Fig. 4. Excitation of the 8$\bar{8}$01 reflection, showing an extinction line along the mirror plane of the whole pattern. The extinction in this case is due to a c glide.

938 K. By analogy with $LiTaO_3$, we conclude that $LiZnTa_3O_9$ at room temperature is paraelectric and that the addition of Zn to $LiTaO_3$ lowers its Curie temperature. The density of $LiTaO_3$, D_m is 7·4564 g cm^{-3}. There are six molecular units per hexagonal

unit cell. For $LiZnTa_3O_9$, $D_m = 7·61$ g cm^{-3} and $Z = 2$ per hexagonal unit cell (Shu *et al.*, 1981).

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X-ray Debye–Waller Factors of Zinc-Blende-Structure Materials:– Dynamic Deformation Effects

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Abstract

A discussion is given on simple grounds, not explicitly involving the dynamical deformation formalism, of the implications of having the outer part of the electron distribution vibrating significantly differently from the core. The use of a lattice dynamical shell model to represent this effect is examined in some detail, with particular reference to the framework within which such a model gives meaningful results. Predictions are given from the 14-parameter shell models and the 11-parameter valence-shell models for the difference between Debye–Waller B values of the shells and cores and also for the effective Debye–Waller factors for the deforming ions in 14 zinc-blende-structure compounds. It is concluded that the effective X-ray Debye–Waller B at very small $\sin\theta/\lambda$ is typically several percent smaller than the core B value, owing to a very substantial reduction in the mean-square displacements of shells compared with cores. Results are also given for the 15-parameter deformation-dipole models for eight materials. These show effects broadly comparable in magnitude to the shell models but more varied in detail. Notably, some models show for the first time a larger rather than smaller Debye–Waller factor for the deforming ion.

Introduction

At least in the past decade, the accurate measurement of Debye–Waller factors has involved concern that not all of the electron distribution of an atom vibrates by the same amount. On the theoretical side one is also concerned that accuracy in calculating the core Debye–Waller factor is wasted if there are moderately

important discrepancies between the theoretical model and reality that have not been investigated at all. With these considerations in mind, it was thought worthwhile to assess whether there could be significant disturbances to an analysis involving Debye–Waller factors from the fact that an atom core and its outer-electron distribution do not vibrate by the same amount. This study is intended to complement the detailed investigation of the Debye–Waller factors of some 17 zinc-blende-structure compounds reported in a previous article (Reid, 1983, hereafter referred to as I). The effect considered has come to be called 'dynamic deformation'. It has been treated in the past through a deformation formalism which, though preserving great generality, has hidden some of the physical arguments involved. [See, for example, March & Wilkins (1978) and Reid & Pirie (1980) for two different approaches.] Before demonstrating that moderate effects are predicted for the materials under discussion, the first section discusses in more detail than has been done before the physical basis of the dynamic deformation effect without explicit recourse to the deformation formalism.

The physical basis of treating dynamic deformation

The current generation of lattice dynamical models used for the zinc-blende-structure materials all take account of the deformation of an ion during vibration and hence implicitly incorporate a different vibration for different parts of the ion. (These models are the shell model, the valence-shell model, the deformation-dipole model and the deformation-ion model, as detailed in I.) We shall consider the well known shell model as the archetype. The intra-ionic degree of freedom, the displacement of the shell relative to the core in pictorial terms, models the deformation. Because of this extra freedom, the absolute shell displacements differ from the core displacements. Hence the shells may have a different temperature-dependent Debye–Waller factor from the cores.

Before looking in detail at the difference between shell and core Debye–Waller factors, it must be mentioned that the shell model includes another feature which has a bearing on the interpretation of the shell. For a finite but very small mass of a shell there are additional very high frequencies of vibration that to some extent model dynamic electronic processes associated with an energy-band spread of many electron volts. These processes may truly produce large very rapid electron-density fluctuations. However, they are not well accounted for by a lattice dynamical model such as a shell model (which gives them a spurious spatial coherence) because only their *time average* influences the normal phonon frequencies and is adequately parameterized by the model.

