

## ELASTIC AND INELASTIC SCATTERING OF NEUTRAL ATOMS BY A CORRUGATED HARD WALL

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A general treatment of the elastic and inelastic scattering of neutral atoms by a corrugated hard wall potential is presented. The influence of the atomic thermal motion is divided into two parts, one corresponding to a translation of the whole profile and due to long wavelength phonons, and the other inducing a deformation of the potential shape corresponding predominately to short wavelength phonons. The Debye–Waller factor (for both the elastic and inelastic contributions) has the expected form and contains terms which correspond to a translation of the profile. However a correction term is introduced by the profile deformation. The one phonon exchange can occur with all the crystal phonons but it appears more important with those of long wavelength. The inelastic cross section is expected to be larger in the vicinity of diffracted peaks of large intensity. The only approximation is made in the determination of the source function where one supposes that a limited and small amount of energy is exchanged between the particle and the crystal.

### 1. Introduction

As the static corrugated hard wall model has proven to be realistic in interpreting the elastic experimental data of thermal neutral helium atoms scattered by a clean crystalline surface, it is now interesting to introduce the thermal motion of the wall. Previous works in this field have been done by Garibaldi et al. [1] who used the eikonal approximation and by Beeby [2], who obtained an approximate solution to the time dependent scattering equation. We present here some results using a time independent approach which treats the thermal motion of the lattice using many-body statistical mechanics in the harmonic approximation. The approximations made are less severe than in the previous works.

### 2. The corrugated hard wall potential including thermal crystal motion

We consider the whole system composed of the scattered particle and the crystal. The hamiltonian is

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$$H = -(\hbar^2 \Delta / 2m) + H^0 + V(r, u), \quad (1)$$

the sum of the particle kinetic energy, the crystal hamiltonian taken in the harmonic approximation, and the interaction potential  $V(r, u)$  which in the following will be represented by the corrugated hard wall potential:

$$\begin{aligned} V(r, u) &= \infty, \quad z < \varphi(R, u), \quad \text{region I}, \\ V(r, u) &= 0, \quad z > \varphi(R, u), \quad \text{region II}. \end{aligned} \quad (2)$$

Here the position vector  $r$  is  $(R, z)$  and  $u$  is the displacement due to the atomic thermal motion.

Generally speaking an incoming atom such as helium experiences a repulsive force very near the surface which is the resultant of the interaction between the helium electron shell and the surface electronic structure. As the helium atom diameter is of the same order of magnitude as the distance between neighbouring crystal atoms, many surface atoms will simultaneously participate in the interaction. However their number will be limited as the forces involved have a short range. Consequently we can consider that the repulsive part of the potential  $V(r, u)$  is formed from the contribution of a limited number of surface atoms located in the vicinity of the helium position  $r$ . For the corrugated hard wall potential this implies that the shape function  $\varphi(R, u)$  will be dependent on the thermal displacements of atoms which belong to the unit cell denoted by the  $R$  value and also, depending on the unit cell dimension, of atoms located in its vicinity. Note that this function is continuous with respect to the  $R$  variable and that  $\varphi(R, u = 0)$  is periodic.

Let us consider now the contribution to the thermal motion of the phonons with wavelength long compared to the unit cell dimension. They produce only a translation of the potential. On the contrary the displacements due to phonons of short wavelength, less than a few unit cell dimensions, will contribute mainly and largely to a deformation or distortion of the potential shape. As the atomic thermal displacement is a sum over all crystal modes we can consider that the thermal motion is made up of two parts, the first corresponding to a translation ( $u_t, u_t^z$ ) and the second to a deformation ( $u_d, u_d^z$ ). Thus we can write

$$\varphi(R, u) = \varphi(R - u_t, u_d, u_d^z) + u_t^z. \quad (3)$$

Let us illustrate this point by a very simple example. We suppose that the potential shape between two atoms labelled 1 and 2 is represented by a straight line. If we restrict the thermal motion to the direction normal to the surface the atoms are located respectively at  $x_1, u_1^z$  and  $x_1 + a, u_2^z$ . We have

$$\varphi(x, u) = (u_2^z - u_1^z) \frac{(x - x_1)}{a} + u_1^z = \frac{(u_2^z - u_1^z)}{2} \left[ \frac{2(x - x_1) - a}{a} \right] + \frac{u_2^z + u_1^z}{2}. \quad (3a)$$

This expression shows clearly that the effects of thermal displacement can be divided into a translational part  $u_t^z = (u_1^z + u_2^z)/2$  (which vanishes for phonons of

short wavelength,  $\sim 2a$ ) and a distortion  $u_d^z = (u_2^z - u_1^z)/2$  (which on the contrary, vanishes for long wavelength phonons).

