J. Appl. Cryst. (1975). **8**, 128

Elastic Diffuse Neutron Scattering on I*h* Ice

BY J. SCHNEIDER AND W. JUST

Institut Laue-Langevin, B. P. 156, 38042 *Grenoble Cedex, France*

(*Received* 29 *April* 1974)

Structural studies showed that oxygen atoms in I*h* ice are well ordered whereas hydrogen atoms are 'statistically' distributed on two possible sites on each O–H–O bond. The entropy of this disorder is in agreement with the 'ice rules' which also imply short-range order. Elastic diffuse neutron scattering on deuterated I*h* single crystals has been performed. The intensity distribution of the [*h*0*l*] zone out to $\kappa \simeq 4$ Å^{-1} can be interpreted in terms of proton–proton correlation functions [Villain, J. & Schneider, J. (1972). Int. Symposium on Physics and Chemistry of Ice, Ottawa].

J. Appl. Cryst. (1975). **8**, 128

Dynamical Diffraction of Thermal Neutrons by Absorbing Magnetic Crystals

BY H. H. SCHMIDT, P. DEIMEL AND H. DANIEL

Physik-Department der Technischen Universität München, D-8046 *Garching, Germany (BRD)*

(*Received* 30 *May* 1974; *accepted* 5 *September* 1974)

Dynamical diffraction of thermal neutrons is treated for a plane single-crystal plate of magnetic neutron-absorbing material. It is shown that the results of the theory of dynamical X-ray diffraction can be used in the case of neutron diffraction, when the Fourier transforms of the polarizability are replaced by the Fourier transforms of the interaction potential divided by the kinetic energy of the neutrons. The Fourier transforms of the magnetic part of the interaction potential are calculated expicitly. In order to take the nuclear part of the interaction into account the method of the Fermi pseudopotential is used. The results are applied to the case of symmetrical Bragg reflexion. There are two solutions for the intensity of the reflected beam as a function of the angle of neutron incidence, corresponding to the two possible directions of the neutron spin, parallel or antiparallel to the magnetic field in the crystal. It is shown that the positions of the maxima and the widths of the curves illustrating the intensity dependence on the angle of neutron incidence are different for the two possible spin directions and depend on the direction of the magnetization in the crystal. The total intensity of the reflected beam for the diffraction of unpolarized neutrons is obtained by averaging the intensities for the two possible spin directions.

Introduction

The dynamical diffraction of thermal neutrons shows close analogy to the dynamical diffraction of X-rays, which has been treated by various authors (Zachariasen, 1945; Borrmann, 1950; Wagner, 1956; Laue, 1960). Goldberger & Seitz (1947) give an equivalent theory for neutrons. Kagan & Afanas'ev (1966), in particular, have treated the phenomenon of anomalous absorption. In both cases only nuclear interaction is taken into account. Magnetic scattering of neutrons has been treated by Schwinger (1937) and by Halpern & Johnson (1939). Halpern, Hamermesh & Johnson (1941) have given a theory for the scattering of neutrons by crystals, taking into account the magnetic interaction. The latter is a kinematical theory, restricted to the case of negligible extinction, and not a dynamical one. The first contributions to the dynamical theory of neutron diffraction by magnetic crystals were given by Ekstein (1949). He treated the case in which the Bragg condition is not fulfilled and the neutron beam is only refracted at the crystal surface. The two-beam case has not been treated because of the lack of magnetic single crystals sufficiently perfect to permit experimental verification of the effects of dynamical diffraction. As it now seems possible to produce such crystals, it will be of interest to extend the dynamical theory of neutron diffraction to the case of magnetic ordered crystals. The aim of this paper is to give a solution of this problem for symmetrical Bragg reflexion by a plane-parallel plate of infinite lateral extension.

General remarks

The dynamical theory of the diffraction of neutrons by perfect single crystals can be treated analogously to