It is relevant here to consider the very-high-frequency model modes because if they were to be included they would contribute a very large *temperature-independent* Debye–Waller factor to the shells, an effect which tends to infinity as the mass of the shell tends to zero. This can be seen as follows. As the mass of the shell (m_s) tends to zero, the high frequencies (ω_s) under consideration tend to infinity such that $m_s\omega_s^2$ remains constant (since it is determined by a mass-independent force matrix). Because the high frequencies always have zero-point energy, every term in the lattice dynamical sum for the mean-square displacement of the shells will contain the factor $(m_s\omega_s)^{-1}$ which tends to infinity as $m_s^{-1/2}$. Indeed, if one looks further at these very-high-frequency modes, one finds that they make a temperature-independent contribution to the total diffuse scattering throughout reciprocal space. As such it is considered that the complete scattering given by these modes of a lattice dynamical model is trying to include processes that give rise to some of the Compton scattering, which is better modelled by other techniques. Hence the (temperature-independent) contribution of the very high frequencies is not included in the sums for the shell Debye–Waller factors. For completeness it should be added that since the cores are almost stationary at these very high frequencies the influence of these frequencies on the core Debye–Waller factors is negligible.

Let us look directly at how the Debye–Waller factor of a shell enters the expression for X-ray Bragg scattering at scattering vector **K**. By keeping within the shell-model picture we can bypass the dynamic-deformation formalism. In general, the Debye–Waller factor W enters in a double summation over unit-cell entities kk' of the form

$$I_B = N \sum_{kk'} f_k \exp(-W_k) f_{k'}^* \exp(-W_{k'})$$

$$\times \exp[i\mathbf{K}\cdot\mathbf{r}(kk')] \, \Delta(\mathbf{K}, \mathbf{G}), \qquad (1)$$

where f_k is the scattering factor of the k entity, $\mathbf{r}(kk')$ the vector between equilibrium positions of the entities and $\mathbf{G}$ is a reciprocal-lattice vector (see, *e.g.*, Willis & Pryor, 1975). If each ion k is now imagined as a core entity, kc, and a shell entity, ks, at the same equilibrium position, then each term in the summation (1) becomes

$$[f_{kc} \exp(-W_{kc}) + f_{ks} \exp(-W_{ks})]$$

$$\times [f_{kc'}^* \exp(-W_{kc'}) + f_{ks'}^* \exp(-W_{ks'})] \exp[i\mathbf{K}\cdot\mathbf{r}(kk')].$$
$$(2)$$

The scattering factor of an atom can be divided between core and shell because the scattering factors depend linearly on the electron charge density, *i.e.*

$$f_k = f_{kc} + f_{ks}.$$

In the present application these scattering factors are considered as functions of the magnitude of **K** only. If

W_{ksc} is the difference in the Debye–Waller factor between core and shell, i.e.

$$W_{ksc} = W_{ks} - W_{kc}, \qquad (3)$$

then (2) becomes

$$[f_{kc} + f_{ks} \exp(-W_{ksc})] \exp(-W_{kc})$$
$$\times [f^*_{kc'} + f^*_{ks'} \exp(-W_{ksc'})] \exp(-W_{kc'}) \exp[i\mathbf{K}.\mathbf{r}(kk')]. \qquad (4)$$

The term W_{ksc} represents in one way the dynamic-deformation effect. Although there is no *a priori* reason why it must be so, it turns out that W_{ksc} is generally negative, often quite substantially so. Hence (4) shows that dynamic deformation effects may (substantially) enhance the scattering factor of the part of the ion identified as the shell. Put in other terms, if (1) has been the essential part in a deduction of scattering factors then the scattering factor of the electrons which are deforming relative to the core will be overestimated proportionally by $\exp(-W_{ksc})$.

The approach to dynamic deformation based on the deformation formalism used by Reid & Pirie (1980) and elsewhere has been to write (2) in terms of an effective Debye–Waller factor, W_k^D, for each site, composed of the core Debye–Waller factor plus a K-dependent modification. Thus

$$W_k^D = W_{kc} + \Delta W_k, \qquad (5)$$

with ΔW_k depending on the magnitude of $\mathbf{K}$. In terms of W_k^D the Bragg scattering is simply

$$I_B = N \sum_{kk'} f_k \exp(-W_k^D) f^*_{k'} \exp(-W_{k'}^D)$$
$$\times \exp[i\mathbf{K}.\mathbf{r}(kk')] \Delta(\mathbf{K}, \mathbf{G}) \qquad (6)$$

and comparing the terms in (6) with (4) gives, after some manipulation,

$$\exp(-\Delta W_k) = [f_{kc} + f_{ks} \exp(-W_{ksc})]/f_k \qquad (7)$$

as the general relationship determining the effective Debye–Waller factor as a function of K. In the limit of small $\sin\theta/\lambda$ (in practice not particularly small) the exponentials in (7) can be expanded to first order giving

