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Theory and Observation of Diffraction Contrast of Electronmicrographs of Dislocation and G. P. Zone

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An approximate expression of the dynamical scattering of electron in imperfect crystal is obtained. In imperfect crystal the transmitted primary and diffracted waves are expressed by superpositions of a number of plane waves. This expression corresponds to diffuse scattering of electron in the kinematical theory of diffraction by imperfect crystal.

The intensity distribution of electron in the electron microscopic images of dislocation are calculated with the use of the wave function. These calculated results explain the several characteristic features of the electronmicrographs of dislocation.

As an application of this imaging theory, the determination of the elastic lattice distortion around G. P. Zone in Cu-Be alloy is performed by the comparison between electronmicrographs and the images calculated from assumed models.

The dynamical theory of electron diffraction in perfect crystal is extended to the diffraction of electron in imperfect crystal so as to know the behaviour of electron waves in the strain field around the fault. The intensity distribution of electron in the electronmicrograph of imperfection is calculated from the wave function on the exit surface of the crystal. The characteristic appearances of the diffraction contrast of dislocations are discussed. The structure of the elastic lattice strain around the G.P. zone in Cu-2%Be alloy is determined by comparing the diffraction contrast calculated from the postulated model and that of the electronmicrographs. This gives an example showing that the theory of imaging of lattice imperfection can be applied to the determination of the strain field around the fault. The relation between this theory and those based upon other treatments is discussed[1),2),3)].

Electron in Imperfect Crystal

A plane wave of electron impinges on the crystal and a kind of lattice plane is in diffraction condition, the electron is diffracted by the plane. The condition of diffraction changes by the irregularity of the lattice along the path of the electron and the diffracted wave (and the transmitted primary wave) cannot be expressed by a plane wave as in perfect crystal. So the wave function of electron is approximately described by a superposition of two groups of plane waves. They are two main waves corresponding to the transmitted primary and the diffracted waves in perfect crystal and many plane waves having wave vectors slightly different from those of main waves (see Fig. 1).

The imperfect crystal, which is a non-periodic scattering potential to the electron due to the strain field around the imperfection, is divided into a number of small regions (blocks) so that the scattering potential can be regarded periodic in each of them. So the wave function of electron on the exit

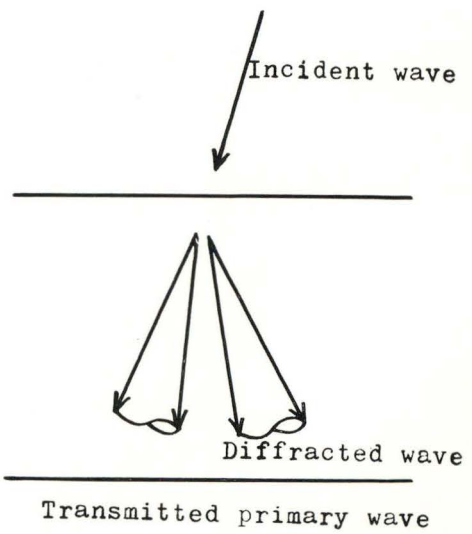

Fig. 1. Waves in imperfect crystal.

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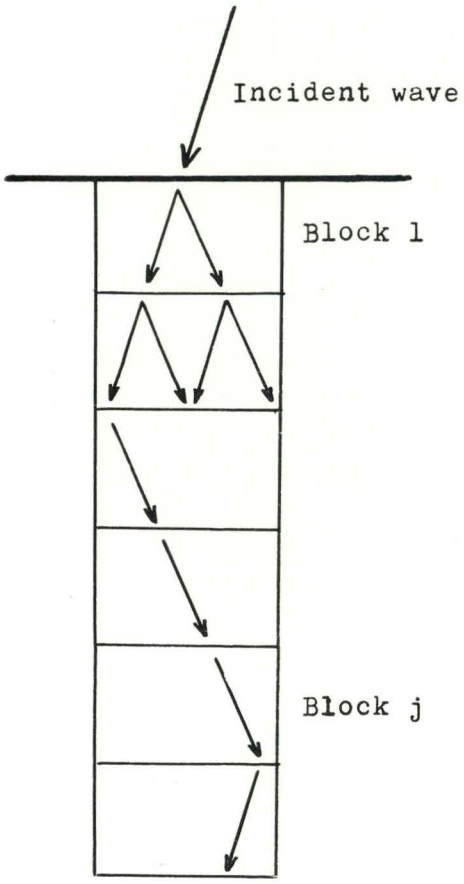

