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Curved-wave corrections to the electron scattering Debye–Waller factor

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Abstract. The influence of atomic movement on the electron scattering is calculated in a curved-wave theory. The contribution in the angular momentum representation of the Green function can be split off into the Debye–Waller factor for the plane-wave scattering and a curved-wave correction. The additional term can be used to correct the expressions for the fine structure in the x-ray absorption spectra or for the angle resolved photoelectron diffraction. The results are applicable to all approximative expressions for these properties. As a main result due to the thermal movement of the atoms the elements of the t -matrix, t_i , have to be replaced by $t_i^{\text{TD}} = t_i + k^2 \sigma_{i0}^2 \bar{t}_i$ where \bar{t} is a modified t -matrix. t and \bar{t} have a different k -dependence. The consequence is a shift in the peaks of the absolute value of the Fourier-transformed spectrum. For nickel we get a shift up to 0.1 au in the single scattering expression for the first nearest neighbour.

1. Introduction

The Debye–Waller factor (DWF) (Debye 1930) was introduced to describe the influence of thermal vibrations on the elastic x-ray scattering from solids. It contains the average square atomic displacement $\langle u^2 \rangle$ and was successfully used to describe the temperature dependence of the measured structure factors. On the other hand the thermal vibration also influences the x-ray absorption fine structure (XAFS) (Beni and Platzman 1976, Teo 1986). In the latter case it is important that the relative phase of the primary and the scattered electron wave is changed by the movement of the emitter R_0 and the scatterer R_j . The average relative atomic displacement $\langle u_{0j}^2 \rangle$ determines the DWF.

High-accuracy intensity measurements indicate that a more detailed investigation of the influence of thermal motion can give additional information. Going beyond the rigid-atom approximation, partial DWF were calculated for different atomic shells (Buyers *et al* 1968, March and Wilkins 1978, Reid 1979, Deutsch *et al* 1989). Furthermore, anharmonic contributions to the mean square displacement were included (Shukla and Hübschle 1989, Shukla and Plint 1989, Wenzel *et al* 1990, Stern *et al* 1991).

In the expression for the x-ray absorption fine structure, curved-wave corrections appear (Lee and Pendry 1975, Müller and Schaich 1983, Fritzsche and Rennert 1984, Barton and Shirley 1985, Fritzsche and Rennert 1986) because we have a local electron source inside the solid instead of an incident plane wave. The curved-wave corrections give an additional contribution to the DWF. Brouder (1988) investigated these

contributions for the static part of the DWF for a given radial distribution, $g(r)$, within the curved-wave approximation of Müller and Schaich (1983) for single scattering.

We investigate the DWF in the general spherical-wave theory of Lee and Pendry (1975) in the single-scattering and multiple-scattering terms of the XAFS expression and also in the angular-resolved photoelectron diffraction. The result is transferable to all curved-wave approximations. In section 2 we review the basic formulae. In section 3 we derive an expression for the propagator, which includes the atomic vibrations. It is shown that it can be reinterpreted as a modified scattering matrix. It is discussed for single scattering in detail in section 4. In section 5 some multiple-scattering loops are discussed and in section 6 numerical results are presented.

2. Basic formulae

The absorption coefficient in the one-electron picture

$$\gamma = \frac{2\pi}{\hbar} \left\langle \psi_i \left| w(\mathbf{r}) \left(-\frac{1}{\pi} \text{Im} G(\mathbf{r}, \mathbf{r}', E_i + \hbar\omega) \right) w(\mathbf{r}') \right| \psi_i \right\rangle \quad (1)$$

and the photoelectron wave function

$$\psi(\mathbf{r}) = \int d^3r' G(\mathbf{r}, \mathbf{r}', E_i + \hbar\omega) w(\mathbf{r}') \psi_i(\mathbf{r}') \quad (2)$$

contain the Green function, G , of the system, which depends on the position of the atoms, \mathbf{R} , and their scattering properties t_j . ψ_i is the initial core state and $w(\mathbf{r})$ is the perturbation by the photon. In the dipole approximation it is proportional to $\mathbf{p} \cdot \mathbf{e}_{\text{photon}}$ or $\mathbf{r} \cdot \mathbf{e}_{\text{photon}}$.

