\theta_l - \beta)/(1-\beta\cos\theta_l). \quad (8)$$

Hence, substituting Eq. (8) in Eq. (7), we obtain

$$\gamma_l = \gamma_e[(1-\beta^2)^{1/2}/(1-\beta\cos\theta_l)]. \quad (9)$$

Finally, from $\gamma_e = \gamma s$ and Eqs. (2) and (9),

$$\gamma_l = s\beta c/d(1-\beta\cos\theta_l). \quad (10)$$

The brehmsstrahlung of an energetic β particle traversing the single crystal in a lattice-directed trajectory along a row of interatomic spacing d will thus be strongly peaked at the wavelengths λ_s with

$$\lambda_s = c/\gamma_l = d(1-\beta\cos\theta_l)/s\beta. \quad (11)$$

In the nonrelativistic limit, this reduces to

$$\lambda_s = d/s\beta. \quad (12)$$

III. CLASSICAL ESTIMATE OF THE MAGNITUDE OF LATTICE-ENHANCED RADIATION

To simplify the calculations we will use nonrelativistic dynamics and assume that the β particle moves in a rectilinear fashion through the interaction potential $V(r)$ of a single-lattice atom. The total energy $S(y,t)$ radiated at the time t of the passage, illustrated in Fig. 1, is given by[13]

$$S(y,t) = \frac{2e^2}{3c^3}\left(\frac{d^2r}{dt^2}\right)^2, \quad (13)$$

where e is the charge of the β particle. Defining $a = d/2$, we obtain the energy $S(y)$ radiated per

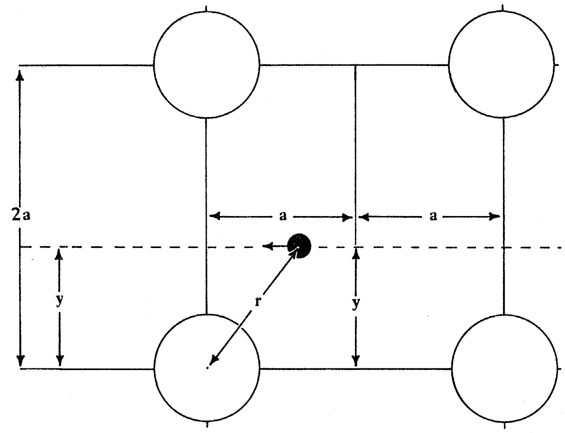

FIG 1. Scattering of an energetic β particle by a lattice atom.

passage

$$S(y)=2\int_0^{a/\beta c} S(y,t)\,dt$$
$$=2\int_0^{a/\beta c}\frac{2e^2}{3c^3m^2}\left(\frac{dV(r)}{dr}\right)^2 dt\,, \qquad (14)$$

where m is the particle rest mass. Using an unscreened Coulomb potential to facilitate integration, we have

$$S(y)=\frac{4e^6}{3c^3m^2}\int_0^{a/\beta c}[y^2+(a-\beta ct)^2]^{-2}\,dt, \qquad (15)$$

to obtain, after defining $f=y/a$,

$$S(f)=K[(1/f^4+f^2)+(\tan^{-1}f^{-1})/f^3]\,, \qquad (16)$$

where $K\simeq 4\times 10^{-22}$ erg/passage.

Let a homogeneous beam of β particles of total beam current I travel into a single crystal aligned with a low-index direction of interatomic spacing $2a$. Assume that such a β particle of initial impact parameter fa travels (nearly) parallel to that low-index direction over a distance $\mu(f)$. Then the total energy radiated per second at the lattice-enhanced frequencies by these lattice-directed β particles can be approximated by

$$S=\int_l^u P(f)S(f)\,df\,.$$

Here, u and l are the upper and lower limits, respectively, of f for which the β particle will be in a lattice-directed trajectory. The function $P(f)\,df$ is the number of passages per second of a lattice atom by a lattice-directed β particle at an impact parameter between af and $a(f+df)$. If $N(f)\,df$ is the number of lattice-directed β particles traveling at a distance from a row axis in the low-index direction between af and $a(f+df)$, we have

$$P(f)\,df=(\beta c/2a)N(f)\,df\;,$$
$$N(f)\,df=(I/e)[\mu(f)/\beta c][2\pi af\,d(af)/4a^2]$$
$$=\pi I\mu(f)f\,df/2e\beta c\,.$$

