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Debye–Waller Factor for Elemental Crystals

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Abstract

A simple model for the Debye-Waller factor is proposed which is based on the familiar high- and low-temperature expansions and allows one to determine this quantity at an arbitrary temperature with a typical accuracy of 2 to 3%. The coefficients in the model are determined from phonon density-of-states curves obtained from neutron inelastic-scattering measurements and are tabulated for 43 elements with the f.c.c., b.c.c., h.c.p. and diamond structures.

Introduction

The Debye-Waller factor, which describes the effect of the lattice vibrations on Bragg-peak intensities, is not accurately known - even for the commonest crystals - in spite of the fact that its importance in crystal-structure determinations has been appreciated since the beginning of X-ray crystallography. For example, in a recent compilation by Butt, Bashir, Willis & Heger (1988) of the best measured values of the Debye-Waller factor of 22 cubic elements at room temperature, the average estimated error is 7%, with many exceeding 10%. The reason is that other effects, most notably absorption, extinction and thermal diffuse scattering, also affect the measured Bragg-peak intensities and are often difficult to make adequate corrections for. On the other hand, an accurate *ab initio* calculation of the Debye-Waller factor is difficult, even when the force constants are known, because anharmonic effects must be taken properly into account.

There are many situations in which an approximate estimate of the Debye-Waller factor of a crystal is required. For example, initial estimates of the Debye-Waller factor are useful in crystal-structure determinations by X-ray or neutron diffraction. An approximate knowledge of the Debye-Waller factor is also required in planning neutron inelastic-scattering experiments or for a preliminary calibration in diffraction thermometry. For applications such as these, one normally uses the familiar Debye model. However, this model does not provide a good representation of the Debye-Waller factor over a wide range of temperatures; if the Debye temperature has been chosen to give a good fit at low temperatures then the model fails badly at high temperatures and *vice versa.*

During the past 30 years, accurate phonon densities of states have been determined for many crystals by neutron inelastic-scattering measurements. Within the quasi-harmonic approximation, these results allow one to obtain a much more reliable estimate of the Debye-Waller factor than is possible using the Debye model. The purpose of the present paper is to summarize these data in a form that will allow one to determine the Debye-Waller factor at an arbitrary temperature without the need for a lengthy numerical calculation.

In particular, we have devised a simple analytical model for the Debye-Waller factor which is based on the familiar high- and low-temperature expansions of this quantity. To the extent that the lattice vibrations are harmonic (or quasi-harmonic), the accuracy of the model is limited by the available data for the phonon density of states, which are used to determine the coefficients in the model, and is about 2 to 3%. These coefficients are tabulated for 43 elements with the f.c.c., b.c.c., h.c.p. and diamond structures.

The Debye–Waller factor

The Debye-Waller factor is denoted by $\exp(-2W)$ and the exponent is in general of the form $2W=(qu)^2$, where q is the wave-vector transfer and u the root-mean-square displacement of an atom perpendicular to the Bragg planes. Since $q=(4\pi/\lambda)\sin\theta$, where λ is the wavelength and θ the Bragg angle, the exponent can be expressed alternatively as

$$2W=2B[(\sin\theta)/\lambda]^2, \qquad (1)$$

in which $B=8\pi^2u^2$. In the harmonic (or quasi-harmonic) approximation, the exponent is given, alternatively, by the expression (*e.g.* Lovesey, 1984)

$$2W=\omega_r\int_0^\infty \coth(\hbar\omega/2kT)[g(\omega)/\omega]\,d\omega. \qquad (2)$$

Here, $\hbar\omega_r=(\hbar q)^2/2m$ is the recoil energy, in which m is the atomic mass, T is the temperature and $g(\omega)$ the phonon density of states which is normalized such that

$$\int_0^\infty g(\omega)\,d\omega=1. \qquad (3)$$

Strictly speaking, the quantity $g(\omega)$ in (2) depends not only on the phonon frequencies but also on the phonon polarization vectors and on the orientation of the reflecting planes relative to the crystallographic axes. It is only in the case of a cubic crystal with one atom per primitive unit cell (*i.e.* a f.c.c. or b.c.c. structure) that $g(\omega)\,d\omega$ is simply the fraction of normal modes with frequency in $d\omega$. Nevertheless, the interpretation of $g(\omega)$ as the phonon density of states may also be valid to an adequate approximation for crystals with the diamond structure, where the Debye-Waller factor is isotropic, or the ideal h.c.p. structure, where it is almost isotropic.

