trypsin inhibitor, tobacco mosaic virus coat protein, rubredoxin, and lysozyme. Mackay's (1974) method is potentially much more rapid, since only a triangularization of **G** is involved, and no eigenvalues. However, in our hands, the resultant coordinates are very sensitive to small errors in **D**, apparently as a result of the inherent instability of Choleski decomposition of nearly singular matrices.

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APPENDIX

Proof of equation (3)

Let $\mathbf{r}_{kl}$ denote the vector from point l to point k; n = total number of points; and O denotes the center-of-mass point. From the definition of the center of mass of an array of points, each of unit mass:

$$\sum_{j=1}^{n} \mathbf{r}_{jO} = \mathbf{0} = \sum_{j=1}^{n} (\mathbf{r}_{1O} + \mathbf{r}_{1j})$$

so that

$$\mathbf{r}_{1O} = -n^{-1} \sum_{j=2}^{n} \mathbf{r}_{1j}$$

and

$$d_{1O}^2 = \mathbf{r}_{1O}\cdot\mathbf{r}_{1O} = n^{-2}\sum_{j=2}^{n}\sum_{k=2}^{n} \mathbf{r}_{1j}\cdot\mathbf{r}_{1k}.$$

By the law of cosines,

$$\begin{aligned} d_{1O}^2 &= (2n^2)^{-1}\sum_{j=2}^{n}\sum_{k=2}^{n}(d_{1j}^2 + d_{1k}^2 - d_{jk}^2) \\ &= (2n^2)^{-1}\left[2(n-1)\sum_{j=2}^{n} d_{1j}^2 - 2\sum_{2=j<k}^{n}\sum d_{jk}^2\right] \\ &= (n-1)/(n^2)\sum_{j=2}^{n} d_{j1}^2 - n^{-2}\sum_{2=j<k}^{n}\sum d_{jk}^2 \\ &= n^{-1}\sum_{j=1}^{n} d_{j1}^2 - n^{-2}\sum_{1=j<k}^{n}\sum d_{jk}^2. \end{aligned}$$

Since the labelling of the points is arbitrary, then we have the general formula

$$d_{iO}^2 = n^{-1}\sum_{j=1}^{n} d_{ij}^2 - n^{-2}\sum_{j=2}^{n}\sum_{k=1}^{j-1} d_{jk}^2.$$

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Diffraction from Dislocations and Grain Boundaries – An Optical Analogue Study

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Optical transforms of the models of atomic configurations around edge and screw dislocations in f.c.c. and b.c.c. lattices as well as grain boundaries have been obtained with the help of a laser diffractometer. The models used were based on computer simulation studies of other workers. It has been observed that the intensity at the reciprocal lattice points splits into annular haloes or takes the 'figure of eight' shape in some cases. The directional dependence of the splitting has been compared with the existing theories. It has also been observed that with ordering of the dislocations at the grain boundaries, the diffraction pattern resembles that of a single dislocation.