$$\Delta W_k = \frac{f_{ks}}{f_k} W_{ksc}. \qquad (8)$$

Finally, it is more convenient to present results for isotropic materials in terms of the Debye–Waller B values rather than the W of the general formulae discussed so far. Since

$$W = B \sin^2 \theta/\lambda^2 \qquad (9)$$

the quantities B_{kc}, B_{ks}, B_{ksc}, etc. are simply related to their W counterparts by dividing by $\sin^2\theta/\lambda^2$. We shall explicitly calculate

$$\Delta B_k = \frac{f_{ks}}{f_k} B_{ksc}, \qquad (10)$$

where the quantity B_{ksc} is the lattice-vibration-determined part of the effective Debye–Waller factor (equivalent to S of Reid & Pirie, 1980). From (3), (9) and the lattice dynamical sum for the Debye–Waller B, B_{ksc} is clearly given by

$$B_{ksc} = \frac{8\pi^2}{3} \frac{1}{N} \sum_{qj} \left(\frac{E}{\omega^2}\right)_{qj} \left\{ \left[\frac{\mathscr{E}(k/qj)}{m_k^{1/2}} + \mathscr{W}(k/qj)\right]^* \right.$$
$$\cdot \left[\frac{\mathscr{E}(k/qj)}{m_k^{1/2}} + \mathscr{W}(k/qj)\right] - [\mathscr{E}^*(k/qj).\mathscr{E}(k/qj)]/m_k \right\}$$
$$= \frac{8\pi^2}{3N} \sum_{qj} \left(\frac{E}{\omega^2}\right)_{qj} \left[\frac{\mathscr{E}^*(k/qj)}{m_k^{1/2}} \cdot \mathscr{W}(k/qj)\right.$$
$$\left. + \mathscr{W}^*(k/qj).\frac{\mathscr{E}(k/qj)}{m_k^{1/2}} + \mathscr{W}^*(k/qj).\mathscr{W}(k/qj)\right], \qquad (11)$$

where $\mathscr{E}(k/qj)$ is the eigenvector of the core in mode j of wavevector $\mathbf{q}$ and $\mathscr{W}(k/qj)$ is the eigenvector of the relative shell–core displacement.

Equations (10) and (11) are the same as equations (8) and (7) in Reid & Pirie (1980) derived through the different approach of the deformation formalism, except that the deformation formalism was followed through only with terms linear in the relative shell–core displacement term $\mathscr{W}(k/qj)$. Since in practice B_{ksc} is negative, the second-order term $|\mathscr{W}|^2$ in (11) when taken into account slightly reduces the magnitude of the effect. This second-order term will be significant if B_{ksc}/B_{kc} (or equivalently S_k/B_{kc} in earlier work) is large.

The following section will present B_{ksc} values calculated using (11) in order that the variation of effective Debye–Waller factors can be estimated through (10), (9), and (5) or the enhancement to the shell scattering factor seen through (4).

The foregoing discussion is phrased in terms of the shell model because in its basic conception the shell model is more than a lattice dynamical model since it has an additional parameter per ion for electronic distortion. The deformation-dipole formalisms emphasize that the lattice dynamical vibrations are determined only by the product of the shell charge $Y(k)$ and shell–core displacement $\mathscr{W}(lk)$, this product being the electronic dipole moment $\mathbf{p}(lk)$ of an ion.

$$\mathbf{p}(lk) = Y(k) e \mathscr{W}(lk), \qquad (12)$$

where e is the magnitude of the electronic charge. Hence, modelled electronic dipole moments can be made the basis of equivalent shell Debye–Waller factors by choosing reasonable values for $Y(k)$ and following through the use of (12).

The shell-model results

Expression (11) for B_{ksc}, the difference between shell and core Debye–Waller factors, was evaluated by direct summation over a uniform mesh of 64 000 wavevectors in the Brillouin zone, for a range of temperatures 1 to 1000 K. The eigendata were generated by the lattice dynamical routines of Kunc & Nielsen (1979b). There is no significant zero-phonon contribution since the relative shell–core displacements tend to zero in the modes where the eigenfrequencies ω tend to zero.