The Green function in (1) and (2) can be written as (Lee and Pendry 1975, Rennert and Chassé 1987)

$$G = G_a + G_a \mathbf{T}^{(a)} G_a \quad (3)$$

$$G = G_a + G_0 \mathbf{T}^{(p)} G_a. \quad (4)$$

The difference between (3) and (4) is due to the position of the variable \mathbf{r} ; in (1) it is near the emitter at \mathbf{R}_0 and in (2) it is far away in the spectrometer. G_a is the atomic Green function, whereas G_0 is the free propagator. In the local description the total scattering matrix \mathbf{T} is a sum over single- and multiple-scattering processes

$$\mathbf{T} = \sum_{\mathbf{R}_1} \mathbf{t}^{\mathbf{R}_1} + \sum_{\mathbf{R}_2 \neq \mathbf{R}_1} \mathbf{t}^{\mathbf{R}_2} G_0 \mathbf{t}^{\mathbf{R}_1} + \dots \quad (5)$$

In the single-scattering term we have the restriction $\mathbf{R}_1 \neq \mathbf{R}_0$. \mathbf{R}_0 is the photoabsorption site. In the second contribution the restriction is $\mathbf{R}_0 \neq \mathbf{R}_2 \neq \mathbf{R}_1 \neq \mathbf{R}_0$ for $\mathbf{T}^{(a)}$ and $\mathbf{R}_2 \neq \mathbf{R}_1 \neq \mathbf{R}_0$ for $\mathbf{T}^{(p)}$, respectively. In the angular momentum representation we rewrite (3) as

$$G = G_a - ik \sum_{L'L} \phi_{L'}(k\mathbf{r}) Y_{L'}(\hat{\mathbf{r}}) X_{L'L}^{(a)} \phi_L(k\mathbf{r}') Y_L(\hat{\mathbf{r}}'). \quad (6)$$

ϕ_l is a solution of the radial Schrödinger equation (in the muffin-tin picture) and Y_L is a spherical harmonic with $L \equiv l, m$. \hat{r} and \hat{e} are unit vectors. The expression

$$\begin{aligned}
 X_{L'L}^{(a)} = e^{i(\delta_l^0 + \delta_l^0)} & \left(\sum_{\mathbf{R}_1} \sum_{L_1} G_{L'L_1}(\mathbf{R}_0 - \mathbf{R}_1) \cdot (-ik) t_{l_1}^{R_1} G_{L_1 L}(\mathbf{R}_1 - \mathbf{R}_0) \right. \\
 & + \sum_{\mathbf{R}_2 \neq \mathbf{R}_1} \sum_{L_2 L_1} G_{L'L_2}(\mathbf{R}_0 - \mathbf{R}_2) \cdot (-ik) t_{l_2}^{R_2} G_{L_2 L_1}(\mathbf{R}_2 - \mathbf{R}_1) \\
 & \left. \times (-ik) t_{l_1}^{R_1} G_{L_1 L}(\mathbf{R}_1 - \mathbf{R}_0) + \dots \right) \quad (7)
 \end{aligned}$$

contains the atomic scattering matrix elements $t_l = -(1/k) \sin \delta_l \exp(i\delta_l)$ and the coefficients $G_{L'L}(\mathbf{R})$. They appear, if a spherical wave

$$h_l(k|\mathbf{R} + \boldsymbol{\tau}|) Y_L(\overline{\mathbf{R} + \boldsymbol{\tau}}) = \sum_{L'} j_{l'}(kr) Y_{L'}(\hat{r}) G_{L'L}(\mathbf{R}) \quad (8)$$

$$G_{L'L}(\mathbf{R}) = \sum_{L''} 4\pi i^{l''+l'-l} h_{l''}^{(1)}(kR) Y_{L''}^*(\hat{\mathbf{R}}) \int d\Omega Y_L(e) Y_{L'}^*(e) Y_{L''}(e) \quad (9)$$

is expanded around another centre (Lee and Pendry 1975, Rennert and Chassé 1987).