Introduction

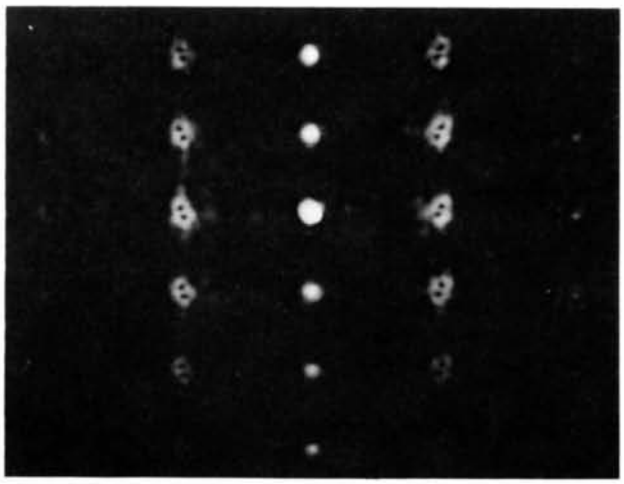
As a result of elastic strain around the lattice defects there is a displacement of atoms from their normal lattice sites. Huang (1947), considering a random distribution of defects, each producing a spherically symmetric displacement field $\mathbf{U} = \mathbf{r}/|\mathbf{r}|^3$, has shown that crystals containing such defects would give rise to a diffuse scattering. Wilson (1949, 1950, 1952, 1955), Vassamillet (1958) and others have given theories of diffraction from crystals containing dislocations and have predicted the nature of the modulation of the intensity distribution. These theories have been further developed by several workers and with improved experimental techniques it has now been possible to obtain the relaxation around the defects from the measurement of the intensity distribution (Dederichs, 1973). Comparison of these theories with the experimental studies of the diffuse scattering is rather difficult because of the interference of the thermal diffuse scattering (TDS) with the defect diffuse scattering (DDS). Of course at liquid-helium temperatures the TDS can be considered to be small with respect to the DDS, but this may not give a true picture of the relaxation field around the defects at room temperature because of the temperature dependence of the atomic bonding, *etc.* Hence it would be helpful if a knowledge of the nature of DDS in different systems could be obtained by numerical computation or by optical diffraction techniques where the system is represented by a mask having static atoms. In the calculation of DDS an enormous amount of numerical calculation is involved and hence often one has to make many simplifying assumptions. Moreover, as shown by Keating & Goland (1971), series-termination effects in such calculations give rise to serious errors in the form of ripples in the intensity distribution. For the above reasons optical transform studies from models containing different types of defects would be of great use. Hence Samantaray, Mathur & Gartia (1975) have used the optical transform method for studying diffuse scattering from point defects.

Previously only Willis (1957*a*,*b*) has used the optical transform technique for studying diffraction from dislocations. He considered only the case of the single edge dislocation and used isotropic elasticity theory for his model. So far no work on the optical diffraction from screw dislocations and dislocation clusters forming grain boundaries has been reported. Therefore, in the present investigation, optical diffraction from edge and screw dislocations and grain boundaries has been treated.

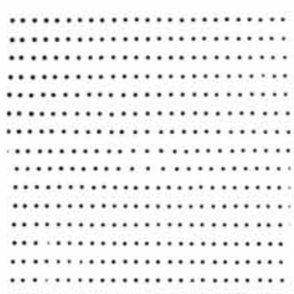
Choice of models

As has been mentioned earlier, most of the above works are based on the elastic continuum model which does not give an accurate representation of the atomic structure in the defect region. The elastic continuum theory fails in the region around the core of the dislocation where, according to this theory, the stresses become infinite. Hence computer simulation methods are employed to obtain a more realistic picture. Excellent reviews of such computer calculations are available in Gehlen, Beeler & Jaffee (1972) and Beeler (1970). In the present investigation the models for the masks of the different defects were made by taking the atomic positions at the defect region from the published works on computer simulation studies.

Masks for the edge and screw dislocation for f.c.c. crystals were made by taking the results of Cotterill & Doyoma (1965, 1966) and Doyoma & Cotterill (1964, 1966). They are shown in Figs. 1(*b*) and 2(*b*) respectively. The core configuration for an edge dislocation in b.c.c. crystal was taken from the results of Bullough & Perrin (1970). The relevant portion of the mask is shown in Fig. 3(*b*). It is well known that stable twist grain boundaries are formed by a crossed grid of screw dislocations. The corresponding mask is shown in Fig. 4(*b*). Masks for the 6° tilt boundary in γ-iron without and with interstitial carbon impurities were made by taking the results of Dohl, Beeler & Bourguin (1972). The cases for the 6° tilt boundary and the 6° tilt boundary with three carbon atoms are shown in Figs. 5(*b*) and 6(*b*) respectively.



(*a*)



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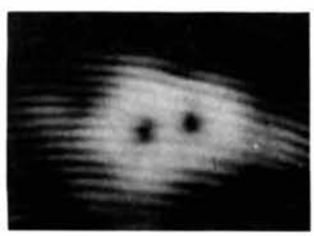


(*c*)

Fig. 1. (*a*) Optical transforms of the projection of six atomic planes around an edge dislocation in a f.c.c. lattice. (*b*) Central portion of the mask. Position of atoms around an edge dislocation in a f.c.c. lattice. It is a projection of six atomic planes. The plane of the figure is (112). (*c*) Figure of eight obtained in f.c.c. edge dislocation optical transform.