Reduced variables

It is convenient to introduce the dimensionless quantities

$$x=\omega/\omega_m, \qquad y=T/T_m, \tag{4}$$

where ω_m is the maximum phonon frequency and $kT_m=\hbar\omega_m$. Then

$$2W=(\omega_r/\omega_m)J(y), \tag{5}$$

in which

$$J(y)=\int_0^1 \coth(x/2y)[f(x)/x]\,dx. \tag{6}$$

Here, $f(x)=\omega_m g(\omega)$ is the reduced phonon density of states and

$$\int_0^1 f(x)\,dx=1. \tag{7}$$

The quantity B in (1) is then given by

$$B=(4\pi^2\hbar/m\omega_m)J(y). \tag{8}$$

Fig. 1 shows $f(x)$ for copper at room temperature obtained from the phonon density of states determined by Svensson, Brockhouse & Rowe (1967) from neutron inelastic-scattering measurements. The corresponding $J(y)$ is illustrated in Fig. 2. These figures also show the results for the conventional Debye model (James, 1965), where T_m is the Debye temperature and

$$f(x)=\begin{cases}3x^2 & 0\le x\le 1\\ 0 & 1<x<\infty.\end{cases} \tag{9}$$

Expansions and model

Expanding the coth term in (6), one obtains the following series expansion of $J(y)$ in inverse powers of y:

$$J(y)=2f_{-2}y+1/6y-f_2/360y^3+\dots, \tag{10}$$

in which

$$f_n=\int_0^1 x^n f(x)\,dx. \tag{11}$$

In (10) we have used the fact that $f_0=1$. For the Debye model, where $f_n=3/(n+3)$, the result obtained by truncating the above series expansion after the third term is shown by the dotted curve in Fig. 3 and compared with the exact result, which is represented by the solid curve.

For any three-dimensional crystal with short-range interatomic forces,

$$f(x)\rightarrow \alpha x^2 \quad \text{as } x\rightarrow 0. \tag{12}$$

For example, $\alpha=3$ for the Debye model (9). It then follows that $J(y)$ has the asymptotic behavior

$$J(y)\rightarrow f_{-1}+(\pi^2/3)\alpha y^2 \quad \text{as } y\rightarrow 0. \tag{13}$$

This result is illustrated for the Debye model by the dashed curve in Fig. 3.

None of the above results are essentially new. In particular, expansions equivalent to (10) and (13) have been known for many years (*e.g.* Barron, Leadbetter, Morrison & Salter, 1966). What is not widely appreciated, however, is the fact that the regions of applicability of these expansions overlap

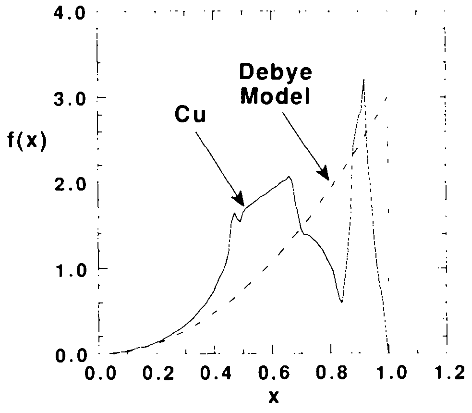

Fig. 1. Reduced phonon density of states for Cu at room temperature (Svensson *et al.*, 1967) and for the Debye model.