Table 1 summarizes the materials and models, listing B_{ksc} at 295 K which can be compared with the B_{kc} values in I to gauge the fractional deficit in mean-square vibrational amplitudes of the shells. The previous discussion demonstrated that a more directly observable quantity is ΔB_k, which in addition depends on the ratio of shell to ion scattering factors (equation 10). The maximum value of ΔB_k therefore occurs at $\mathbf{K} = 0$.

$$\Delta B_k(\mathbf{K} = 0) = Y_k B_{ksc}/Z_k^{\text{total}}, \qquad (13)$$

where Z_k^{total} is the total number of electrons in the k ion. Table 1 shows the values given by the models for this maximum as a fraction of B_k. For larger K this ratio will decrease at a rate that depends on the detail of the distorting electron distribution, which in turn depends on the number of electrons effectively participating in the distortion.

Broadly speaking, the $\Delta B_k(\mathbf{K} = 0)$ are a few percent of B_{kc}, with different models for the same material typically differing by a factor of two. As might be expected, the lighter ions tend to show the largest effects. All the shell models predict a smaller shell vibration than core vibration. Most of the valence-shell models have 'large Z', that is an ionic charge about 2, and give positive shell charges for the cation. There is no clear evidence that these positive charges arise from the time-averaged effects of holes at the top of the valence band: it is most likely that they are an artefact of obtaining a suitable balance of forces with a limited number of parameters in the dynamical matrix. Whatever their dynamical significance, it is certainly true that for scattering purposes Y_k and Z_k^{total} in (13) refer to numbers of real electrons and hence for these models Y_k has simply been interpreted as the average number of electrons significantly participating in the distortion.

Some support for the generally small values of shell vibration comes from the analysis of molecular beam scattering experiments by Johansson & Persson (1980). The Debye–Waller factor determined from this scattering, which is dominated by the outer electrons, is generally found to be appreciably smaller than the core Debye–Waller factor. Unfortunately the materials

Table 1. B_{ksc} is the difference between shell and core B values at 295 K calculated from equation (11)

The sources of shell model (SM) parameters and valence-shell model (VSM) parameters are given in I. The final columns show by what fraction the effective Debye–Waller factor for the whole atom differs from the core Debye–Waller factor (B_{kc}) in the limit of $\sin \theta/\lambda = 0$. The values are calculated from equation (13). (ΔB_k is zero for a rigid ion.) For ions marked * the modelled shell charge is positive but is taken as negative in equation (13) for the reasons discussed in the text. For the ion †, the modelled shell charge exceeds the ionic charge but could be reduced to a reasonable value by the transformation discussed in the final section without much affecting the table entry.

| | | B_{ksc} (Å^2) | | $\Delta B_k(\mathbf{K} = 0)/B_{kc}$ (%) | |
	Model	Cation	Anion	Cation	Anion
GaP	SM	−0·30	−0·42	−3·0	−8·4
	VSM	−0·07	−0·13	−2·3*	−3·4
GaAs	SM	−0·36	−0·42	−2·9	−6·9
	VSM	−0·07	−0·14	−2·2*	−1·9
GaSb	SM(A)	−0·30	−0·20	−6·6	−2·9
	SM(B)	−0·21	−0·30	−4·8	−4·3
	VSM	−0·14	−0·18	−2·5*	−1·3
InP	VSM	−0·10	−0·14	−1·5*	−2·4
InAs	VSM(A)	−0·10	−0·17	−1·3*	−1·8
	VSM(B)	−0·08	−0·17	−1·4*	−1·9
InSb	SM	−0·63	−0·38	−3·8	−4·0
	VSM	−0·12	−0·30	−1·0*	−1·9
ZnO	VSM	−0·06	−0·12	−3·0*	−4·3
ZnS	VSM(Ia)	−0·27	−0·03	−6·4	−1·6
	VSM(IIa)	−0·11	−0·13	−3·0*	−2·4
ZnSe	VSM	−0·11	−0·18	−2·7*	−1·9
ZnTe	VSM(I)	−0·05	−0·20	−0·2	−2·1
	VSM(II)	−0·25	−0·15	−3·1*	−0·8
CdTe	SM(I)	0·90	−0·33	−1·6	−2·6
	SM(II)	−0·81	−0·24	−2·3	−2·1
CuCl	SM	−2·01	−0·57	−0·1	−0·9
CuBr	SM(I)	−0·07	−0·95	−1·7	−1·8
	SM(II)	−1·59	−1·17	−2·7	−1·6
CuI	SM	−0·69	−0·04	−0·1	−2·9†

Table 2. Showing the effect of altering the shell charge Y_k through the parameter N discussed in the text for GaAs at 295 K