### 3. Solution of the Schrödinger equation

The incident plus scattered state function  $\psi_i^+$  (i.e. the solution of the Schrödinger equation) must be equal to zero in region I. This condition is fulfilled by writing that the product  $V\psi_i^+$  is equal to zero in this region.

In region II,  $V = 0$ , and the product  $V\psi_i^+$  also vanishes. The solution of the Schrödinger equation is of the form

$$\psi_i^+ = \sum_j a_j \phi_j |n_j\rangle, \quad (4)$$

$\phi_j$  being a plane wave and  $|n_j\rangle$  a crystal state. At the boundary  $z = \varphi(R, u)$ ,  $\psi_i^+$  must be equal to zero but its first derivative with respect to  $z$  has a discontinuity. The quantity  $\Delta\psi_i^+$  is consequently a Dirac delta function at the surface. If  $\psi_i^+$  is to satisfy the Schrödinger equation the product  $V\psi_i^+$  must also have the same behaviour.

It is also clear that the transition operator  $T$  operating on an unperturbed state should give the same result as the potential operating on  $\psi_i^+$ . Therefore the following two relations

$$V\psi_i^+ = T|\phi_i n_i\rangle = L^{-3/2} f(R, u) \delta[z - \varphi(R, u)] \exp(iK_0 \cdot R) |n_i\rangle, \quad (5)$$

$$\psi_i^+[R, z = \varphi(R, u)] = 0, \quad (6)$$

are necessary and sufficient to determine  $\psi_i^+$  everywhere [3].

Note that  $L^{-3/2}$  is the box normalization factor and  $K_0$  the surface parallel component of the incident particle wavevector  $k_0 = (K_0, k_0^z)$ .

Starting with the Lippmann–Schwinger equation [3] together with relation (5) one obtains:

$$\begin{aligned} \psi_i^+ = |\phi_i n_i\rangle - im(2\pi\hbar)^{-2} L^{-3/2} \sum_j |n_j\rangle \int \int_{-\infty}^{+\infty} dK_j (k_j^z)^{-1} \exp(iK_j \cdot R) \\ \times \langle n_j | \int \int_{-\infty}^{+\infty} dR' f(R', u) \exp\{i[(K_0 - K_j) \cdot R' + k_j^z z - \varphi(R', u)]\} |n_i\rangle, \end{aligned} \quad (7)$$

with  $m$  the mass of the incident particle and

$$k_j^z = [(E_i^c - E_j^c) 2m\hbar^{-2} + |k_0|^2 - |K_j|^2]^{1/2}, \quad (8)$$

where  $E_j^c$  is the energy of the crystal state  $|n_j\rangle$ .

Eq. (8) expresses the fact that in the hard wall formalism only those intermediate states which conserve the total energy contribute to the scattering process.

For  $z$  greater than the maximum value of  $\varphi(R, u)$ ,  $\psi_i^+$  is the sum of an incoming plane wave, outgoing diffracted waves, and inelastically scattered waves, and corresponds to the expected form (4) of the Schrödinger equation. Thus the solution is uniquely specified if the emitting or source function  $f(R, u)$  can be evaluated by applying the boundary condition (6) to  $\psi_i^+$  of eq. (7).

#### 4. Determination of the source function

If the surface profile is translated as a whole in the direction normal to the surface by a quantity  $u^z$ , it is easy to show that the source function is multiplied by a phase factor  $\exp(-ik_0^z u^z)$ . Thus using the decomposition (3) we can write:

$$f(R, u) = f(R - u_t, u_d, u_d^z) \exp(-ik_0^z u_t^z). \quad (9)$$

Introducing this expression into (7) together with (3) and making the change of variable  $S = R - u_t$  gives an expression for  $\psi_i^+$  where the  $\varphi$  and  $f$  functions are now dependent only upon that part of the thermal displacement which produced a deformation of the corrugation shape  $(u_d, u_d^z)$ . The boundary condition (6) gives:

