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A diffraction pattern caused by thermal diffuse scattering of X-rays in a pyrolytic graphite crystal.

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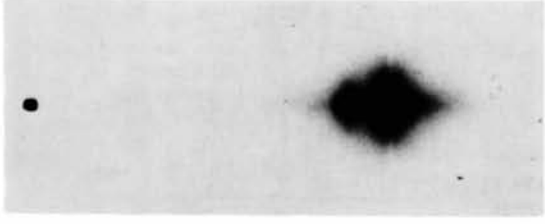
Abstract

A defect line across the 002 diffuse spots scattered from a pyrolytic graphite plate has, for the first time, been clearly observed in X-ray films taken with unfiltered radiation from a copper target. The line was caused by the 002 Bragg reflection of the thermal diffuse scattering.

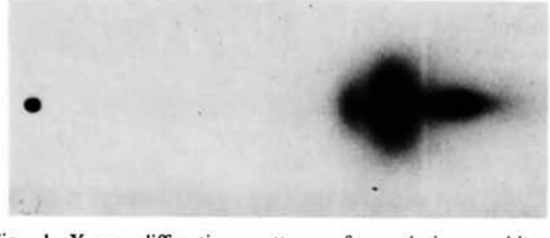
The present authors have recently succeeded in separating inelastic and elastic scattered intensities and found a dip in the inelastic intensity profile of the 200 Bragg reflection from a LiF crystal (Kashiwase & Minoura, 1981) with energy resolution of about 10^{-8} eV by means of the Mössbauer diffraction with 14·4 keV γ-rays, a nuclear resonant absorber and a position-sensitive proportional detector. The dip was suggested to be caused by the thermal diffuse scattering (TDS) which is secondarily reflected by net planes in the same crystal (Kainuma, 1961). Dips of the same kind were also observed in the 002, 004 and 006 Bragg reflections from KCl (Kashiwase, Kainuma & Minoura, in preparation). The defect line corresponding to the dip was observed in the 002 diffuse spot from a urea nitrate crystal (Kashiwase, Kainuma & Minoura, 1981). The purpose of the present paper is to justify this interpretation by the film observation of the diffraction patterns of X-rays from a pyrolytic graphite crystal. The specimen crystal was chosen for the following reasons. The crystal has a layered structure with a low-lying phonon branch. X-ray film observation of the defect line across the diffuse spot scattered from the crystal was expected to be easy. A dip in the inelastic intensity profile at the 002 Bragg reflection from a pyrolytic graphite plate using 14·4 keV Mössbauer γ-rays has been observed (Zasimov, Lobanov, Rudiger & Kusmin, 1976), although the cause of the dip has been attributed to other effects.

Unfiltered radiation from a copper target in a sealed-off X-ray tube operated at 30 kV and 10 mA was incident with glancing angle θ on a flat surface parallel to the (001) planes of the pyrolytic graphite plate. The plate had a rectangular surface 10 × 15 mm, thickness 1 mm. The crystal plate was mounted on a goniometer head of a Laue camera. The incident beam was collimated with a tube of length 60 mm and a hole of diameter 0·5 mm. The distance between the source and the crystal was about 130 mm. The camera length between the crystal and the film was about 100 mm. X-ray films for cosmic-ray observations were used.

Figs. 1(*a*) and (*b*) show X-ray diffraction patterns taken at glancing angles of 13·3 and 15·3°, respectively. The schematic illustration of these patterns are shown in Figs. 2(*a*) and (*b*). The large spot *A* and the small one *B* were caused by the TDS of $K\alpha$ and $K\beta$ X-rays near the 002 reciprocal-lattice point, respectively. Figs. 1(*a*) and 2(*a*) show the case in which the glancing angle θ nearly equals the Bragg angle $\theta_B = 13{\cdot}3°$ for the 002 reflection of Cu $K\alpha$ radiation. The spot *E* is due to the incident beam penetrating the crystal and a thin lead sheet set before the film. The sharp long defect line *D* is clearly seen across the middle of the diffuse spot *A* and the Laue spot *C*. In Figs. 1(*b*) and 2(*b*), the deviation angles between the spot *A* and the line *D* and between the spot *C* and the line *D* are the same. They are



(*a*)



(*b*)

Fig. 1. X-ray diffraction pattern of pyrolytic graphite. The dimensions of the figures are those of the original ones.