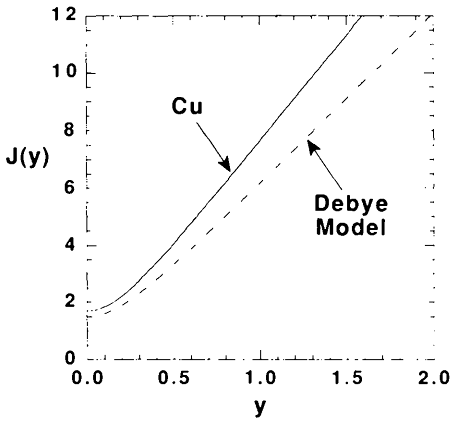

Fig. 2. Integral $J(y)$ calculated from (6) for Cu and the Debye model from the reduced phonon density-of-states curves shown in Fig. 1.

in the neighborhood of $y = 0{\cdot}2$ so that the model

$$J(y) = \begin{cases} f_{-1} + (\pi^2/3)\alpha y^2 & y < 0{\cdot}2 \\ 2f_{-2}y + 1/6y - f_2/360y^3 & y \geq 0{\cdot}2 \end{cases} \qquad (14)$$

provides a good approximation to $J(y)$ for all y. The validity of this statement for the Debye model is evident from Fig. 3. In the next section we show that it is true quite generally.

Analysis

We have calculated $J(y)$ by a numerical integration of (6), together with the coefficients in the approximate model (14), for all the elements in the Periodic Table with the f.c.c., b.c.c., h.c.p. or diamond structure for which published values of the phonon density of states, and hence $f(x)$, are available. In almost all cases, the phonon density of states had been constructed from the interatomic force constants obtained from phonon dispersion curves measured by coherent neutron inelastic scattering. The only exceptions are vanadium, for which $f(x)$ was obtained directly from incoherent neutron inelastic-scattering measurements, and xenon, for which $f(x)$ was obtained from a published theoretical calculation. Most of the data were taken at room temperature; the exceptions include cryogenic crystals (like Ne) and high-temperature phases (like f.c.c. Fe). The results are summarized in Table 1, together with the references for the $f(x)$ data. We also list the coefficients for the Debye model.

The phonon density of states of Cu at room temperature has been measured very precisely by two different groups - Svensson *et al.* (1967) and Nicklow, Gilat, Smith, Raubenheimer & Wilkinson (1967) - and the corresponding f_n values differ by 1 to 2%. The discrepancies between the values of f_n obtained by these authors and the values we have calculated from their published phonon density-of-states curves are typically 0·1 to 0·3%. Thus, it appears that the accuracy of the results in Table 1 is mostly limited by the original data and not by the accuracy with which we were able to extract the f_n values from the published results.

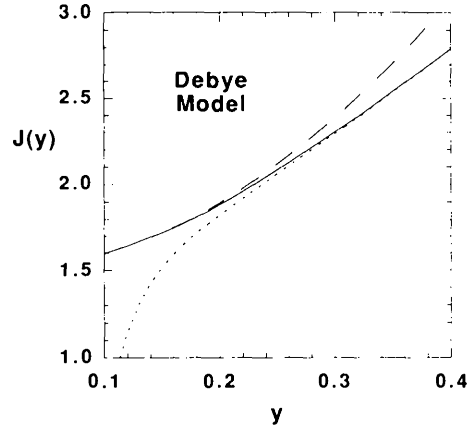

Fig. 3. Integral $J(y)$ for the Debye model. The solid curve shows the exact result calculated from (6), the dotted curve the first three terms in the series expansion (10) and the dashed curve the asymptotic expansion (13).

We have investigated the rate of convergence of the expansions (10) and (13) for all 46 elements and structures in Table 1. We find that if (10) is truncated beyond the third term, then the error is, on average, less than 0·2% if $y \geq 0{\cdot}3$, while the error in (13) is generally less than 0·4% if $y \leq 0{\cdot}1$. When $y = 0{\cdot}2$ the error in both (10) and (13) is typically 2%. Thus, the maximum error in the model expression (14) is evidently no worse than the accuracy of the available data for the coefficients themselves.