Fig. 2. Scattering of electron in a block and a path of multiple scattering.

surface of the crystal is obtained from the calculation of dynamical scattering of electron in each block taking account of the elastic lattice distortion and that of multiple scattering among the blocks taking account of the displacement of the lattice (see Fig. 2).

Electronmicrographs

From the wave function thus calculated the intensity distribution of electron in the micrograph is calculated. Numerical calculation of the diffraction contrast of dislocations have been performed under various conditions of diffraction (for example, see Fig. 3). The calculated results are compared with the electronmicrographs and the agreement between them is satisfactory.

The determination of the structure of the lattice displacement around the G.P. zone in Cu-2%Be alloy has been performed applying this theory. The specimen thinned electrolytically, which is previously agehardened at 300°C for about twenty minutes, is examined by transmission electron microscope (Hitachi HU-11). An example of the electronmicrograph of G.P. zone is shown in Fig. 4. They are thin lines parallel to (100) plane of matrix with dark and white contrast according to the condition of diffraction of electron.

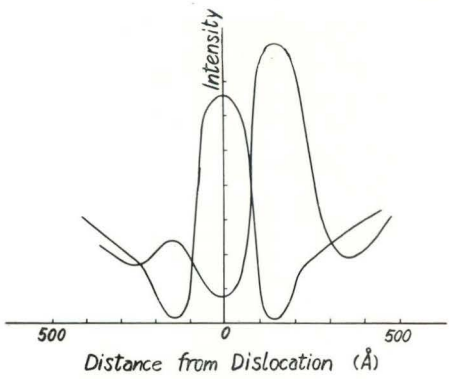

Fig. 3. Calculated diffraction contrast of screw dislocation parallel to the crystal surface. Net plane in diffraction condition is perpendicular to the Burgers vector. Condition of diffraction is shown by t.

The most simple structure of this kind of precipitate is that the solute beryllium atoms coagulate on (100) plane and form a pair of dislocations. The intensity distribution of electron in the electron microscopic image is calculated from this model and two examples are shown in Fig. 5.

These calculations show that the model is inadequate to explain Fig. 4.

So we can expect that the lattice distortion is dominant in a region shown in Fig. 6. The region is a plate parallel to (100) plane of matrix and the thickness is about 20~40Å and the diameter is more than 100Å. As we cannot observe the intermediate lattice structure in the electron diffraction pattern, the coagulated beryllium atoms do not form regular lattice. The lattice distortion may be due to the irregular distribution of these beryllium atoms in the region.

Relation between the present theory and those based upon other treatment

Here in this treatment we took account of two factors i.e. (a) the change in the condition of diffraction by lattice distortion and (b) the phase change of electron by lattice displace-