Hence

$$S=\frac{\pi I}{4ea}\int_l^u f\mu(f)S(f)\,df\,. \qquad (17)$$

A brehmsstrahlung spectrum corresponding to a random motion through the crystal (or a motion through a random material) will be generated by the initially random β particles and those β particles with $\mu(f)<\delta$, where δ is the minimum distance to be travelled through the crystal before emission. If we define

$$F(f)\,df=N(f)\,df/\int_0^1 N(f)\,df\,,$$

we find that the fraction F with

$$F=\int_0^l F(f)\,df+\int_u^1 F(f)\,df$$

of the β particles will be randomized upon entering the crystal. The energy S_1 radiated by these β particles is given by

$$S_1=\int_0^1 P_1(f)S(f)\,df\,,$$

where $P_1(f)\,df$ is the average number of passages per second of a lattice atom by such an initially random β particle at an impact parameter between af and $a(f+df)$. Assume that such a β particle travels an average distance $m\delta$ through the crystal with an average collision frequency $n(\beta c/2a)$, then

$$P_1(f)\,df=\frac{2mnI}{4ea}F\delta\,df\,,$$

where m and n are numbers of order 1. Hence

$$S_1=\frac{2mnI}{4ea}\int_0^1 F\delta S(f)\,df\,. \qquad (18)$$

We obtain the second contribution to the random brehmsstrahlung spectrum by the β particles that have left their lattice-directed trajectories from

$$S_2=\int_0^1 P_2(f)S(f)\,df\,.$$

Here

$$P_2(f)\,df=\frac{2mnI}{4ea}\int_{f'}[\delta-\mu(f')]F(f')\,df'\,df\,,$$

and the integral is taken over those ranges of f' with $\mu(f')<\delta$ and $l\leqslant f'\leqslant u$. The total "background" brehmsstrahlung S_0 is thus given by

$$S_0=S_1+S_2\,;$$

hence,

$$S_0=\frac{2mnI}{4ea}\int_0^1\{\delta F+\int_{F'}[\delta-\mu(f')]F(f')\,df'\}S(f)\,df\,. \qquad (19)$$

Finally, we obtain from Eqs. (17) and (19) the ratio of the energies radiated in the two components of the total brehmsstrahlung spectrum:

$$\frac{S}{S_0}=\frac{(\pi/2mn)\int_l^u f\mu(f)S(f)\,df}{\int_0^1\{\delta F+\int_{f'}[\delta-\mu(f')]F(f')df'\}S(f)\,df}\,. \qquad (20)$$

Let us determine the value of (S/S_0) for a few cases. For a channelled positron in a transmission experiment, we can write $\mu(f')=\delta$ for all $l\leqslant f'\leqslant u$, and find $S_2=0$. Furthermore, since $u=1$ and $\int_0^l F(f')\,df'=l^2$, we obtain from Eq. (20)

$$\frac{S}{S_0}=\frac{\pi}{2mnl^2}\int_l^1 fS(f)\,df\Big/\int_0^1 S(f)\,df \;. \qquad (21)$$

Observing that the terms in the first integral of Eq. (21) are f times smaller than the corresponding terms in the second integral of Eq. (21), while $f\geqslant l$, we obtain from Eq. (21)

$$S/S_0 \geqslant \pi/2mnl \;. \qquad (22a)$$

For (100) axial channelling in a simple cubic lattice, we have $n^{-1}=5.4$ if a scattering is assumed to take place when the projectile passes the lattice site within one-fifth of the interatomic spacing. Under those conditions we can approximate $m=1.7$ and $l=0.2$, and obtain

$$S/S_0 \geq 25 \;. \qquad (22b)$$

Furthermore, for a perfectly collimated beam of 1-MeV positrons, we get from Eq. (17)

$$S\simeq 2\times10^{-11}\ \mathrm{J/sec}\ \mu\mathrm{A}\;. \qquad (22c)$$

In a transmission experiment with energetic electrons, the electrons will be blocked by the low-index direction and only for sufficiently thin crystals will the contribution of S_2 to S_0 be negligible. For a thickness $\delta\simeq 2600$ Å and 1.7-MeV electrons along the (111) axis in Au, we obtain (using the results of a computer simulation of the electron trajectories[5])

$$S/S_0 \simeq 5 \;. \qquad (23)$$

The values of l and u will be difficult to estimate in a reflection or implantation experiment with either type of β particle. Only for small penetration or implantation depths, will $\mu(f)$ be larger than δ and in both cases F will not be very small. However, the largest part of the lattice-enhanced radiation will be emitted in the forward direction (nearly) parallel to the direction of motion of the β particles,[14] i.e., along the low-index direction. Hence, we can experimentally increase the ratio S/S_0 be selecting the appropriate detection direction of the brehmsstrahlung.

IV. CONCLUSIONS

The brehmsstrahlung spectrum of energetic β particles travelling in lattice-directed trajectories will be strongly peaked around integral multiples of the frequency of the interaction between the β particle and the individual lattice atoms. The effect should be readily observable under the appropriate experimental conditions.

ACKNOWLEDGMENTS

The authors are grateful to E. P. George and Paul Bryce for critical evaluation and discussion, and to the Australian Research Grants Committee for support.

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