The boundary, $y = 0{\cdot}2$, in (14) is somewhat arbitrary and certainly not optimal. For example, it is evident from Fig. 3 that the value $y = 0{\cdot}24$ would be a better choice for the Debye model. However, for the elements we have studied, $y = 0{\cdot}2$ is a good overall compromise. One could, of course, treat the boundary as an additional parameter in the model, but there is little point in doing this. If the exact position of the boundary becomes an important consideration, one probably should not be using this kind of model in the first place.

The quantity B, as expressed by (8), is given in units of Å^2 by

$$B = (39{\cdot}904/M\nu_m)J(y), \qquad (15)$$

where $M = N_A m$ is the atomic weight in g mol^{-1} (N_A being Avogadro's number) and $\nu_m = \omega_m/2\pi$ is the maximum phonon frequency in THz. With ν_m in THz, T_m is given in units of K by $T_m = 47{\cdot}993\nu_m$. Table 2 shows a comparison of values of B at $T = 293$ K calculated from (14) and (15) with the corresponding experimental values compiled by Butt *et al.* (1988). The experimental values were obtained directly from diffraction measurements and have an estimated average error of 7%. The error in the calculated values is assumed to be 3%. The difference between the calculated and experimental values in Table 2 is, in most cases, less than twice the standard error of the difference.

Concluding remarks

Equations (14) and (15), together with the coefficients listed in Table 1, enable one to quickly estimate the Debye-Waller factor at an arbitrary temperature for any of the elements and structures in the table. The accuracy of the model is presently limited to at best 2 to 3% by the available data for the phonon density of states which were used to determine the coefficients.