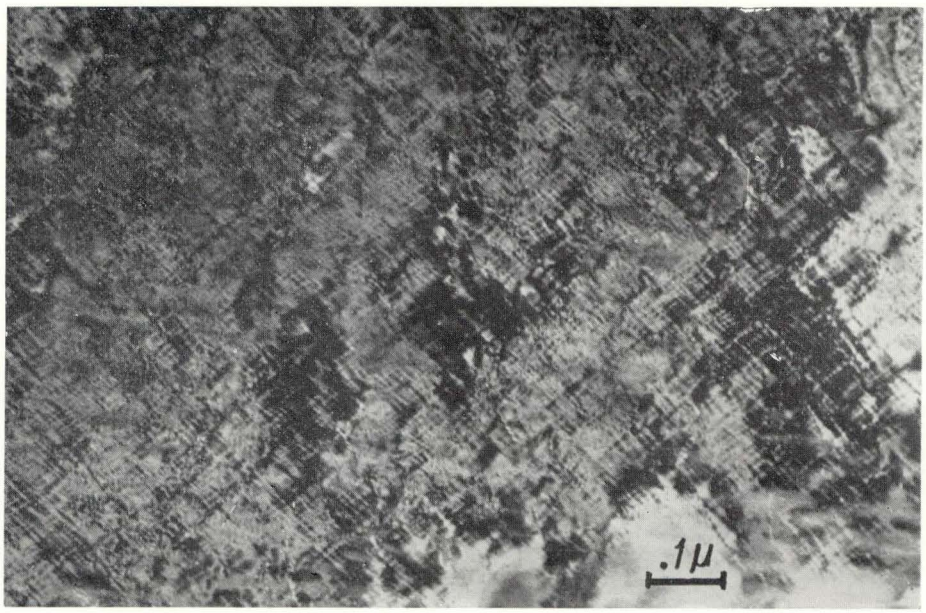

Fig. 4. Electronmicrograph of G. P. zone in Cu-2% Be alloy.

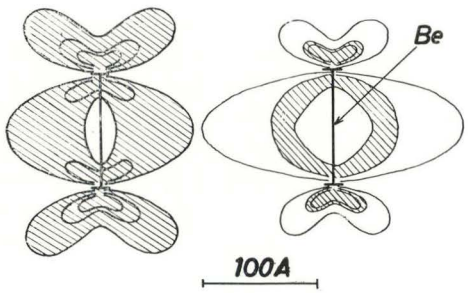

Fig. 5. The intensity distribution of electron in the electron microscopic image calculated from the pair of dislocations' model. The plane in diffraction condition is perpendicular to the Burgers vector of dislocations.

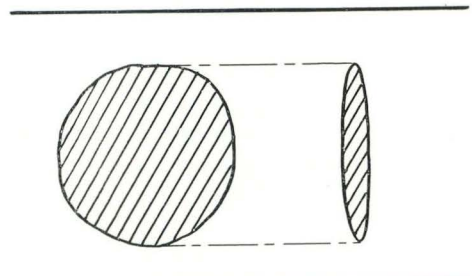

Fig. 6. The structure of G. P. zone.

ment. In general these two factors must be considered. But in the case of the images of stacking fault, only (b) has to be considered because the lattice distortion is negligibly small[3]. In the case of the images of an edge dislocation perpendicular to the crystal surface, only (a) has to be considered[1]. Kato[2] obtained a matrix expression of the wave function of electron in imperfect crystal where (a) is neglected.

So we can obtain the same expression of the wave function of electron in imperfect crystal as those reported by several authors quoted here when we make appropriate model of imperfect crystal in this theory.

The applicability of column assumption (or block assumption here) is common difficulty in these imaging theories.

References

1 H. Hashimoto and M. Mannami: Acta Cryst. **13** (1960) 363. M. Mannami: To be published.
2 N. Kato: Private communication; Acta Cryst. to be published.
3 M. J. Whelan and P. B. Hirsch: Phil. Mag. **2** (1957) 1303.

DISCUSSION

J.M. WHELAN: Dr. Howie has pointed out that the theory we have developed can be extended to cover the case of different displacements in neighbouring columns. However, in our notation, T and S are not only functions of depth z but also of some lateral coordinates. The simple column approximation differential equations are replaced by partial differential equations in two or more variables. The only assumption is that you can describe the wave field at a point in terms of plane waves T and S. The equations are however very difficult to handle with a computer.

S. MIYAKE (to M. Mannami): In Kato's theory a criterion for the limit of its applicability has been pointed out. What will be about it in your theory?

N. KATO: I would like to make a comment on the treatments for lateral distortions among blocks and tilting between blocks. I think it is necessary to make sure in this sort of work that a way of dividing a crystal into blocks does not influence the final results. Of course I appreciate your physical pictures, but I would like to know a justification more in details.

H. HASHIMOTO: On the behalf of Dr. Mannami may I reply to you? We did not yet such a theoretical criterion like that of Kato. From the strict theoretical point of view this theory may not be good. But the results can explain the observed contrast fairly well, and we have a feeling that this theory may be rather good. The theoretical criterion of the applicability of this theory will be studied in near future.