Acta Cryst. (1976). A**32**, 299

Bragg Diffraction from Curved Surfaces*

BY J. S. DESJARDINS

Department of Physics, University of Rhode Island, Kingston, Rhode Island, U.S.A.

(*Received* 10 *July* 1975; *accepted* 9 *September* 1975)

Hamilton's equations for secondary extinction are considered in the light of Riemann's integration of the hyperbolic differential equation. It is shown that Green's function for diffraction from a crystal in the Bragg geometry is determined by an integral equation. The equation is valid for an arbitrarily shaped crystal boundary curve as long as the boundary does not become tangent to the incident or diffracted beam directions.

Introduction

Werner & Arrott (1965), and later Werner, Arrott, King & Kendrick (1966) have considered the propagation of Bragg diffracted neutrons in mosaic crystals bounded by plane surfaces. The starting point of these calculations is the coupled differential equations of Hamilton (1957) which, in turn, are generalizations of the one-dimensional equations describing secondary extinction in a uniformly illuminated infinite slab (Zachariasen, 1945; Bacon & Lowde, 1948). In their first paper, Werner & Arrott reformulated Hamilton's equations in integral form and calculated the forward and diffracted currents under a large slab with a plane boundary for an incident neutron beam of infinitesimal width by explicit consideration of the multiple scattering formulation of the theory. The re-emerging diffracted current density along the surface constitutes a Green function for this geometry.

* This work was supported by the U. S. Atomic Energy Commission.

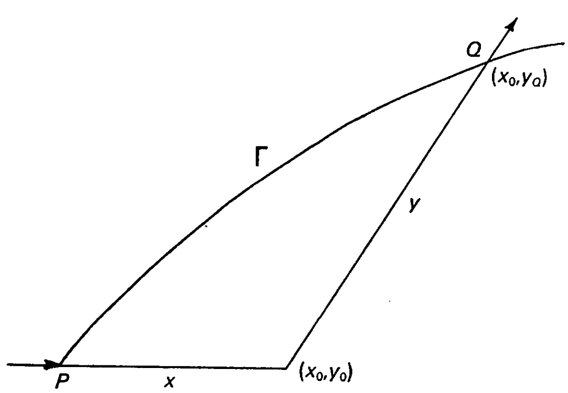

Fig. 1. Geometry for the Bragg Green function. A neutron is incident at point P on the crystal surface bounded by the curve Γ. We are considering the response arising from this unit source as the diffracted current emerging from the surface (in the y direction) at some other point on the surface (x_0, y_Q).

The purpose of this paper is to show that even though an explicit expression for the Bragg Green function is no longer available when the surface becomes of arbitrary shape, this function is still determined through an integral equation for a class of arbitrarily shaped surfaces.

Green's function for the Bragg case

The problem we wish to solve is illustrated in Fig. 1. A neutron beam of singularity is incident at point P and we wish to determine the diffracted current density, $U_d(x,y)$, that re-emerges at the point Q located on the boundary curve Γ. The coordinates of the point Q on the crystal surface are (x_0, y_Q) in a non-orthogonal (Bragg) coordinate system. x and y are taken along the incident and diffracted current directions respectively. Hamilton's equations for the forward and diffracted neutron current densities U_i and U_d are

$$\begin{aligned} \frac{\partial U_i}{\partial x} &= -(\beta+\mu)U_i+\beta U_d \\ \frac{\partial U_d}{\partial y} &= -(\beta+\mu)U_d+\beta U_i \end{aligned} \tag{1}$$

where β is the reciprocal mean free path for Bragg scattering, while μ is the reciprocal mean free path for all other processes that can occur which cause neutrons to become unavailable for further Bragg scattering. If we set

$$U_i = \exp\left[-(\beta+\mu)\,(x+y)\right]u_i(x,y)$$

and

$$U_d = \exp\left[-(\beta+\mu)\,(x+y)\right]u_d(x,y)$$

and substitute in equation (1) we obtain

$$\frac{\partial u_i}{\partial x} = \beta u_d$$

and

$$\frac{\partial u_d}{\partial y} = \beta u_i \,.$$

We will refer to u_i and u_d as the reduced current densities.

Both u_i and u_d satisfy the equation

$$\frac{\partial^2 u}{\partial x \partial y} = \beta^2 u \,. \tag{2}$$

Equation (2) is a hyperbolic, self-adjoint equation in normal form. Characteristic curves for this equation in the xy plane are the lines x=constant or y=constant.