3. Inclusion of atomic vibrations

Now we consider atoms at \mathbf{r}_R

$$\mathbf{r}_R = \mathbf{R} + \mathbf{u}_R \quad (10)$$

which move around its position \mathbf{R} . We calculate the influence of this movement. Usually it is characterized by a Debye-Waller factor (DWF). If we describe the movement by phonons, then

$$\mathbf{u}_R = \text{Re} \sum_{\mathbf{q}\nu} \mathbf{u}_{\mathbf{q},\nu} \exp[i(\mathbf{q} \cdot \mathbf{R} - \omega_{\mathbf{q},\nu} t)] \quad (11)$$

where \mathbf{u} is a sum over contributions to different wave numbers \mathbf{q} and polarizations ν . In the adiabatic approximation we have to consider expressions (7) and (9) with positions \mathbf{r}_R instead of \mathbf{R} . Using (9) again

$$\begin{aligned}
 G_{L'L}(\mathbf{R} + \mathbf{u}) & = \sum_{\Lambda''} 4\pi i^{\lambda''+l'-l} h_{\lambda''}^{(1)}(k|\mathbf{R} + \mathbf{u}|) Y_{\Lambda''}(\overline{\mathbf{R} + \mathbf{u}}) \\
 & \times \int d\Omega Y_L(e) Y_{L'}^*(e) Y_{\Lambda''}^*(e) \\
 & = \sum_{\Lambda''} 4\pi i^{\lambda''+l'-l} \sum_{\Lambda'} j_{\lambda'}(ku) Y_{\Lambda'}(\hat{\mathbf{u}}) \sum_{L''} 4\pi i^{l''+\lambda'-\lambda''} h_{l''}^{(1)}(kR) Y_{L''}^*(\hat{\mathbf{R}}) \\
 & \times \int d\Omega' Y_{\Lambda''}(e') Y_{\Lambda'}^*(e') Y_{L''}(e') \int d\Omega Y_L(e) Y_{L'}^*(e) Y_{\Lambda''}^*(e)
 \end{aligned}$$

and the plain wave expansion

$$e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}'} = \sum_{\Lambda'} 4\pi i^{\lambda'} j_{\lambda'}(ku) Y_{\Lambda'}(\hat{\mathbf{u}}) Y_{\Lambda'}^*(\mathbf{e}') \quad (12)$$

we get

$$G_{L'L}(\mathbf{R} + \mathbf{u}) = \sum_{L''} 4\pi i^{l''+l'-l} h_{l''}^{(1)}(kR) Y_{L''}^*(\hat{\mathbf{R}}) \int d\Omega Y_L(\mathbf{e}) Y_{L'}^*(\mathbf{e}) Y_{L''}(\mathbf{e}) e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}} \quad (13)$$

$$G_{L'L}(-\mathbf{R} - \mathbf{u}) = \sum_{L''} 4\pi i^{l-l'+l''} h_{l''}^{(1)}(kR) Y_{L''}^*(\hat{\mathbf{R}}) \int d\Omega Y_L(\mathbf{e}) Y_{L'}^*(\mathbf{e}) Y_{L''}(\mathbf{e}) e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}}. \quad (14)$$

The parity $Y_L(-\mathbf{e}) = (-1)^l Y_L(\mathbf{e})$ was used. If we restrict the considerations to a radial movement, $\mathbf{u} \parallel \mathbf{R} \parallel \mathbf{e}_z$ then (13) reduces to equation (A17) in the paper of Brouder (1988). Using (13) and (14) instead of (9), the atomic movement can be included into the expression for XAFS (1) and angle-resolved photoelectron diffraction (2) in the single-scattering and multiple-scattering terms of the curved-wave theory.

In the plane-wave approximation the Hankel function is approximated by $h_l(x) = i^{-l} h_0(x)$ and (13) reduces to

$$G_{L'L}(\mathbf{R} + \mathbf{u}) = 4\pi i^{l'} Y_{L'}^*(\hat{\mathbf{R}}) h_0^{(1)}(kR) i^{-l'} Y_{L'}(\hat{\mathbf{R}}) e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}_R}. \quad (15)$$

We get the DWF in the plane-wave approximation from averaging the factor $\exp(2i\mathbf{k}\mathbf{u}\cdot\mathbf{e}_R)$, which appears in (1).