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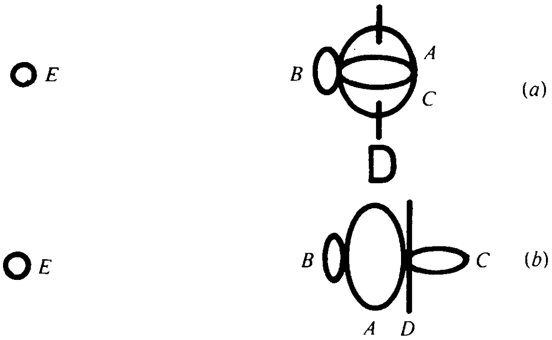

Fig. 2. Schematic illustration of the patterns in Fig. 1. (*a*) and (*b*) correspond to Fig. 1(*a*) and (*b*).

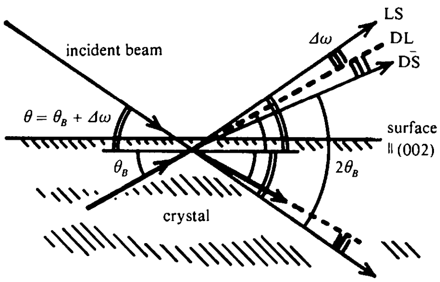

Fig. 3. Propagation direction of the radiation in the present X-ray diffraction experiment.

nearly equal to the deviation angle $\Delta\omega$ of the glancing angle from the Bragg angle θ_B.

The origin of the defect line is explained as follows. Fig. 3 illustrates schematically the propagation of the X-rays in real space. We consider the Bragg case in which the surface of the crystal is parallel to the reflecting net planes in the crystal. The deviation angle $\Delta\omega$ of the glancing angle of the incident beam from the 002 Bragg angle is less than a few degrees. A Laue spot (LS) is caused in the direction with scattering angle $2\theta_B + 2\Delta\omega$ by the mirror reflection of the incident white radiation. Intensity maximum of a diffuse spot (DS) due to the TDS is observed in the direction with scattering angle close to $2\theta_B$. If a cone of the TDS is incident on the 002 reflection planes with the Bragg angle θ_B in the crystal, the direction of the TDS is changed by the 002 reflection in the crystal. Thus the defect line (DL) is caused in the diffuse spot. It will be easily understood from Fig. 3 that the defect white line is observed in the middle between the Laue spot and the diffuse spot.

We therefore conclude that the defect line, *i.e.* the diffraction pattern caused by the Bragg reflection of TDS, was observed in the 002 diffuse spot from the pyrolytic graphite crystal.

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On some X-ray diffuse scattering effects on Cu–Al single crystals.

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Abstract

A change in the diffuse scattering intensity distribution as a function of Al concentration in the α-phase Cu–Al solid solution is examined. The shape and intensity of the diffuse $\bar{1}11$ and 020 reflexions are shown to change with increasing Al concentration. With 10 at.% Al as the starting point, new diffuse reflexions appear. These are interpreted in terms of the formation of new Al atom configurations.

Recently, the Cu–Al system has been the subject of a number of detailed studies, and so far the structure type occurring in the α-phase solid solution of this compound has not been elucidated. Measurement of diffuse scattering shows that with ~11 at.% Al as the starting point, these alloys reveal short-range order (Iveronova & Katsnelson, 1977). At lower Al concentrations the diffuse scattering is weak, and quantitative results on the structures are not reliable (Epperson, Fürnrohr & Ortiz, 1978). Analysis of the diffuse scattering distribution, however, gives qualitative evidence for the variations in the state of the alloying component at concentrations less than 10 at.% Al. The X-ray patterns correlate with the behaviour of the mechanical characteristics of the alloy (Braude, Gluzman, Demirsky & Komnic, 1981).

Experimental

Studies were carried out on single crystals of Cu and its alloys. Initial materials were of 99·996% Cu and 99·999% Al purity. The samples were annealed at ~1273 K for 8 h in

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