$$\begin{aligned} 0 = & \exp\{i[K_0 \cdot (S + u_t) - k_0^z(\varphi(S, u_d, u_d^z) + u_t^z)]\} |n_i\rangle - \frac{im}{(2\pi\hbar)^2} \int_{-\infty}^{+\infty} \frac{dK_j}{k_j^z} \\ & \times \exp\{i[K_j \cdot (S + u_t)]\} |n_j\rangle \langle n_j| \int_{-\infty}^{+\infty} dS' \exp\{i[K_0 - K_j] \cdot (S' + u_t) - ik_0^z u_t^z\} \\ & \times \exp\{ik_j^z[\varphi(S, u_d, u_d^z) - \varphi(S', u_d, u_d^z)]\} f(S', u_d, u_d^z) |n_i\rangle, \end{aligned} \quad (10)$$

with

$$k_j^z = [(E_i^c - E_j^c) \frac{2m}{\hbar^2} + k_0^2 - |K_j|^2]^{1/2}.$$

In order to obtain a manageable integral equation we suppose now that  $E_j^c$  is not very different from  $E_i^c$ , that is to say we suppose that the exchange of energy between the particle and the crystal is very small. Thus the sum over  $|n_j\rangle$  reduces to a projector and the boundary condition becomes:

$$\begin{aligned} 0 = & \exp\{i[K_0 \cdot S - k_0^z \varphi(S, u_d, u_d^z)]\} + \frac{ab}{(2\pi)^2} \int_{-\infty}^{+\infty} \frac{dK_j}{k_j^z} \exp(iK_j \cdot S) \\ & \times \int_{-\infty}^{+\infty} dS' \exp\{i(K_0 - K_j) \cdot S'\} \exp\{ik_j^z[\varphi(S, u_d, u_d^z) - \varphi(S', u_d, u_d^z)]\} \\ & \times F(S', u_d, u_d^z), \end{aligned} \quad (11)$$

with  $F = (-im/\hbar^2 ab)f$ , and  $ab$  is the area of the surface unit cell. This integral

equation which determines the source function  $F$  is dependent only upon that part of the thermal motion which produces a deformation of the infinite barrier shape. This is a reasonable result from a physical viewpoint as the part of the motion giving only a profile translation should not modify the source function apart from a phase factor.

Eq. (11) is still rather difficult to handle since it depends on a large number of phonon variables. We now proceed to give two different approximations which lead to manageable equations. The first consists in neglecting the influence of the thermal deformation  $(u_d, u_d^z)$ . The  $\varphi$  and  $F$  functions are now periodic and the integral over  $S'$  which extends over the whole surface can then be reduced to an integral over a single surface cell together with a sum over all surface reciprocal lattice vectors  $G$ . We recover the integral equation which determines the source function in the purely elastic case and which has recently been solved exactly [4,3]. In fact this approximation leads to an exact result if one considers in the elastic or inelastic cross section calculation the influence of the thermal translation alone. Therefore the results obtained will be certainly good if the influence of the thermal deformation is comparatively less than the translational effects. In either case the exchange of energy between particle and crystal should be small as we have supposed above. This should correspond to a system with particles scattered around each diffraction peak which are due mainly to single phonon exchange.

A more elaborate and perhaps less severe approximation consists in linearizing first the  $\varphi$  and  $F$  functions

$$\begin{aligned}\varphi(S, u_d, u_d^z) &= \varphi(S) + \xi(S) \cdot u_d + \xi^z(S) u_d^z, \\ F(S, u_d, u_d^z) &= F(S) + \eta(S) \cdot u_d + \eta^z(S) u_d^z,\end{aligned}\tag{12}$$

and then taking the thermal average of (11). As the thermal average of  $\varphi$  and consequently of  $F$  are periodic, eq. (11) contains only periodic functions of  $S$ . The same procedure as above reduces this equation to an integral over a unit cell with a sum over reciprocal lattice vectors. The four unknown functions,  $F$ ,  $\eta^x$ ,  $\eta^y$  and  $\eta^z$  can be determined by a procedure like those used in the preceding case if the thermal averaged value of  $u_d^x$ ,  $u_d^y$ , and  $u_d^z$  are known. This leads to functions which are temperature dependent.

