Textures and Microstructures, 1991, Vols 14–18, pp. 431–436
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INTERPRETATION OF PREFERRED ORIENTATION IN NATURALLY AND EXPERIMENTALLY DEFORMED CHALCOPYRITE ORES BY NEUTRON DIFFRACTION TEXTURE ANALYSIS

E. M. JANSEN[1)], P. MERZ[2)], H. SIEMES[1)], G. WILL[2)]

1) Institut für Mineralogie und Lagerstättenlehre der RWTH Aachen, Wüllnerstr. 2, D-5100 Aachen, FRG

2) Mineralogisches Institut der Universität Bonn, Arbeitsgruppe Neutronenbeugung in der KFA Jülich, Poppelsdorfer Schloß, D-5300 Bonn, FRG

The chalcopyrite ($CuFeS_2$) structure is a tetragonal derivative of the sphalerite structure with a ratio of c_o/a_o = 1.97. Therefore in X-ray diffraction experiments either the tetragonal reflections are not distinguishable from the cubic sphalerite reflections or the cubic sphalerite reflections are splitted into two very close adjacent tetragonal ones. In X-ray texture goniometry they cannot be resolved because of the rather wide open slits which are used in order to minimize the defocussing effects and are measured as pseudo-cubic double reflections. The poles of the most important, strong reflections with low multiplicity factors (112) and (220/204) are therefore of pseudocubic symmetry (1, 2). Because of the similarity of the sphalerite and chalcopyrite structure the sphalerite mechanisms were assumed to be activated during deformation. X-ray, optical and TEM studies of chalcopyrite single crystals have shown that several tetragonal slip and twinning modes were activated (3) in deformation experiments. In order to check whether the preferred orientation of chalcopyrite is caused by pseudo-cubic or by true tetragonal behaviour of the deformation modes it is necessary to use a position sensitive detector combined with a profile analysis program in order to seperate the overlapping peaks. This could be realized by means of a neutron diffraction texture goniometer at the FRJ-2 reactor of the KFA Jülich (4).

Two chalcopyrite samples with different preferred orientations were investigated. The first one, is an experimentally undeformed sample from the Frood Mine, Sudbury, Canada. The X-ray pole figure showed a quasi single crystal orientation with a maximum of the pseudo-cubic a-axes close to the centre of the projection. This maximum could be either a tetragonal c-axis maximum, a tetragonal a-axis maximum or a mixture of both. The neutron pole figures of several true tetragonal reflections revealed a mixture of two preferred orientations. Figure 1 and 2 show the measured (008), (400), (220), (204) and (112) pole figures with two single crystal orientations A and B in comparison with the modelled (001), (100), (110), (102) and (112) pole figures after Matthies et. al. (5). The greater fraction of crystallites is contributing with their a-axes (A), the smaller fraction with their c-axes (B) to the maximum close to the centre of the projection. With the exception of one small maximum for each of the (008) and (220) pole figures, which cannot be explained by the simple modelling, the measured pole figures are in good agreement with the modelled ones.

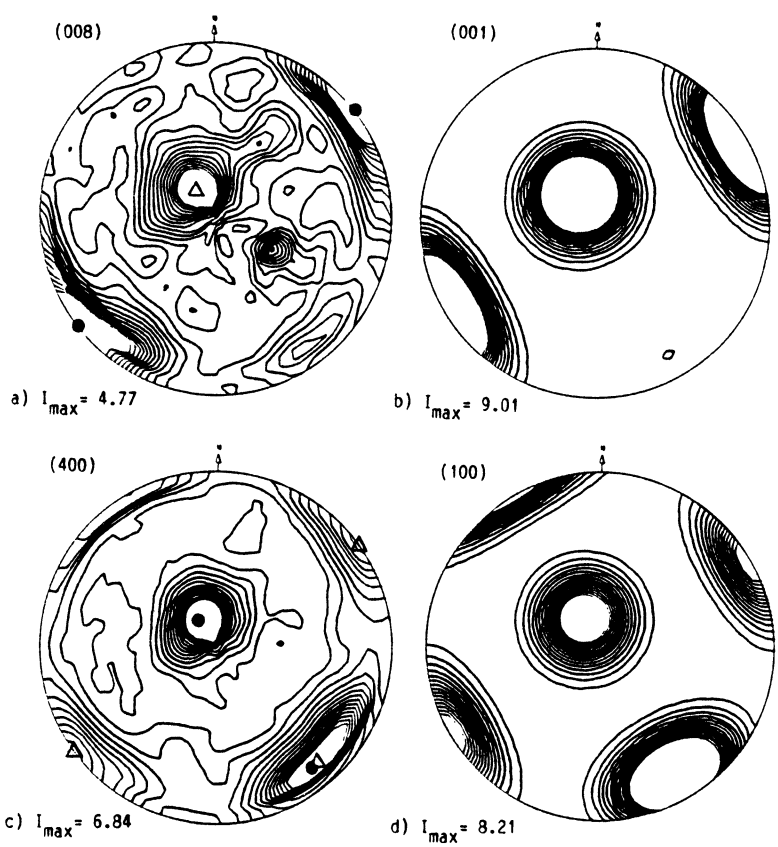

Figure 1 Neutron diffraction measured complete (008) and (400) pole figures (a and c) with single crystal orientations A (●) and B (△) of a naturally deformed sample of the Frood Mine, Sudbury, in comparison with the modelled (001) and (100) pole figures (b and d), equal area projection