The quantities listed are those of Table 1. For this table the sums were performed over only 1000 wavevectors in the Brillouin zone but the resulting loss of accuracy is not significant.

| | Y_k (−|e|) | | B_{ksc} (Å^2) | | $\Delta B_k(\mathbf{K} = 0)/B_{kc}$ (%) | |
N	Ga	As	Ga	As	Ga	As
0·5	0·78	1·87	−0·496	−0·541	−2·0	−4·4
1·0	1·56	3·74	−0·361	−0·417	−2·8	−6·9
2·0	3·13	7·47	−0·209	−0·245	−3·3	−8·0
3·0	4·69	11·21	−0·146	−0·172	−3·4	−8·5
5·0	7·82	18·68	−0·090	−0·107	−3·6	−8·7

studied were not the zinc-blende-structure compounds of interest here.

The variation of the shell Debye–Waller term with temperature is generally similar to that of the core term, resulting in quite a stable value for $\Delta B_k/B_{kc}$. The percentages shown in Table 1 vary typically by

between one half to one as the temperature is lowered, usually becoming more negative but not always so.

Other models

Pirie & Reid (1981) recently discussed how an extra parameter (N) could be introduced into any shell model to change the amount of charge in the shell and to redistribute the forces amongst the force constants. The notable feature about this extra parameter is that it does not alter the model frequencies or, indeed, the core eigenvectors. Increasing N from its implied value of 1·0 puts more charge into the shell and makes the ions more rigid. Reducing N towards zero weakens all the forces holding the shell and correspondingly reduces the shell charge. Hence the B_{ksc} values in Table 1 purely represent the shell models as traditionally parameterized ($N = 1$). As N is reduced from 1 towards 0, the relative shell–core displacements increase by a factor $1/N$. It happens for at least a sample of the materials examined that this at first reduces B_{ks} and hence increases B_{ksc}. However, as N approaches zero what is left of the shells flops around with very large amplitude and correspondingly large B_{ks}. All this happens without any change in the behaviour of the cores.

If the B value of the deforming electrons, represented by B_{ks}, is essentially observable then such an observation will determine N and hence provide insight into the relative strengths of shell–shell, shell–core and core–core forces. If, on the other hand, only ΔB_k is observable then this will provide a quantity independent of B_{kc} that is more of a check on the model as a whole. The difference arises because $Y_k B_{ksc}$ is not nearly so dependent on N, having a variation due only to the second-order term $|\mathscr{W}(k/\mathbf{q}j)|^2$ in B_{ksc}. Illustrative data are tabulated in Table 2. Therefore, although fitting a shell model to phonon frequencies in no way determines the motion of the shells, the dynamic deformation effect is moderately well predicted. The decrease with K of ΔB_k will depend somewhat on N if one interprets the model literally in that for large N more of the ion is associated with the shell and hence one would on the whole expect a slower decrease in the scattering factor f_{ks} with K.

Finally, to test a different set of models, the deformation-dipole models were investigated using the subroutines of Kunc & Nielsen (1979a) even though the parameterized deformable-bond approximation has been shown in I to be only moderately successful at predicting B_k values. For all materials except SiC a notional charge of 8 electrons was used to produce shell displacements $\mathscr{W}$ through (12), displacements that were sufficiently small to emphasize the linear terms in (11) for B_{ksc}. For SiC a charge of 2 was used. As has been seen, if the effects are modest then the actual shell charge does not much influence $\Delta B_k / B_{kc}$.

Table 3. *The deformable-dipole model predictions for the effect of dynamic deformation on the Debye–Waller factor of the whole atom as tabulated in Tables 1 and 2*

The model parameter sources are given in I. HgTe and SiC do not have corresponding shell models in Table 1. SiC shows an unusually large temperature dependence. The line marked (L) gives results at 1 K; that marked (H), results at 1000 K. All other materials were evaluated at 295 K and seldom show variations over temperature in the tabulated percentage of greater than one.

| | $\Delta B_k(\mathbf{K} = 0)/B_{kc}$ (%) | |
	Cation	Anion
GaP	−0·8	4·0
GaAs	−0·6	−4·2
InSb	1·0	3·3
ZnS	0·4	0·7
ZnSe	2·7	5·9
HgTe	−0·0	−2·1
CuI	−1·6	−1·5
SiC	8·5$^{(L)}$ / 0·7$^{(H)}$	−1·7$^{(L)}$ / −7·9$^{(H)}$