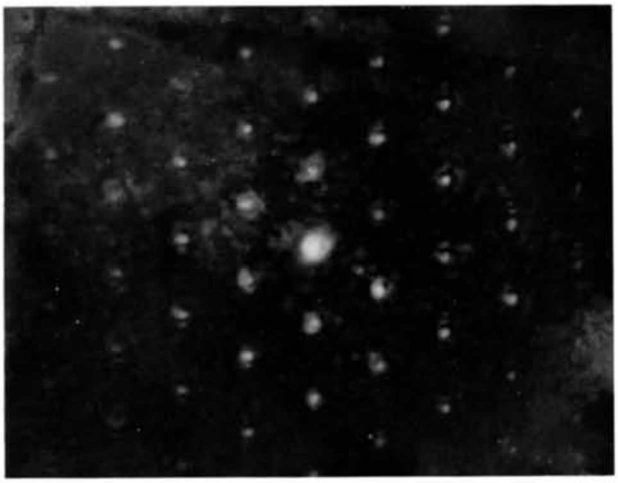
Experimental

Drawings of the atomic configurations at the defects were made on a white sheet of paper by plotting atomic coordinates obtained from the computer-simulated models described earlier. The atomic positions were blackened with Indian ink and photographs were taken with a reduction ratio of 100 : 1. Enough atoms were taken in each model for the strain field of the defects to decrease to negligible value. This was around 10^3 atoms. The negatives placed between two optical flats were used as the masks for obtaining the diffraction patterns. An optical diffractometer was constructed with a geometry similar to the well known Lipson diffractometer, but with the conventional Hg source replaced by a 1 mW Spectra Physics He–Ne laser. The optical diffraction patterns were recorded on 22 DIN–125 ASA films and were all processed under the same conditions. The optical diffraction patterns shown in Figs. 1(*a*)–6(*a*) correspond to the masks shown in Figs. 1(*b*)–6(*b*) respectively.

Results and discussion

The optical transform of the f.c.c. edge dislocation is shown in Fig. 1(*a*). It is observed that the *hk* ($h \neq 0$) reflections have the shape of a figure of eight. One of the *hk* reflections has been enlarged and is shown in Fig. 1(*c*). In the case of 1*k* reflections a continuous figure-of-eight pattern is obtained, while for higher values of *h*, the spot breaks into several spots which lie on a contour of figure-of-eight shape. However, no change in the 0*k* reflections is observed.

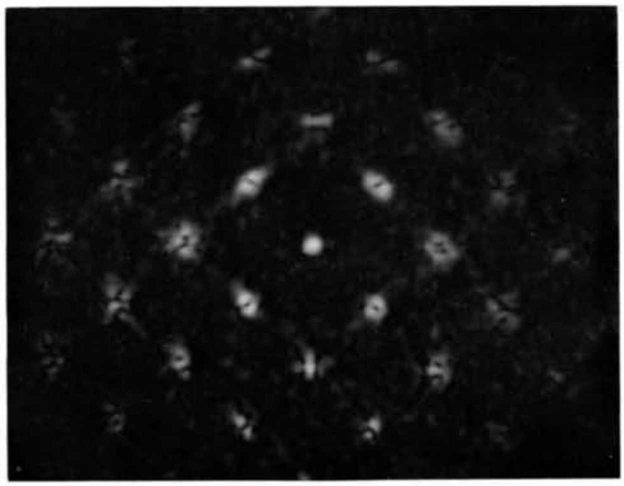
Two different theories have been proposed for the diffraction from dislocations. Using Hall's (1950) model for displacements, Wilson (1950) calculated the intensity distribution for the edge dislocation. He observed that 0*k* reflections are unaffected by the presence of dislocations, where *k* refers to the direction normal to the Burgers vector. He also observed that *hk* intensity distributions are drawn out into hollow rings and the diameter of the rings is independent of *k* but increases with *h*. On the other hand, Suzuki (1957) and Suzuki & Willis (1956) showed by considering the



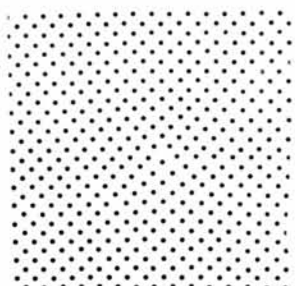
(*a*)

(*b*)

Fig. 2. (*a*) Optical transform of a screw dislocation in a f.c.c. lattice. (*b*) Central portion of the mask. Position of the atoms around a screw dislocation in a f.c.c. lattice. The figure shows a (111) plane immediately above the slip plane.