Riemann's integration of the hyperbolic equation is treated by Sommerfeld (1964) and may be summarized for the particular case of equation (2) with the help of Fig. 2. Note that the following general considerations regarding the integration of equation (2) take place in an abstract two-dimensional xy space within which x and y are plotted along *orthogonal* axes as shown in Fig. 2. We assume that u, $\partial u/\partial x$, and $\partial u/\partial y$ are given on the curve Γ, which does not become tangent to a characteristic. Then, with the help of the characteristic function $v(x,y)$, defined below, the value of u at some point R off the curve Γ is shown by Sommerfeld to be given by the expression

$$u_R = \int_\Gamma \{X \cos(n,x) + Y \cos(n,y)\} \mathrm{d}s + \tfrac{1}{2}\{(vu)_P + (vu)_Q\} \tag{3}$$

where, in the particular case of equation (2)

$$X = \tfrac{1}{2}\left(v\frac{\partial u}{\partial y} - u\frac{\partial v}{\partial y}\right)$$

$$Y = \tfrac{1}{2}\left(v\frac{\partial u}{\partial x} - u\frac{\partial v}{\partial x}\right) .$$

The characteristic function $v(x,y)$ has the following properties:

1. v satisfies (2) in the region S.
2. $v=1$ at the point R with coordinates x_0, y_0.
3. $\partial v/\partial y = 0$ on the characteristic $x=x_0$.
4. $\partial v/\partial x = 0$ on the characteristic $y=y_0$.

In equation (3), the integration along the curve Γ is in the sense from Q down to P, while n is the outward normal from the region S in Fig. 2. From the modified Bessel function solution to (2) given by Werner, Arrott, King & Kendrick (1966), it is not difficult to verify that the characteristic function appropriate in the case of equation (2) is

$$v(x,y) = I_0[2\beta\sqrt{(x-x_0)(y-y_0)}] \,.$$

We note, however, since $x \le x_0$, $y \ge y_0$ in S, that the argument of the modified Bessel function is imaginary so that $v(x,y)$ should be rewritten as

$$v(x,y) = J_0[2\beta\sqrt{(x_0-x)(y-y_0)}] \,. \tag{4}$$

That is, the modified Bessel function solution turns over into an ordinary Bessel function for the case at hand. To find the neutron Green function, we will choose u in equation (3) to be u_i. The reduced current density u_i generated by the incident-beam singularity at point P has the value zero at point P. This is because the incident-beam singularity moving along the x direction does not contribute directly to the reduced current densities u_i and u_d within the material. Hence, we can take $u_i=0$ everywhere on the curve Γ so that Riemann's solution (3) is simplified to

$$u_i(x_0,0) = \int_\Gamma \{X \cos(n,x) + Y \cos(n,y)\} \mathrm{d}s$$

where we have set the y coordinate of the point R in Figs. 1 and 2 equal to zero without loss in generality. From $u_i=0$ on Γ we have

$$\frac{\partial u_i}{\partial y} = -\frac{\partial u_i}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}y}$$

along Γ. Furthermore, $\partial u_i/\partial x = \beta u_d$, so that (3) reduces further to

$$u_i(x_0,0) = \beta \int_0^{x_0} v u_d \mathrm{d}x \tag{5}$$

where v and u_d are considered as functions of x alone along the crystal boundary curve Γ, which we imagine given by $y=f(x)$. We can make an independent evaluation of $u_i(x_0,0)$ by noting that along the incident direction, U_i must satisfy the equation

$$\frac{\mathrm{d}U_i}{\mathrm{d}x} = -(\beta+\mu)U_i + \beta^2 \exp[-(\beta+\mu)x]$$