## 5. Transition rate

The transition matrix element between final (f) and initial (i) states is given by:

$$T_{fi} = \langle n_f \phi_f | V \psi_i^+ \rangle = \langle n_f \phi_f | T | \phi_i n_i \rangle \equiv \langle n_f | t_{fi} | n_i \rangle.$$

As above using the  $V \psi_i^+$  product expressed by relation (5), the decomposition (3) (which implies relation (9)), and the change of variables  $S = R - u_t$  one gets

$$t_{fi} = L^{-3} \exp \{ -i [\Delta K \cdot u_t + (k_i^z + k_f^z) u_t^2] \} \int_{-\infty}^{+\infty} dS f(S, u_d, u_d^z) \\ \times \exp \{ -i [\Delta K \cdot S + k_f^z \varphi(S, u_d, u_d^z)] \}, \quad (13)$$

with

$$\Delta K = K_f - K_i.$$

The mean transition rate is then deduced in the usual way and one finds:

$$W_{fi} = \hbar^{-2} \int_{-\infty}^{+\infty} dt \exp \{ i t (\hbar)^{-1} (E_f^p - E_i^p) \} \langle\langle t_{fi}^*[u(0)] t_{fi}[u(t)] \rangle\rangle, \quad (14)$$

in which  $E^p$  denotes the particle energy and  $\langle\langle \rangle\rangle$  indicates that one has to make the thermal average over crystal states. In general the effect of this last operation is to produce the exponential of mean square and mean correlated displacements which gives a so-called Debye–Waller factor, and the exponential of a time dependent correlation function between displacements. If this latter exponential factor is expanded in powers of the correlation function, the zeroth order term is just the elastic case, the first order term gives the single phonon scattering and the higher order terms give the multiphonon events. The Debye–Waller factor, of course, appears in all of these terms. An important result of the thermal averaging of eq. (14) is that it leaves the transition rate independent of all phonon variables. In the integral over  $S$  appearing in  $t_{fi}$  the part of the integrand depending on  $\varphi$  and  $f$  becomes periodic in  $S$  as the thermal average of  $\varphi$  and consequently of  $f$  are periodic in  $S$ . The integral can be reduced to an integral over a single unit cell with the sum over reciprocal lattice vectors and, with the exception of the elastic case, over phonon momenta parallel to the surface. In all cases the source function is determined by one of the procedures outlined in section 4.

## 6. Elastic events

In this section, and in the following section on inelastic events, we will assume the linearization of the  $\varphi$  and  $F$  functions given by eq. (12). Formally, one can readily include the higher order terms and the associated thermal averages can be carried out. However, we will make the reasonable assumption that the coefficients of these higher order terms are small and hence their influence can be neglected. The elastic reflection coefficient is composed of a sum of three terms which give respectively the influence of  $F(S)$ ,  $\eta(S)$  and  $\eta^z(S)$ , and the influence of the coupling between  $F$  and  $\eta$ . As the terms depending upon  $\eta$  and  $\eta^z$  seem to give much smaller contributions certainly the contributions of higher order terms in the expansion of  $F$  can be neglected. As a zeroth order approximation one has:

$$R_{f=G,i} = (k_0^z k_G^z)^{-1} |A_G|^2 \exp(-2W_{t,G}), \quad (15)$$

with

$$A_G = \int \int_{u.c} dS F(S) \exp\{-i[G \cdot S + k_G^z \phi(S)]\} \exp[-W_{d,G}(S, T)], \quad (16)$$

where  $W_{d,G}$  is a temperature dependent function given by

$$W_{d,G} = k_G^z \langle\langle [(k_i^z + k_G^z) u_i^z + G \cdot u_t] [\xi(S) \cdot u_d + \xi^z(S) u_d^z] \rangle\rangle \\ + \frac{1}{2} (k_G^z)^2 \langle\langle (\xi(S) \cdot u_d + \xi^z(S) u_d^z)^2 \rangle\rangle, \quad (17)$$

$$W_{t,G} = \frac{1}{2} \langle\langle [(k_i^z + k_G^z) u_i^z + G \cdot u_t]^2 \rangle\rangle. \quad (18)$$

The reflection coefficient contains the term  $\exp(-2W_{t,G})$  which is similar to a Debye-Waller factor. We note that this Debye-Waller factor is of the same form as the corresponding factor which is often used in an ad hoc manner for interpreting experimental data [5], however, we have shown that it results naturally from a general formalism and is not restricted to the Born or eikonal approximation. It contains only the translational thermal displacement part, that is to say the influence of phonons of wavelength long compared to the unit cell dimension. The effect of the distortional phonons is to introduce a position dependent correction to this Debye-Waller factor through the deformation displacement term  $\exp[-W_{d,G}(S, T)]$ . The reason one obtains this position dependent term is because of the unusual manner in which the distortional phonons enter the potential. Standard treatments of the Debye-Waller factor, such as for neutron or electron diffraction, depend on a potential of the form  $\sum_l v(\mathbf{r} - \mathbf{r}_l - \mathbf{u}_l)$  or  $V(\mathbf{r} - \mathbf{u})$ . If the phonon operators do not appear in the potential in the linear form  $\mathbf{r} - \mathbf{u}$  one immediately lead to a much more complicated analysis, which in the present case gives rise to the position dependent correction. The physical interpretation is that due to distortions, the effective shape of the surface corrugation in the unit cell can change with temperature and hence give a redistribution of the relative intensities of the diffracted beams.