(*a*)



(*b*)

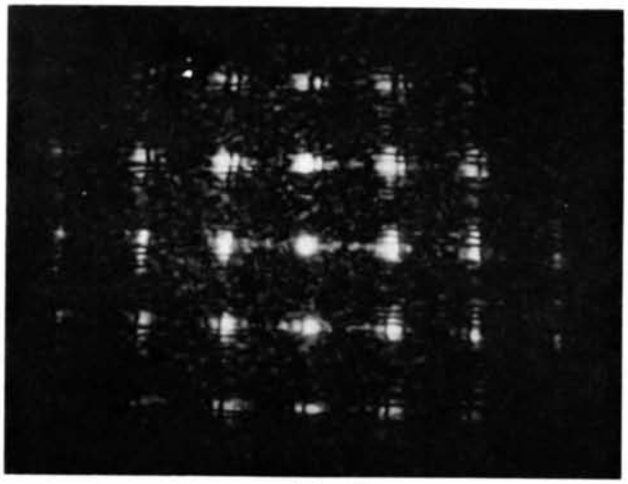
Fig. 3. (*a*) Optical transform from a two-layer projection of an edge dislocation in a b.c.c. lattice. (*b*) Central portion of the mask. A (010) projection of a b.c.c. edge dislocation with Burgers vector *a*, [100]. There are no displacements in the [010] direction. It is a projection of two layers.

model given by isotropic elasticity theory (Reed, 1953) that the intensity distribution in the neighbourhood of a *hk* point is more complex and depends on both *h* and *k*. They observed that the *h*0 reflection is of the shape of a figure of eight and the 0*k* reflection is of the shape of a cross. Willis (1957*a*,*b*) took the optical transform for both the models and showed that the optical transforms agree with the theoretical predictions. In the present case the models were made on the basis of the results of the computer simulation studies. If we look at Fig. 1(*a*), we find that the *h*0 and *hk* reflections resemble the Suzuki case whereas the 0*k* reflections resemble the Wilson case. None of the theories fully explains the diffraction pattern obtained in the present case.

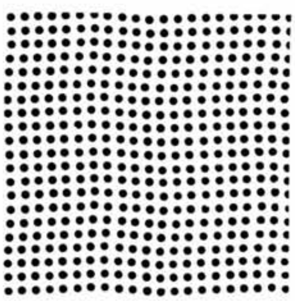
Fig. 2(*a*) is the optical transform of the atoms in a (111) plane immediately above the slip plane for the screw dislocation in a f.c.c. lattice. It is observed that an annular halo forms around the spots. The radius of the halo increases with the increase in the order. Formation of these rings is as predicted by Wilson (1949). The central spot inside every halo is present because only one plane was considered for the purpose of taking the optical transform. However, if the entire screw dislocation is considered, possibly the halo will increase in intensity with a corresponding decrease in the intensity at the reciprocal lattice point. The optical method could not be applied to verify this because of difficulties in representing in a two-dimensional grating the repetition in a third direction of a two-dimensional configuration of atoms.

In the optical transform of a b.c.c. edge dislocation (Fig. 3*a*), it is observed that the different *hk* reflections have different shapes depending upon their indices. 11-type reflections are found to have a ring shape, whereas 20-type reflections have the figure-of-eight shape. The 02-type reflections have a cross shape similar to the one obtained for the Suzuki case.

One common feature among all the optical transforms is the existence of weak diffuse scattering. This is present in the form of streaks joining the reciprocal lattice points. In case of the f.c.c. edge dislocation the streaks are observed to be parallel to the *h* and *k* directions, whereas in b.c.c. edge dislocation they are observed to be parallel to the diagonal.

