SHORT COMMUNICATIONS

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An exact analytical expression for the primary extinction factor for a perfect spherical crystal in the limit $\theta_{oh} \to \pi/2$

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Abstract

Based on the boundary-value Green-function technique, an analytical expression for the primary extinction factor for a perfect non-absorbing spherical crystal has been found in the Bragg limit, $\theta_{oh} \to \pi/2$. The asymptotic behaviour is also outlined.

1. Introduction

In a previous paper (Thorkildsen & Larsen, 1998), hereafter denoted TL, we have shown how to obtain solutions for the Takagi–Taupin equations (Takagi, 1962, 1969; Taupin, 1964) by a series-expansion approach utilizing boundary-value Green functions. The primary extinction factor, y_p, for a perfect spherical crystal was found and its angular dependence discussed. For the pure Laue transmission case, $\theta_{oh} \to 0$, using the calculated terms up to fifth order:

$$y_p(x, \theta_{oh} \to 0) = 1 - (4/5)x^2 + (12/35)x^4 - (16/189)x^6 + (4/297)x^8 - (16/10\,725)x^{10} + \ldots,$$

it was shown that y_p may be given analytically as a hypergeometric function†

$$y_p(x, \theta_{oh} \to 0) = {}_1F_2[\tfrac{1}{2}; 1, \tfrac{5}{2}; -4x^2], \qquad (1)$$

where θ_{oh} is the Bragg angle and $x = R/\Lambda_{oh}$. R is the radius of the sphere and $\Lambda_{oh} = V_c/[r_e\lambda C(F_h F_{\bar{h}})^{1/2}]$ denotes the extinction length. The other symbols have their standard interpretation: V_c is the volume of the unit cell, r_e the classical electron radius, λ the wavelength of the incident radiation, C the polarization factor and F_h the structure factor associated with the reflection h.

It is interesting to note that this functional form is similar to the primary extinction factor expression for Laue transmission through a perfect semi-infinite crystal plate of thickness t (Zachariasen, 1945):

$$y_p^{(\text{plate,Laue})}(x_p, \theta_{oh} \to 0) = (1/x_p)\sum_{n=0}^{\infty} J_{2n+1}(2x_p) \equiv {}_1F_2[\tfrac{1}{2}; 1, \tfrac{3}{2}; -x_p^2],$$

where $x_p = t/\Lambda_{oh}$ and J is the Bessel function.

It is of importance to obtain an exact analytical expression for y_p in the Bragg limit, $\theta_{oh} \to \pi/2$, *e.g.* in order to establish reference points for evaluating and assessing more approximative approaches (Sabine, 1988, 1995). In this short contribution, we report the finding of such an expression.

† For a general definition of the hypergeometric function consult for instance Gradshteyn & Ryzhik (1980).

2. y_p in the Bragg limit

In TL, it was shown that the primary extinction factor for a perfect sphere is given by

$$y_p = \sum_{n=0}^{\infty}(-1)^n f_n^{(s)}(\theta_{oh})(x/\sin 2\theta_{oh})^{2n}. \qquad (2)$$

Here, $f_n^{(s)}$ denotes the series-expansion coefficient for the scattering order n in the θ_{oh} interval s.

Owing to the asymptotic properties of these coefficients, we were able to calculate the terms in the expansion up to $n = 5$ in the limit $\theta_{oh} \to \pi/2$:

$$y_p(x, \theta_{oh} \to \pi/2) = 1 - (4/5)x^2 + (32/35)x^4 - (1088/945)x^6 + (15\,872/10\,395)x^8 - (1\,415\,168/675\,675)x^{10} + \ldots.$$

By comparing these six terms with the result for a perfect semi-infinite plate (Darwin, 1922; Zachariasen, 1945), expressed as a series expansion in x_p,

$$y_p^{(\text{plate,Bragg})}(x_p, \theta_{oh} \to \pi/2) = (\tanh x_p)/x_p = \sum_{n=0}^{\infty}[2^{2(n+1)}(2^{2(n+1)} - 1)/(2n+2)!]B_{2n+2}x_p^{2n}, \qquad (3)$$

we obtain the following generalization:

$$y_p(x, \theta_{oh} \to \pi/2) = \sum_{n=0}^{\infty} \frac{3 \times 4^n\, 2^{2(n+1)}(2^{2(n+1)} - 1)}{(2n+2)!(2n+3)} B_{2n+2}x^{2n}. \qquad (4)$$

B_{2n} are the Bernoulli numbers, defined according to

$$B_{2n} = (-1)^{n-1}[2 \times (2n)!/(2\pi)^{2n}]\sum_{k=1}^{\infty}(1/k^{2n}). \qquad (5)$$

The above series solution for the primary extinction factor, equation (4), is convergent for $0 \leq x < \pi/4$. The following sum of well defined functions represents its analytic continuation (Lewin, 1981; Titchmarsh, 1985) and is valid for all $x \geq 0$:

$$y_p(x, \theta_{oh} \to \pi/2) = (3/4x^3)\{x^2 + x\ln[1 + \exp(-4x)] - \tfrac{1}{4}\mathrm{Li}_2[1 + \exp(-4x)] - (\pi^2/48)\}, \qquad (6)$$

where Li_2 is the dilogarithm function (Abramowitz & Stegun, 1965), defined as the integral $\mathrm{Li}_2(z) = -\int_1^z \mathrm{d}t\, \ln t/(t-1)$. Equation (6) has been obtained by means of *Mathematica* (Wolfram, 1991).†

† The *Mathematica* representation of the dilogarithm function is `PolyLog[2, 1 - z]` $\equiv \mathrm{Li}_2(z)$.

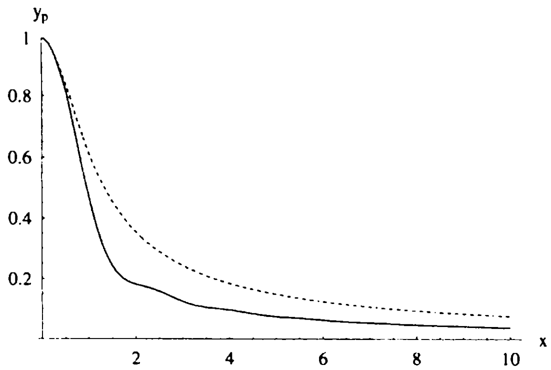

Fig. 1. The primary extinction factor as a function of the expansion parameter $x = R/\Lambda_{oh}$. Solid line: Laue limit $\theta_{oh} \to 0$; dashed line: Bragg limit $\theta_{oh} \to \pi/2$.

3. Conclusions

An analytical expression for y_p in the Bragg limit for a perfect non-absorbing spherical crystal is derived. The result, presented in equation (6), is useful for calculating primary extinction factors for all values of x. In Fig. 1, we have compared the Laue and Bragg limits, *i.e.* equations (1) and (6).

For $x > 2$, the asymptotic expansions, valid within an absolute error of less than 10^{-4}, are:

$$y_p(x, \theta_{oh} \to \pi/2) \sim (3/4x)(1 - \pi^2/48x^2) \quad (7)$$

for the Bragg case; and

$$y_p(x, \theta_{oh} \to 0) \sim (3/8x)\{1 - [\pi/(2\pi x)^{3/2}]\cos(4x - 5\pi/4) + 1/16x^2\} \quad (8)$$

for the Laue case.

Equation (8) is obtained using a procedure given by Luke (1969).

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