Table 3 shows values of $\Delta B_k / B_{kc}$ that are rather different from those of the shell models. Five ions always show equivalent shells with more vibration than the cores, giving a positive ΔB_k. This effect can be achieved in the shell model if one sets Pirie & Reid's parameter N as negative, which reverses the sign of the inter-ion core–shell force constants subscripted T and reverses the sign of the shell charge. These reversals affect both ions. Additional effects not seen in the table are that the anions of ZnS and HgTe and the cations of GaAs and InSb exhibit a linear term in (11) which changes sign at one temperature, though the actual ΔB_k changes sign at a different temperature due to the influence of the second-order term in $\mathscr{W}$. Some equivalent shell displacements are quite large, causing the second-order term to increase the effect substantially as the shell charge is made smaller. This occurs particularly for both ions in SiC and also for the anions of GaP, ZnS and ZnSe.

Since most of the ions under discussion have the bulk of their electron density as a fairly rigid core, it is clear that all the lattice dynamical evidence points to substantially different vibrations being associated with the outer levels of the electron distribution. The size of the effect predicted by the models is linked to the relative size of different forces that act on the ion, as has been detailed, but it is clear that the models that predict core Debye–Waller B values reasonably will all predict much smaller vibrations for the 'shell' electrons. If the ions are treated as a whole, the effective Debye–Waller B will differ from the core B value for low-index reflections at the highest level of accuracy (a few percent) for many or the ions discussed here.

concerning the interpretation of the very-high-frequency shell-model modes.

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Wavelength-Dependent Measurements of Extinction in an Extended-Face Crystal of Zinc Selenide

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Abstract

The effect of extinction on Bijvoet ratios is demonstrated. It is suggested that an observed anomaly in the wavelength dependence of ZnSe Bijvoet ratios is due to the Borrmann effect. It is shown that wavelength-dependent studies of extinction may be used to obtain extinction parameters from relative intensity measurements without resorting to a refined scale factor.

Introduction

The importance of the extinction problem derives from the common necessity of using available crystals which satisfy neither the perfection criteria of dynamical theory nor those of kinematic theory.

The most commonly used extinction theory is that first derived by Zachariasen (1967) from a set of transfer equations and later revised by Becker & Coppens (1974a,b). Various authors have discussed the shortcomings of Zachariasen's theory, the main criticisms being its kinematical nature and resulting inapplicability in the case of severe primary extinction (Werner, 1969; Lawrence, 1972), its neglect of the angle dependence of the effective path length through the crystal (Cooper & Rouse, 1970) and its failure in cases of severe extinction (Cooper & Rouse, 1970; Becker & Coppens, 1974a). Most tests of the validity of this theory known to us include a simultaneous refinement of the extinction parameter(s) and a scale factor (*e.g.* Zachariasen, 1968a; Cooper, Rouse & Fuess, 1973), notwithstanding the high correlation

usually observed between these parameters (Lander & Mueller, 1970; Stevens & Coppens, 1975).

The ZnSe specimen used in this study has the cubic zinc-blende structure. The noncentrosymmetric nature of this structure and the presence of anomalous dispersion effects results in the manifestation of non-zero Bijvoet ratios, which has been discussed by McIntyre, Moss & Barnea (1980) (hereafter referred to as MMB) and corresponds to a breakdown of Friedel's law (Friedel, 1913).

The work described in this paper arose from the observation that measurements of Bijvoet ratios may be significantly affected by extinction [see Ramaseshan & Abrahams (1975) for discussions on this subject and Cole & Stemple (1962) and Fukamachi, Hosoya & Okunuki (1976) regarding the intensity ratio of Friedel-pair reflections]. In attempting to estimate the effects of extinction upon the Bijvoet ratios at various wavelengths, we found that we could derive values of extinction parameters without resorting to refined scale factors. However, we encountered a distinct region between the K absorption edges of zinc and selenium in which the derivation of consistent parameters proved impossible. We suggest that the systematic inconsistency in this region is due to an enhanced contribution from the Borrmann effect (Borrmann, 1941; Zachariasen, 1968b,c).

The most common method of obtaining values of the conventional extinction parameters r and g (the mean radius of the perfect-crystal domains and the quantity in the isotropic Gaussian distribution law describing the misalignment of the domains, respectively) is to carry out least-squares refinements of data obtained at two different wavelengths (λ). In so doing one obtains two