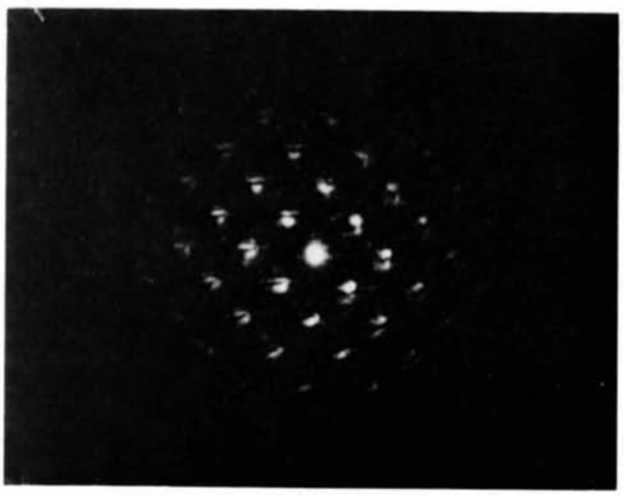


(*a*)

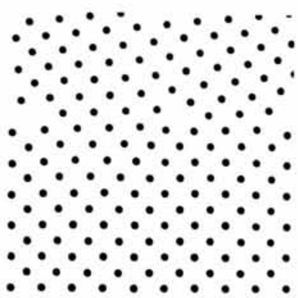


(*b*)

Fig. 4. (*a*) Optical transform of twist boundary formed by a crossed grid of screw dislocations. (*b*) Central portion of the mask. Twist boundary formed by a crossed grid of screw dislocations (sectional).



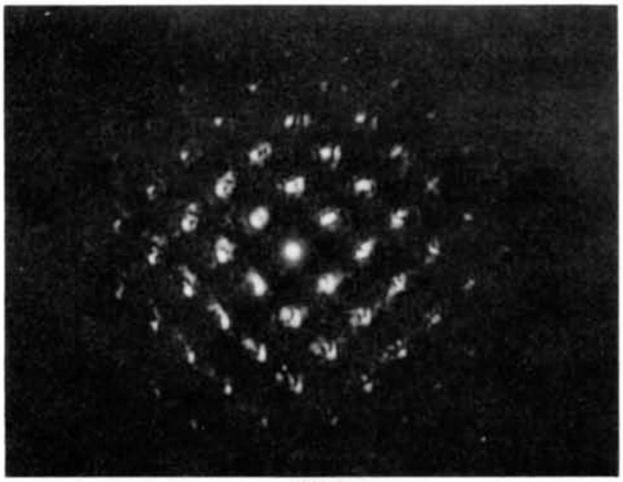
(*a*)



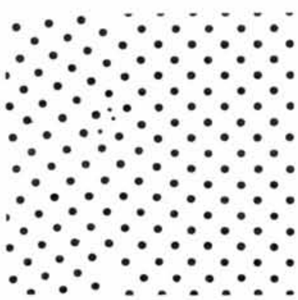
(*b*)

Fig. 5. (*a*) Optical transform of a 6° tilt grain boundary in the (100) plane of γ-iron. (*b*) Central portion of the mask.

Optical transform of grain boundaries have been shown in Figs. 4(*a*)–6(*a*). In the optical transforms of a section of a crossed grid of a screw dislocation giving rise to a twist boundary (Fig. 4*a*) it is observed that each of the spots splits into a large number of parallel spots. Further strong diffuse streaks are also found to join the reciprocal lattice points. In case of a 6° tilt grain boundary in γ-iron (Fig. 5*a*) the spots are found to bifurcate. With the addition of a carbon impurity atom at the bad-fit region it is observed from computer-simulation experiments that there is an ordering of the dislocations forming the grain boundaries. In the optical transform it is observed that the splitting of the spots becomes rounded to resemble the diffraction from an edge dislocation. On addition of two more carbon atoms there is further ordering of the dislocations forming the grain boundaries. The optical transform (Fig. 6*a*) further improves and resembles the diffraction pattern from an edge dislocation. There is much similarity between Fig. 3(*a*) and Fig. 6(*b*). Thus it is observed that when there is an ordering of dislocations at the grain boundaries the diffracted intensities greatly resemble that from a single dislocation.



(*a*)



(*b*)

Fig. 6. (*a*) Optical transform of a 6° tilt grain boundary with three carbon interstitials in the bad fit region. (*b*) Central region of the mask.

Hence we see that optical-analogue methods can be effectively used for corroborating and distinguishing between different theories of diffraction and for studing their limitations. In the present case we find that the displacement fields produced because of dislocations are quite complex and the different diffraction theories which assume the simple elastic continuum approach do not explain the results fully.

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