4. Single-scattering expression

We start from the expression in (7). The abbreviations $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$, $\mathbf{e}_{ij} = \mathbf{R}_{ij}/R_{ij}$ and $\mathbf{u}_{ij} = \mathbf{u}_{R_i} - \mathbf{u}_{R_j}$ are used. Sometimes we cancel the indices altogether. We insert (13) and (14) and get

$$\begin{aligned} \sum_{L_1} G_{L'L_1}(-\mathbf{R})(-ik) t_{L_1}^R G_{L_1L}(\mathbf{R}) &= \sum_{L_1} \sum_{L''} 4\pi i^{l_1-l'+l''} \\ &\times h_{l''}^{(1)}(kR) Y_{L''}^*(\hat{\mathbf{R}}) \int d\Omega_2 Y_{L'}^*(\mathbf{e}_2) Y_{L_1}(\mathbf{e}_2) Y_{L''}(\mathbf{e}_2) e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}_2} (-ik) t_{L_1}^R \\ &\times \sum_{\Lambda''} 4\pi i^{\lambda''+l_1-l} h_{\lambda''}^{(1)}(kR) Y_{\Lambda''}^*(\hat{\mathbf{R}}) \\ &\times \int d\Omega_1 Y_{L_1}^*(\mathbf{e}_1) Y_L(\mathbf{e}_1) Y_{\Lambda''}(\mathbf{e}_1) e^{i\mathbf{k}\mathbf{u}\cdot\mathbf{e}_1}. \end{aligned} \quad (16)$$

Due to the atomic movement we have to average the factor

$$\langle e^{i\mathbf{k}\mathbf{u}_{10}\cdot(\mathbf{e}_2+\mathbf{e}_1)} \rangle = \exp\left[-\frac{1}{2}k^2\langle(\mathbf{u}_{10}\cdot(\mathbf{e}_2+\mathbf{e}_1))^2\rangle\right] \quad (17)$$

and we restrict the expansion to the second moment.

In an isotropic Debye model we can sum over the polarization. The mean value $\langle u_{q,\nu}^2 \rangle$ is independent of ν . We get $\langle (e_1 \cdot u_{10})^2 \rangle = \langle (e_2 \cdot u_{10})^2 \rangle = \sigma_{10}^2$ and $\langle (e_1 \cdot u_{10})(e_2 \cdot u_{10}) \rangle = e_1 \cdot e_2 \sigma_{10}^2$ with

$$\sigma_{10}^2 = \sum_q \langle u_q^2 \rangle (1 - \cos(q \cdot R)). \tag{18}$$

The thermal average reduces to

$$\langle e^{ik u_{10} \cdot (e_2 + e_1)} \rangle = \exp[-k^2 \sigma_{10}^2 (1 + e_1 \cdot e_2)] = e^{-2k^2 \sigma_{10}^2} (1 + k^2 \sigma_{10}^2 (1 - e_1 \cdot e_2) + \dots). \tag{19}$$

The term containing $1 - e_1 \cdot e_2$ describes the curved-wave corrections. In the plane-wave approximation we have only contributions for $e_1 = e_2 = e_{10}$ and $1 - e_1 \cdot e_2$ vanishes. Therefore we include only the lowest order of $1 - e_1 \cdot e_2$ into the curved-wave corrections.