Table 1. *Coefficients for the model Debye-Waller factor*

Element	Z	M (g mol^{-1})	Structure	ν_m (THz)	T_m (K)	α	f_{-2}	f_{-1}	f_2	Reference
He	2	4·0026	H.c.p.	1·74	83·5	18·476	11·285	2·837	0·219	(*a*)
			F.c.c.	4·00	192	5·318	4·595	1·853	0·435	(*b*)
Li	3	6·941	B.c.c.	9·07	435	8·677	5·552	1·909	0·492	(*c*)
Be	4	9·0122	H.c.p.	20·29	974	2·225	3·139	1·611	0·479	(*d*)
C	6	12·011	Diamond	40·09	1924	2·352	3·114	1·552	0·576	(*e*)
Ne	10	20·179	F.c.c.	1·69	81·1	3·184	3·569	1·676	0·479	(*f*)
Na	11	22·990	B.c.c.	3·84	184	5·386	4·558	1·800	0·494	(*g*)
Mg	12	24·305	H.c.p.	6·49	311	3·557	3·723	1·702	0·475	(*d*)
Al	13	26·982	F.c.c.	9·75	468	3·670	4·029	1·778	0·445	(*h*)
Si	14	28·086	Diamond	15·85	761	6·933	6·943	2·136	0·497	(*e*)
Ar	18	39·948	F.c.c.	2·03	97·4	3·300	3·603	1·675	0·490	(*i*)
K	19	39·098	B.c.c.	2·38	114	5·251	4·818	1·859	0·474	(*j*)
Ca	20	40·078	F.c.c.	4·71	226	3·914	3·568	1·625	0·539	(*k*)
			B.c.c.	4·97	239	7·917	5·220	1·885	0·470	(*l*)
Sc	21	44·956	H.c.p.	7·22	347	3·054	3·511	1·651	0·506	(*m*)
Ti	22	47·88	H.c.p.	8·74	419	2·766	3·772	1·743	0·453	(*n*)
V	23	50·942	B.c.c.	8·10	389	5·424	3·845	1·655	0·506	(*o*)
Cr	24	51·996	B.c.c.	9·71	466	1·502	2·443	1·428	0·594	(*p*)
Fe	26	55·847	B.c.c.	9·54	458	3·079	3·310	1·602	0·522	(*q*)
			F.c.c.	7·43	357	3·585	3·453	1·608	0·543	(*r*)
Ni	28	58·69	F.c.c.	8·97	430	2·639	3·364	1·642	0·491	(*s*)
Cu	29	63·546	F.c.c.	7·29	350	3·681	3·737	1·699	0·479	(*t*)
Zn	30	65·39	H.c.p.	6·29	302	4·060	5·991	2·147	0·381	(*d*)
Ge	32	72·59	Diamond	9·20	442	4·518	7·495	2·245	0·476	(*e*)
Kr	36	83·80	F.c.c.	1·50	72·0	3·743	3·673	1·685	0·485	(*u*)
Rb	37	85·468	B.c.c.	1·51	72·5	7·054	5·304	1·911	0·468	(*v*)
Sr	38	87·62	B.c.c.	2·69	129	6·581	4·877	1·833	0·495	(*w*)
Y	39	88·906	H.c.p.	4·76	228	2·394	3·454	1·661	0·503	(*x*)
Zr	40	91·224	H.c.p.	6·29	302	3·485	4·136	1·803	0·440	(*y*)
Nb	41	92·906	B.c.c.	6·50	312	3·668	3·544	1·637	0·511	(*z*)
Mo	42	95·94	B.c.c.	7·96	382	1·841	2·607	1·461	0·578	(*aa*)
Pd	46	106·42	F.c.c.	6·88	330	5·556	4·526	1·828	0·439	(*bb*)
Ag	47	107·87	F.c.c.	5·09	244	4·488	4·131	1·769	0·458	(*cc*)
Sn	50	118·71	Diamond	6·07	291	5·199	10·087	2·480	0·499	(*dd*)
Xe	54	131·29	F.c.c.	1·32	63·4	4·618	4·136	1·771	0·450	(*ee*)
Cs	55	132·91	B.c.c.	1·09	52·3	8·845	5·835	1·980	0·446	(*ff*)
Ba	56	137·33	B.c.c.	2·28	109	4·653	4·429	1·809	0·471	(*gg*)
La	57	138·91	F.c.c.	2·57	123	2·833	3·427	1·635	0·520	(*hh*)
Tb	65	158·93	H.c.p.	3·28	157	3·043	3·470	1·647	0·502	(*ii*)
Ho	67	164·93	H.c.p.	3·44	165	2·244	3·291	1·637	0·492	(*jj*)
Ta	73	180·95	B.c.c.	5·12	246	2·324	3·061	1·573	0·514	(*kk*)
W	74	183·85	B.c.c.	6·74	323	1·872	2·652	1·483	0·551	(*ll*)
Pt	78	195·08	F.c.c.	5·15	247	4·227	3·874	1·705	0·490	(*mm*)
Au	79	196·97	F.c.c.	4·69	225	7·453	5·439	1·982	0·405	(*cc*)
Pb	82	207·2	F.c.c.	2·22	107	4·357	4·439	1·836	0·456	(*nn*)
Th	90	232·04	F.c.c.	3·51	168	3·641	4·205	1·816	0·439	(*oo*)
Debye						3·000	3·000	1·500	0·600	

