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SHORT COMMUNICATIONS

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

By H. HERMANN, *Central Institute of Solid State Physics and Materials Research, Dresden, Helmholtzstrasse* 20, *O*-8027 *Dresden, Germany*, and K. RÖSKE and M. HENTSCHEL, *Martin Anderson Nexö College Dresden, Kretschmarstrasse* 27, *O*-8053 *Dresden, Germany*

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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 $i\,(i=1,\dots,n)$ 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, $i=1,\dots,n$, 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 incident beam, V is the volume of the sample and c_i the volume fraction of phase i. Multiple scattering is neglected in (1). For homogeneous materials ($\mu = \mu_1$, $c_1 = 1$),

$$I/I_0 = 1/2\mu \qquad (3)$$

is valid.

The absorption in heterogeneous multiphase substances may be described by an effective absorption coefficient μ'_i that is valid for a beam scattered from particles of phase i.

$$I_i/I_{0,i} = 1/2\mu'_i. \qquad (4)$$

Characterizing the size of i-type particles by the mean chord length $\bar{l}_i$, one can solve (1) exactly for the following limiting cases.

(i) Very small particles ($\mu_i \bar{l}_i \ll 0.1$):

$$I_i/I_{0,i} = 1/2\bar{\mu}, \quad \bar{\mu} = \sum_k c_k \mu_k. \qquad (5)$$

(ii) Very large particles ($\mu_i \bar{l}_i \gg 1$):

$$I_i/I_{0,i} = 1/2\mu_i. \qquad (6)$$

The deviation of the absorption effect from these limiting cases is called 'microabsorption'. Brindley (1945) pointed out that besides the size of scattering particles the absorption contrast ($\mu_i - \bar{\mu}$) should play a decisive role. Suortti (1972) investigated porous single-phase substances and proved experimentally the effective linear absorption coefficient μ' to be a function of mean chord length $\bar{l}$ and volume fraction c. He also gave evidence for the influence of the surface roughness of the samples on μ'.

Here we start with a stochastic germ-grain model and use it to describe the bulk structure of the scattering regions (phase i). The model is constructed in two steps. In the first step a random (Poisson) point field is generated and in the second one grains are placed on each germ whereby the grains may overlap. For details see Stoyan, Kendall & Mecke (1987). In recent papers we applied this model to solve (1) using Poisson polyhedra as grains for porous (Hermann & Ermrich, 1987) and multiphase (Hermann & Ermrich, 1989*a*, *b*) materials. In the latter case we obtained for $c_i \ll 1$, $\mu_i \bar{l}_i \ll 1$ the expression

$$\mu'_i = \bar{\mu}/[1 - 2(1 - c_i)(\mu_i - \bar{\mu})\bar{l}_i]. \qquad (7)$$

Now we consider equally sized spheres as primary grains which represent a good contrast to a set of randomly shaped Poisson polyhedra. [The random polyhedra are produced by means of a tessellation of the space by random planes. The mean value b of the breadth or the mean chord length $\bar{l}$ characterizes the particle size. For a Boolean structure composed by Poisson polyhedra we have $\bar{l}_i = b_i/(1 - c_i)$ in the limit of low volume fraction $c_i \ll 1$, and $\bar{l}_i = 4r_i/3(1 - c_i)$ for spheres with radius r_i as grains (Stoyan *et al.*, 1987).]

As was shown by Hermann & Ermrich (1989*a*), the mean value L_i of the path x_i through phase i for fixed scattering angle θ and depth of the scattering region parallel to the surface can be used to evaluate (1):

$$L_i = 2 \int_0^{L/2} C_{ii}(r)/c_i \, \mathrm{d}r. \qquad (8)$$

L is the geometrical length of the beam through the sample and $C_{ii}(r)$ is the probability of finding two arbitrary points with distance r both lying in an i-type region. For spheres, the correlation function is (Stoyan *et al.*, 1987)

$$C_{ii}(r) = \begin{cases} 2c_i - 1 + (1 - c_i) & \\ \quad \times \exp\{-[\ln(1 - c_i)][r^3/16r_i^3 - 3r/4r_i]\}, & r \le 2r_i \\ c_i^2, & r > 2r_i \end{cases} \qquad (9)$$

and the corresponding expression for Poisson polyhedra is

$$C_{ii}(r) = p_i^2 + p_i(1 - p_i)\exp(-r/b_i). \qquad (10)$$

The correlation functions (9), (10) are used to calculate the mean values L_i of the path x_i of the beam through phase i by means of (8). Then (1) is evaluated replacing x_i by L_i and $x_{(i)}$ by $L - L_i$. For $c_i \ll 1$ and $|\mu_i - \bar{\mu}|\bar{l}_i \ll 1$, the result is easy to calculate and we obtain

$$I_i/I_{0,i} = (c_i/2\bar{\mu})[1 - k(1 - c_i)(\mu_i - \bar{\mu})\bar{l}_i] \qquad (11)$$

with

$$k = \begin{cases} 9/8 & \text{for spheres} \\ 2 & \text{for Poisson polyhedra.} \end{cases}$$

Expression (11) shows that the intensity of an X-ray beam reflected symmetrically by a planar sample does not only depend on the absorption contrast ($\mu_i - \bar{\mu}$) and the mean chord length $\bar{l}_i$ but also on the shape of the scattering particles. Because of the restriction $c_i \ll 1$, within the random set produced by the Boolean model only few overlaps of grains appear. Therefore, the shape of the scattering regions of the present structure model is similar to that of the grains used for the construction of the random set, and we may conclude from (11) that the absorption caused by a random arrangement is remarkably enhanced with increasing polydispersity and irregularity of the particles.

The present results can be used to carry out a refined absorption correction of scattering data which is of interest in quantitative phase analysis.

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