Now we rearrange (16) for the curved-wave correction in (19), looking at the sum over L_1 (writing L instead of L_1)

$$\begin{aligned} 4\pi \sum_L (-1)^l t_l Y_L(e_1) Y_L^*(e_2) (1 - e_1 \cdot e_2) &= \sum_l (-1)^l (2l + 1) t_l P_l(\zeta) (1 - \zeta) \\ &= \sum_l (-1)^l [l t_{l-1} + (2l + 1) t_l + (l + 1) t_{l+1}] P_l(\zeta) \\ &= 4\pi \sum_L (-1)^l \tilde{t}_l Y_L(e_1) Y_L^*(e_2) \end{aligned} \tag{20}$$

with $\zeta = e_1 \cdot e_2$ and using $(2l + 1)\zeta P_l = (l + 1)P_{l+1} + lP_{l-1}$. The factor $1 - e_1 \cdot e_2$ can be included by introducing a modified t -matrix with elements

$$\tilde{t}_l = \frac{1}{2l + 1} [l t_{l-1} + (2l + 1) t_l + (l + 1) t_{l+1}]. \tag{21}$$

Thus, due to the thermal vibration (19) we have the usual DWF $\exp(-2k^2 \sigma_{10}^2)$ and modified scattering properties described by

$$t_l^{TD} = t_l + k^2 \sigma_{10}^2 \tilde{t}_l. \tag{22}$$

This is the main result of the paper.

In the curved-wave theory we have a scatterer at the position $R + u$, which produces a scattered wave with angular momentum l . It is described by a scatterer at the position R , which produces a scattered wave with angular momentum l and $l \pm 1$. If we include higher-order terms in (19) we get additional l values.

This result was developed in the general angular momentum expansion (5) (Lee and Pendry 1975). Thus, it can also be used for all approximate expressions (Müller and Schaich 1983, Fritzsche and Rennert 1984, Barton and Shirley 1985, Fritzsche and Rennert 1986). A scattering amplitude \tilde{f} calculated with \tilde{t} instead of t has the property $\tilde{f}(\pi) = 0$, in accordance with the statement that the correction vanishes in the plane-wave approximation.

5. Multiple-scattering expressions

We do not write down the contributions to the DWF in detail, because they are very lengthy (even in the plane-wave approximation). Let us look at a second-order process, $R_0 \rightarrow R_1 \rightarrow R_2 \rightarrow R_0$. This is a contribution in (7) containing

$$G_{L'L_2}(R_0 - R_2)(-ik)t_{l_2}^{R_2} G_{L_2L_1}(R_2 - R_1)(-ik)t_{l_1}^{R_1} G_{L_1L}(R_1 - R_0).$$

Including in G the atomic vibrations (13) and (14) and averaging according to (17), we have an additional factor

$$\text{DWF} = \exp\left[-\frac{1}{2}k^2 \langle (u_{20} \cdot e_3 + u_{21} \cdot e_2 + u_{10} \cdot e_1)^2 \rangle\right]. \quad (23)$$

Mean square displacements like (18) appear containing trigonometric functions with $q \cdot (R_1 - R_0)$, $q \cdot (R_2 - R_1)$, and $q \cdot (R_2 - R_0)$ instead of $q \cdot R$. An expansion like (19) is possible, but the angles $e_{20} \cdot e_{21}$, $e_{21} \cdot e_{10}$ and $e_{10} \cdot e_{20}$ appear explicitly. In the curved-wave corrections, $e_3 \cdot e_2$ and $e_2 \cdot e_1$ can be included into a modified t-matrix (21) for both the scattering processes, but $e_3 \cdot e_1$ remains separate.

We can get a simple expression for the multiple-scattering loops with shadowed atoms, which are the most important ones. If we consider a process

$$R_0 \rightarrow R_1 \rightarrow R_2 \rightarrow R_1 \rightarrow R_0 \quad \text{with } R_2 = 2R_1$$

then we get an exponent (23) containing

$$\begin{aligned} u_{10} \cdot e_4 + u_{21} \cdot e_3 + u_{21} \cdot e_2 + u_{10} \cdot e_1 &= u_{20} \cdot (e_3 + e_2) + u_{10} \cdot (e_4 - e_3 - e_2 + e_1) \\ &\simeq u_{20} \cdot (e_3 + e_2) \end{aligned} \quad (24)$$

where we used $u_{21} = u_{20} - u_{10}$. A rearrangement is possible (24) and the last term can be neglected, because (due to the special positions in the loop) we have contributions for just $e_4 = e_3 = e_2 = e_1 = e_{10}$ in the plane-wave approximation. The movement of the atom at R_1 gives a higher-order correction in the curved-wave theory for this loop. It remains the same DWF as for the single-scattering loop $R_0 \rightarrow R_2 \rightarrow R_0$ with the t-matrix t^{TD} (22) only at R_2 .