References: (*a*) Reese, Sinha, Brun & Tilford (1971); (*b*) Eckert, Thomlinson & Shirane (1977); (*c*) Smith, Dolling, Nicklow, Vijayaraghavan & Wilkinson (1968); (*d*) Young & Koppel (1964); (*e*) Dolling & Cowley (1966); (*f*) Skalyo, Minkiewicz, Shirane & Daniels (1972); (*g*) Gilat & Dolling (1964); (*h*) Gilat & Nicklow (1966); (*i*) Fujii, Lurie, Pynn & Shirane (1974); (*j*) Cowley, Woods & Dolling (1966); (*k*) Stassis, Zarestky, Misemer, Skriver, Harmon & Nicklow (1983); (*l*) Heiroth, Buchenau, Schober & Evers (1986); (*m*) Wakabayashi, Sinha & Spedding (1971); (*n*) Stassis, Arch, Harmon & Wakabayashi (1979); (*o*) Page (1967); (*p*) Shaw & Muhlestein (1971); (*q*) Minkiewicz, Shirane & Nathans (1967); (*r*) Zaretsky & Stassis (1987); (*s*) Birgeneau, Cordes, Dolling & Woods (1964); (*t*) Svensson, Brockhouse & Rowe (1967); (*u*) Skalyo, Endoh & Shirane (1974); (*v*) Copley & Brockhouse (1973); (*w*) Mizuki & Stassis (1985); (*x*) Sinha, Brun, Muhlestein & Sakurai (1970); (*y*) Stassis, Zarestky, Arch, McMasters & Harmon (1978); (*z*) Sharp (1969); (*aa*) Powell, Martel & Woods (1977); (*bb*) Miiller & Brockhouse (1971); (*cc*) Lynn, Smith & Nicklow (1973); (*dd*)Price & Rowe (1969); (*ee*) Gupta & Gupta (1969); (*ff*) Nücker & Buchenau (1985); (*gg*) Mizuki, Chen, Ho & Stassis (1985); (*hh*) Stassis, Loong & Zarestky (1982); (*ii*) Houmann & Nicklow (1970); (*jj*) Nicklow, Wakabayashi & Vijayaraghavan (1971); (*kk*) Woods (1964); (*ll*) Higuera, Brotzen, Smith & Wakabayashi (1985); (*mm*) Ohrlich & Drexel (1968); (*nn*) Stedman, Almqvist & Nilsson (1967); (*oo*) Reese, Sinha & Peterson (1973).

The accuracy is also limited by the assumption that anharmonic effects are negligible. The formal theory of the effect of anharmonic interactions on the Debye-Waller factor has been developed by a number of authors (*e.g.* Maradudin & Flinn, 1963; Cowley, 1963; Kashiwase, 1965; Wolfe & Goodman, 1969; Willis, 1969). In the harmonic approximation at high temperature $2W$ is proportional to q^2T, while the leading anharmonic correction is found to be proportional to q^2T^2, so that anharmonic effects can be expected to become important at sufficiently high temperature. There is also a term proportional to q^4T^3, but this term is almost always negligible. In practice, the information necessary to implement the theory for any particular crystal is often not available but, when it is, large-scale computer calculations are required.

One effect of the anharmonic interactions is thermal expansion, which produces a change in the effective force constants, and hence in the phonon frequencies, so that $g(\omega)$ becomes temperature dependent. This

Table 2. *Comparison of values of B at $T = 293$ K calculated from* (14) *and* (15) *with the corresponding experimental values compiled by Butt et al.* (1988); *B is in units of* Å^2

Element	Structure	B (calc.)	B (exp.)
Li	B.c.c.	4·9 (1)	4·1 (6)
Na	B.c.c.	6·6 (2)	7·9 (2)
Al	F.c.c.	0·81 (2)	0·86 (1)
Si	Diamond	0·52 (2)	0·45 (1)
K	B.c.c.	10·7 (3)	12 (2)
V	B.c.c.	0·58 (2)	0·55 (3)
Cr	B.c.c.	0·263 (8)	0·26 (1)
Fe	B.c.c.	0·34 (1)	0·35 (1)
Ni	F.c.c.	0·34 (1)	0·37 (1)
Cu	F.c.c.	0·56 (2)	0·57 (1)
Ge	Diamond	0·61 (2)	0·57 (1)
Nb	B.c.c.	0·45 (1)	0·49 (2)
Mo	B.c.c.	0·220 (7)	0·25 (2)
Pd	F.c.c.	0·45 (1)	0·45 (6)
Ag	F.c.c.	0·73 (2)	0·79 (2)
Ta	B.c.c.	0·32 (1)	0·32 (1)
W	B.c.c.	0·161 (5)	0·18 (1)
Pt	F.c.c.	0·37 (1)	0·32 (2)
Au	F.c.c.	0·62 (2)	0·57 (4)
Pb	F.c.c.	2·11 (6)	2·42 (7)

effect contributes to part of the q^2T^2 term mentioned above and can be seen in the work of Nicklow *et al.* (1967) who determined the phonon density of states for copper at 49 and 298 K. We find from their results that f_{-2} changes by almost 3% over this temperature range while f_{-1} and f_2 change by about 1%. This suggests that the error in the present model may be more like 3 to 5% when it is applied at a temperature much different from the one at which $g(\omega)$ was measured.