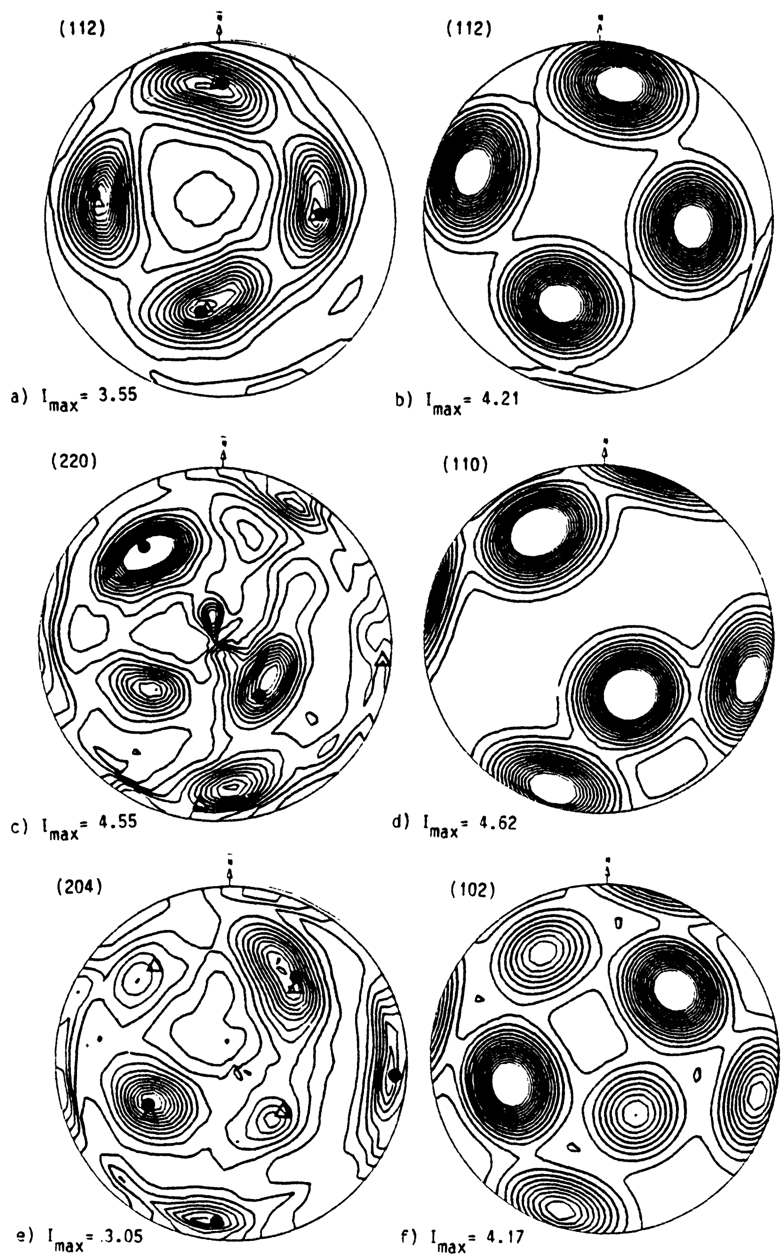

Figure 2 Neutron diffraction measured complete (220), (204) and (112) pole figures (a, c and e) with single crystal orientations A (●) and B (△) of a naturally deformed sample of the Frood Mine, Sudbury, in comparison with the modelled (110), (102) and (112) pole figures (b,d and f), equal area projection