6. Numerical results

We want to prove the importance of the curved-wave corrections developed in the preceding sections. We consider a single-scattering loop and calculate the first-nearest-neighbour contribution to XAFS in a nickel crystal. According to (22) we calculate two spectra: one is calculated with t_l and the other one with \tilde{t}_l (21). Figure 1 shows the result of the calculation where the contributions are multiplied by k and k^3 , respectively. Thus, the factor k^2 appearing in (22) is still included. There is an additional factor of 1/40 in the second contribution to give nearly the same maximum value.

The most important result is the difference in the length of the oscillations. This length is determined by $2kR$ on the one hand and by the k dependence of the phase of the scattering amplitude on the other hand. Figure 1 shows that there is

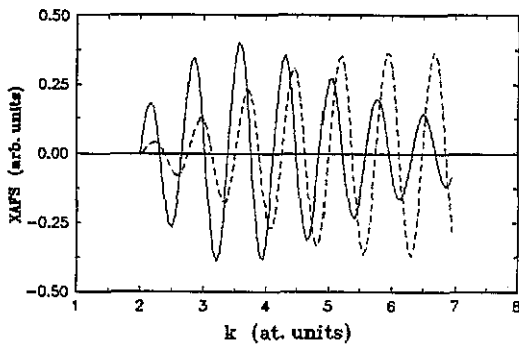


Figure 1. First-nearest-neighbour contribution to XAFS for a nickel atom times a factor k calculated with t (full line). The dashed line shows the same expression calculated with \tilde{t} and multiplied by k^3 and a factor $1/40$ for scaling.

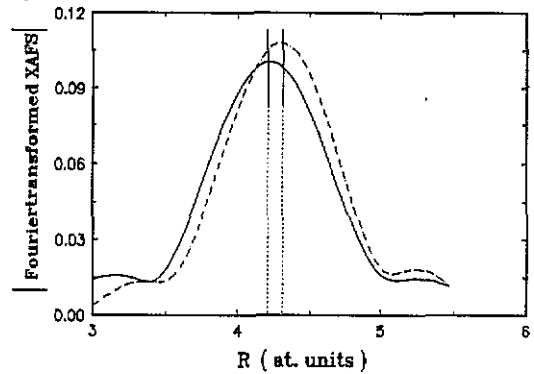


Figure 2. The absolute value of the Fourier-transformed spectra of figure 1. The difference in the maximum position is indicated.

a different k dependence of t and \tilde{t} . Figure 2 contains the absolute value of the Fourier-transformed spectra. Due to the mentioned k dependence of the phase, the position of the maximum of the Fourier-transformed spectrum differs from R (or $2R$). This has to be included if we evaluate a spectrum to determine neighbour distances. Neglecting the curved-wave corrections, an error of up to 0.1 au can arise according to the difference in the maximum position of the two curves in figure 2.

The actual error depends on the weight of the second contribution in (22). Due to the above-mentioned factor of $1/40$ in the considered example both contributions in (22) have nearly the same weight in the Fourier-transformed spectrum if $40\sigma_{10}^2 (\text{au})^{-2}$ is equal to one. This is the case for $\sigma_{10}^2 = 0.025 (\text{au})^2$ or $\sigma_{10}^2 \approx 0.006 \text{ \AA}^2$. This is the order of magnitude of the mean square displacement at room temperature.

7. Summary

We have calculated the influence of the movement of the atoms on the Debye-Waller factor in a curved-wave theory for the electron scattering. In the general angular momentum expansion they can be expressed by a modified coefficient $G_{L'L}$ (13). It is possible to split off a Debye-Waller factor known from the plane-wave scattering. However, there remain curved-wave corrections. In the single-scattering expression they can be included by adding a contribution to the t -matrix, which has a modified dependence on the phase shift and a weight containing the mean square displacement and a factor k^2 . The curved-wave corrections can be important if the modified t -matrix, \tilde{t} , differs in its k dependence in comparison to t .

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