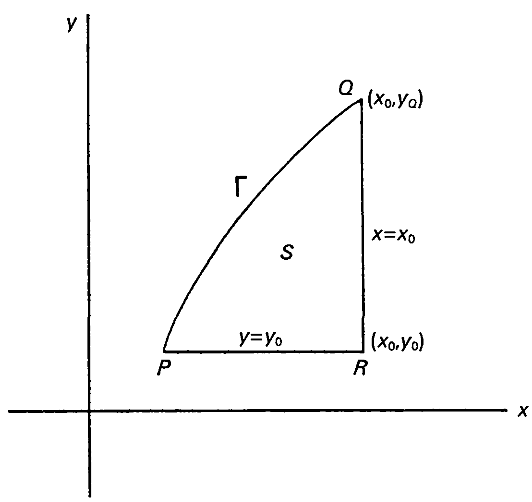

Fig. 2. General diagram for a hyperbolic boundary value problem of the first kind (Sommerfeld, 1964). $u, \partial u/\partial x, \partial u/\partial y$ are given on the curve Γ while u satisfies the equation $\partial^2 u/(\partial x \partial y) = \beta^2 u$ for the case considered here. Riemann's integration gives the value of u at the point R with the aid of the characteristic function $v(x,y)$.

with $U_i(0,0)=0$. The first term in this equation is obvious, while the second term is produced by the incident current singularity. This singularity, which is itself distinct from the current densities determined by Hamilton's equations, nevertheless contributes to the derivative of the forward current density along the x axis a term $\beta^2 \exp[-(\beta+\mu)x]$ due to twice-scattered neutrons whose second scattering occurs within the immediate neighborhood of the x axis. The solution for $U_i(x,0)$ is therefore

$$U_i(x,0)=\beta^2 x \exp[-(\beta+\mu)x],$$

so that $u_i(x_0,0)=\beta^2 x_0$. Substituting this result into (5) we obtain the following relationship which involves the unknown diffracted reduced current density u_d

$$\beta x_0=\int_0^{x_0} v u_d \mathrm{d}x \,. \tag{6}$$

If we now take the derivative of both sides of (6) with respect to x_0, keeping in mind the form of $v(x,y)$ from equation (4), we obtain the following Volterra equation for the reduced neutron current density at point (x_0,y_Q) on the surface Γ:

$$u_d(x_0)=\beta+\beta\int_0^{x_0} K(x,x_0)u_d(x)\mathrm{d}x \tag{7}$$

where the kernel is given by

$$K(x,x_0)=\frac{J_1[2\beta\sqrt{(x_0-x)f(x)}]}{\sqrt{(x_0-x)f(x)}}f(x).$$

J_1 is the ordinary Bessel function of first order. It is necessary to remember for computational purposes that the actual relation $y=f(x)$ must be written in the non-orthogonal coordinate system.

Formula (7) has been numerically compared with the known Green function for the case $y=Cx$ with $C=$ constant (plane surface) and found to be in agreement.

The integral equation (7) determines the diffracted current due to a unit source for a given shape of intervening surface $y=f(x)$. It is valid as long as the intervening surface does not become tangent to the incident or diffracted beam directions between the entrance and exit points of the beam. As stated in the introduction, the derivation was motivated by a desire to extend the previous result of Werner & Arrott (1965) for flat surfaces. As such, its most obvious application is to the effects of secondary extinction in large neutron monochromating crystals employed in the Bragg geometry. To proceed from a knowledge of the Green function to a realistic assessment of the diffracted intensity when a finite portion of the surface is illuminated, one must perform an integration of the Green function over the outgoing current and incoming source positions on the crystal surface. This is carried out in detail for the plane-surface Green function by Desjardins (1970) and the considerations of that article apply here in essentially the same way.

As far as the more general unsolved problem is concerned of assessing the effects of secondary extinction on small cylindrical crystals of arbitrarily shaped cross section totally immersed in a uniform beam, equation (7) itself is perhaps of less interest than the general method employed in arriving at it. To our knowledge there is still no systematic method of treating this latter problem short of direct numerical integration of equation (1).

References

BACON, G. E. & LOWDE, R. D. (1948). *Acta Cryst.* **1**, 303–314.

DESJARDINS, J. S. (1970). *J. Appl. Cryst.* **3**, 361–371.

HAMILTON, W. C. (1957). *Acta Cryst.* **10**, 629–634.

SOMMERFELD, A. (1964). *Lectures on Theoretical Physics.* Vol. VI. *Partial Differential Equations of Physics.* New York: Academic Press.

WERNER, S. A. & ARROTT, A. (1965). *Phys. Rev.* A**140**, 675–686.

WERNER, S. A., ARROTT, A., KING, J. S. & KENDRICK, H. (1966). *J. Appl. Phys.* **37**, 2343–2350.

ZACHARIASEN, W. H. (1945). *Theory of X-Ray Diffraction in Crystals.* New York: John Wiley.