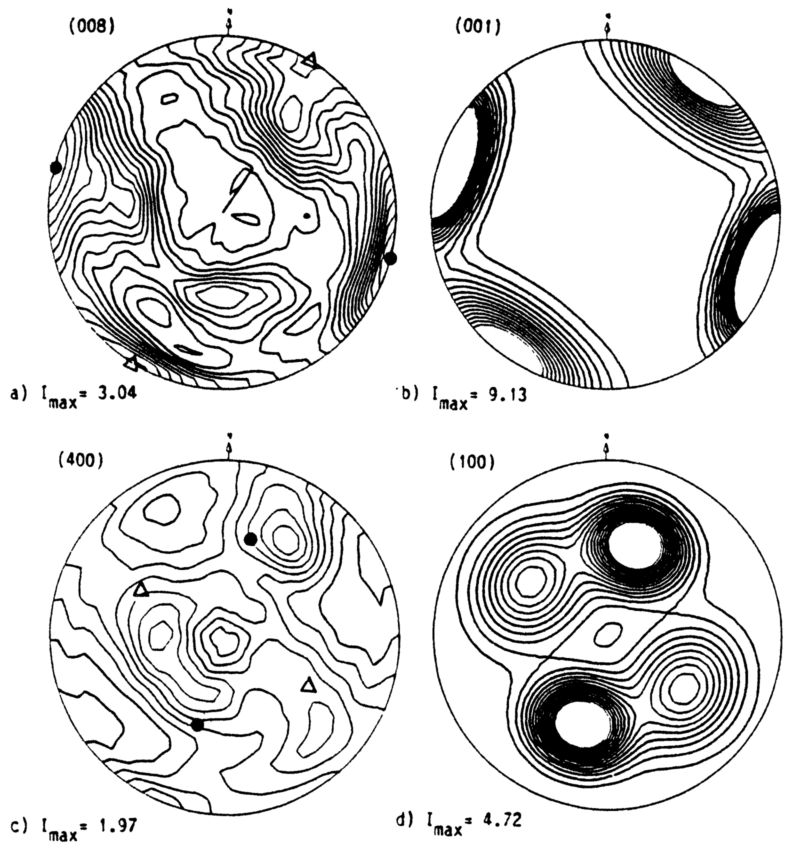

Figure 3 Neutron diffraction measured complete (008) and (400) pole figures (a and b) with single crystal orientations A (●) and B (△) of an experimentally deformed sample of the Mt.Isa Mine, Australia, in comparison with the modelled (001) and (100) pole figures (b and d), equal area projection

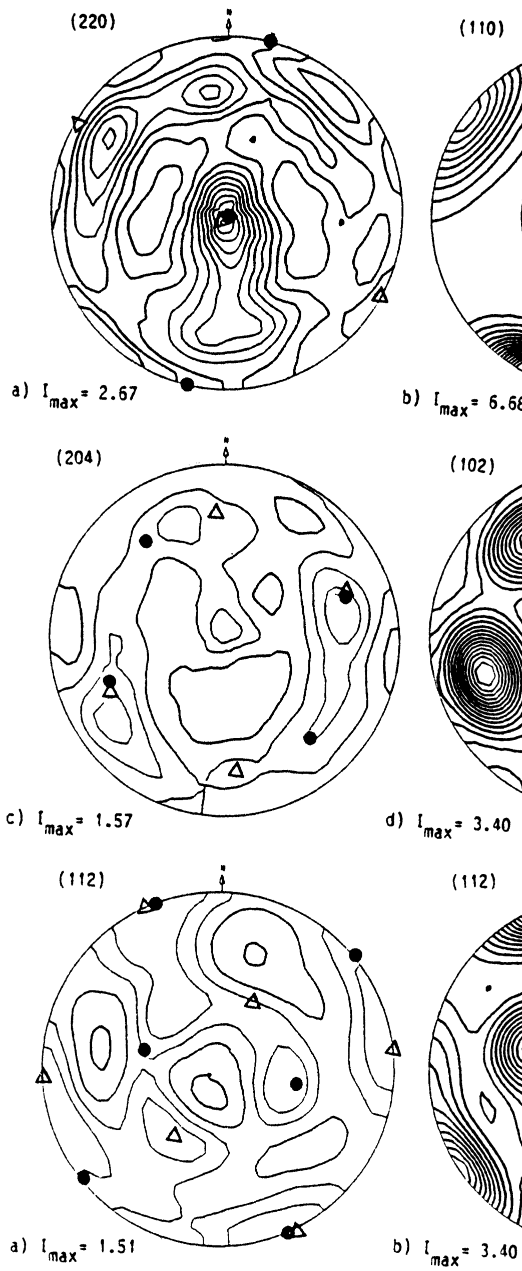

Figure 4 Neutron diffraction measured complete (220), (204) and (112) pole figures (a, b and e) with single crystal orientations A (●) and B (△) of an experimentally deformed sample of the Mt.Isa Mine, Australia, in comparison with the modelled (110), (102) and (112) pole figures (b, d and f), equal area projection

The second sample from Mt. Isa, Australia has been experimentally shortened 15% by axial compression under a confining pressure of 150 MPa, at a temperature of 200°C and a strain rate of $6.8*10^{-6}s^{-1}$. The X-ray pole figure of this sample showed a preferred orientation of (220/204) perpendicular to the axis of compression, which has been described already for room temperature experiments by Lang (1). The (220/204) maximum could be either a maximum of the tetragonal prism (110), a maximum of the tetragonal pyramid (102) or a mixture of both. In figure 3 and 4 the (008), (400), (220), (204) and (112) neutron pole figures are also compared with the modelled (001), (100), (110), (102) and (112) pole figures after Matthies (5). The neutron pole figures show two main idealized c-axes orientations perpendicular to the compression axis. These orientations correspond to a (110) maximum in the centre of the projection. This true tetragonal preferred orientation is consistent with tetragonal deformation modes of chalcopyrite. Further interpretation of chalcopyrite preferred orientation will be done in more detail by ODF analysis.

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