In the case of helium atoms scattered by the (100), (110) or (111) faces of copper no diffracted peaks have been observed experimentally. This means certainly that the amplitude of the surface corrugated wall is very small. Therefore we may suppose that the correction introduced by the  $\xi$  functions is negligible. Taking a  $u_i^z$  displacement equal to the average displacement of atoms belonging to a surface unit cell we recover a previous result for the Debye-Waller factor which has given a good understanding of the rather high effective surface Debye temperature found experimentally [5,6].



## 7. One phonon events

In order to obtain a result consistent with previous calculations we suppose now that the  $\sigma$  components of  $u_t$  and  $u_d$  are respectively given by

$$u_{tL}^\sigma = \frac{1}{n} \sum_{r=1}^n \alpha_r u_{Lr}^\sigma, \quad u_{dL}^\sigma = \frac{1}{n} \sum_{s=1}^n \beta_s u_{Ls}^\sigma,$$

where the  $n$  atoms considered belong to the unit cell  $L$  or  $L'$ ,  $\alpha_r$  being a positive coefficient whereas  $\beta_s$  can be positive or negative. As mentioned above the thermal average reduces the  $\varphi$  and consequently the  $F$  functions to periodic functions on the surface. Thus the integrals over  $S$  are reduced to a single unit cell and in doing so the summation over all lattice cells gives a  $\delta$  function which guarantees the momentum conservation.

Using the linearization of  $\varphi$  and  $F$  (expression 12)) and neglecting as above the terms given by the  $\eta$  functions one gets for the differential scattering intensity

$$\frac{dR}{dE d\chi} = \frac{\pi ab}{(2\pi)^3 K} \frac{|k_f|}{|k_i^z|} \frac{A(\Omega)}{\Omega} \sum_G \exp(-2W_{t,G+q})(P_{tt} + P_{td} + P_{dd}). \quad (19)$$

$W_{t,G+q}$  and  $W_{d,G+q}$  which enter into eq. (20) below are given respectively by (18) and (17) upon replacing  $k_G^z$  by  $k_f^z$  and  $G$  by  $G + q$ , and

$$K_f = K_0 + G + q,$$

$$k_f^z = [2m(\hbar)^{-2}\hbar\omega + |k_0|^2 - |K_0 + G + q|^2]^{1/2},$$

where  $q$  is the parallel phonon momentum. The function  $A(\Omega) = n(\Omega)$  for phonon annihilation and equals  $n(\Omega) + 1$  for phonon creation, with  $n(\Omega)$  the mean number of phonons of the dimensionless frequency  $\Omega = (M/K)^{1/2} \omega$ ,  $M$  being an atom mass and  $K$  a constant force of the harmonic lattice taken as reference. The three  $P$  terms are given by:

$$P_{tt} = \left[ \sum_{\sigma\alpha} \Delta K^\sigma \Delta K^\alpha \Delta_i^\sigma(q) (\Delta_i^\alpha(q))^* \rho^{\sigma\alpha}(\Omega, q) \right] |C_{G+q}^0|^2,$$

$$P_{dd} = (k_f^z)^2 \sum_{\sigma\alpha} \Delta_d^\sigma(q) (\Delta_d^\alpha(q))^* \rho^{\sigma\alpha}(\Omega, q) (C_{G+q}^\sigma)^* C_{G+q}^\alpha, \quad \sigma, \alpha = x, y \text{ or } z,$$

$$P_{td} = 2k_f^z \operatorname{Re} \left[ \sum_{\sigma\alpha} \Delta K^\sigma (\Delta_i^\sigma(q))^* \Delta_d^\alpha(q) \rho^{\sigma\alpha}(\Omega, q) (C_{G+q}^0)^* C_{G+q}^\alpha \right],$$

with

$$\Delta K^{x,y} = (G + q)^{x,y}, \quad \Delta K^z = k_i^z + k_f^z,$$

$$C_{G+q}^\alpha = \int \int_{\text{u.c.}} dS H^\alpha(S) \exp\{-i[(G + q) \cdot S + k_f^z \varphi(S)]\} \exp\{-W_{d,G+q}(ST)\}, \quad (20)$$

$$H^\alpha(S) = F(S) \xi^\alpha(S), \quad H^0(S) = F(S);$$

$\rho^{\sigma\alpha}(\Omega, q)$  is the spectral density for given  $q$  between direction  $\sigma$  and  $\alpha$  for the surface plane [7], and

$$\Delta_{t(d)} = \frac{1}{n} \sum_{r(s)=1}^n \alpha_r(\beta_s) \exp(iq \cdot R_{r(s)}^0), \quad R_{r(s)}^0 = R_{r(s)} - R_{L(L')}.$$