In metals, the anharmonic contribution to the Debye–Waller factor remains at the few-percent level until the temperature exceeds about half the melting point (*e.g.* Pathak & Shah, 1979). Near the melting point the measured anharmonic shift in B is typically 25% but, even here, the present model may continue to be useful if a rough estimate of the Debye–Waller factor is all that is needed.

Finally, it is unlikely that the discrepancies between the directly measured values of B in Table 2 and those calculated from the present model are primarily due to anharmonic effects because the discrepancies appear to be largely random in both magnitude and sign. Furthermore, one would not expect anharmonic effects to be large here because, in most cases, $g(\omega)$ and the measured values of B were both determined from room-temperature experiments and this temperature is well below the melting point of most of the elements in Table 2. One notable exception is Na, for which $g(\omega)$ was determined at 90 K while the temperature, 293 K, at which B was measured is very near the melting point, 371 K. In this case, the large 20% discrepancy may well arise mainly from anharmonic effects.

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SHORT COMMUNICATIONS

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Microabsorption of X-rays and its dependence on the shape of scattering particles.

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Abstract

The absorption of X-rays scattered by isotropic random multiphase materials is shown theoretically to depend not only on volume fraction, linear absorption coefficient and mean particle size of each phase but also on the shape of the scattering particles. The absorption effect is remarkably enhanced with increasing polydispersity and irregularity of the scattering phase.

In the present note we consider the absorption of X-rays in heterogeneous materials and its dependence on the shape of the scattering particles. The specimen is supposed to be planar and to consist of n crystalline phases. The particles of each phase $i\,(i=1,\ldots,n)$ should be randomly distributed. The intensity I_i of the X-ray beam scattered by phase i is mainly determined by the volume fraction c_i of the scattering particles. However, interaction processes such as the generation of photoelectrons by the X-rays attenuate the intensity of the beam. In a homogeneous single-phase material, this attenuation is described by the linear absorption coefficient μ_i of the corresponding phase. The situation is more complicated in heterogeneous materials. In general, the beam penetrates not only the scattering phase i but also regions filled with particles of the other phases. If all particles are very small compared with the penetration depth of the X-rays, the beam will pass through many regions of all phases. Then the path length through particles of the scattering phase is given by the geometrical path length of the beam in the whole sample multiplied by the volume fraction of the scattering particles. Considering a series of samples of the same composition but with increasing particle size, the length of the path of the beam through the scattering phase exceeds the above-mentioned value more and more, and in the limit of very large particles the whole path of the beam through the sample is within a single scattering particle at the surface of the sample. With the supposition that the linear absorption coefficients μ_i, $i=1,\ldots,n$, are different, it is obvious that the strength of the absorption effect varies with the size of scattering particles (Brindley, 1945; Suortti, 1972). The present calculation will show that the absorption effect depends also on the shape of scattering particles.

The intensity I_i of a symmetrically diffracted beam is

$$I_i/I_{0,i}=\int_V \exp\left[-\mu_i x_i-\mu_{(i)}x_{(i)}\right]\mathrm{d}V/Q_0. \qquad (1)$$

The scattering phase is denoted by i, x_i is the path length of a ray through particles of phase i and $x_{(i)}$ is the path length through the regions of the (planar) sample that do not belong to phase i. μ_i is the linear absorption coefficient of phase i and

$$\mu_{(i)}=(1-c_i)^{-1}\sum_{j\neq i}c_j\mu_j \qquad (2)$$

describes the mean value of the absorption coefficient for all regions of the sample outside phase i. $I_{0,i}/2\mu_i$ is the intensity of an i-type single-phase reference specimen ($c_i=1$) obtained under the same experimental conditions as the scattering intensity I_i of the multiphase sample (external standard method). Q_0 is the cross-section area of the

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