The two first terms  $P_{tt}$  and  $P_{dd}$  give a predominant one phonon cross section for long and short wavelength waves respectively as they come from the translation and deformation part of the thermal displacement. This behaviour is produced by the form of the  $\Delta_t$  and  $\Delta_d$  factors which, for example are equal respectively to  $\frac{1}{2}(1 + \exp iqa)$  and  $\frac{1}{2}(1 - \exp iqa)$  for the very simple model depicted in section 2. The modulus of  $\Delta_t$  varies continuously from 1 to 0 while  $|\Delta_d|$  varies from 0 to 1 as  $q$  increases from 0 to  $\pi/a$ .

The  $P_{td}$  term gives the interference of  $u_t$  and  $u_d$  as it is composed of the product  $\Delta_t \Delta_d$ . It will be maximum for phonons of medium wavelength.

The appearance of the factors  $\Delta_t$  and  $\Delta_d$  in eq. (19) represents an extension of previous work [5] based on a simpler model exhibiting no distortion. With the present model the one phonon exchange can occur for phonons over the entire Brillouin zone. However it seems that the cross section for phonons of parallel momentum falling near or in the vicinity of the Brillouin zone edge will be small due to the presence of the  $\xi(S)$  function in the integral giving the  $C_{G+q}^0$  matrix element.

Another important fact should be pointed out here. The inelastic matrix element  $C_{G+q}^0$  and the elastic matrix element  $A_G$  are very similar as we have  $C_G^0(\Omega = 0) = A_G$ . In an experimental situation in which there are several neighbouring diffracted peaks which are large compared to the surrounding peaks it is clear that the corresponding  $A_G$  are large. One can then expect that  $C_{G+q}^0$  will also be large for scattering angles near these peaks and in fact will probably exhibit a maximum. In other words the inelastic matrix elements should be large for roughly the same scattering conditions in which the elastic matrix elements are large. Physically, this implies that in a given scattering experiment, wherever one finds strong elastic peaks these should also be a strong inelastic background. It is likely that the inelastic scattering will be particularly important at angles near to the classical rainbow angles.

## 8. Conclusion

The results presented here have been obtained in a closed form using the two important facts:

— The thermal average over crystal states of the shape corrugation function  $\langle\langle \phi(R, u) \rangle\rangle$  is periodic over the surface. As a consequence the same average of the emitting or source function is also periodic.

— The thermal atomic motion can be decomposed into two parts. The first induces a translation of the whole surface profile and corresponds to the motion given by phonons of long wavelength. The second implies a deformation or a distortion of the profile shape and corresponds to the motion given by phonons of short wavelength. The only approximation is introduced in the determination of the source or emitting function. For that we have supposed that the exchange of energy between the particle and the crystal is small. Furthermore we assume that the shape corrugation function  $\varphi(\mathbf{R}, u_d, u_d^z)$  which depends only upon that part of thermal motion which produces the distortion  $(u_d, u_d^z)$  is periodic. This is strictly true for the thermal average of this function but for the function itself this is not exact as far as the phonons of medium or intermediate wavelength are concerned. The zeroth order approximation is equivalent to taking the source function of the purely elastic case. Note that these approximations are made only for the determination of the source function and are not made at any other point in the formalism.

Independent of the determination of the source function two important results have been obtained:

- The Debye–Waller factor for the elastic and inelastic cases is of the same form as the factor usually used in the interpretation of the experimental data. We note that it is obtained in a general formalism and not as previously done with the help of the Born or eikonal approximations. However, one has to take account of a correction term which is position dependent. Its importance should be evaluated in each particular system studied.
- The one phonon exchange can occur with phonons of parallel momentum  $q$  lying in the entire Brillouin zone. However the cross section seems to be more important with phonons of small  $q$  corresponding to a translation of the profile, and seems to decrease as  $q$  approaches the Brillouin zone edge, corresponding to a deformation of the profile shape. Finally one can expect a greater one phonon cross section in the vicinity of the diffracted peaks of large intensity.

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