A Theoretical Analysis of the Dislocation Contrast in LACBED Patterns

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Introduction: LACBED (Large Angle Convergent Beam Electron Diffraction) technique has been widely used to investigate strain fields or the nature of dislocations in specimens[1,2]. Cherns and Preston[1] have devised a simple rule to determine the Burgers vector, **b**, of a dislocation from LACBED patterns. They noted that high index **g**-reflection lines would split into n-fringes at the region intersecting by a dislocation line, and |**g.b**|=n. The purpose of this work is to clarify this rule further by computer simulations of the patterns for various cases, using a new form of theory for dislocation contrasts.

Theory: First, to calculate dislocation contrasts in LACBED patterns, it has been newly formulated the form of theory in which the inclination of the entrance surface and the slip plane of dislocation are taken into account. It was hoped that this formulation might give better understanding of the contrast behavior. The form of theory is, in brief, as follows.

In Fig. 1 **ns** and **nd** are normal vectors to the entrance surface and slip planes respectively. It is assumed that the each slab of A and B is a perfect crystal but displaced each other by **R(r)** due to a defect. This model is then essentially the same as multi-layered stacking fault configurations, and the formulation of the diffraction theory for this case have been done and verified experimentally by the author [3]. With slight modification of the eqn. (12) in [3], one can easily obtained the N-beam diffracted intensity including absorption effects at the E in the exit surface of the column drawn in Fig. 1 as,

$$I_g = \left| \sum_m \exp[2\pi i(\gamma_z^{(m)} t) \sum_j \chi_n^{(j,m)} C_g^{(j,m)} \right|^2 \qquad (1)$$

For the meanings of symbols in (1) and other details, one should refer to the [3]. It must be noted that in (1) the column approximation is employed. With the assumption that **ns** //

nd, and parallel to the beam direction, (1) can be easily manipulated to the well known Howie-Whelan(HW) equations.

Simulations: As examples for calculations, the specimen of cobalt (in fcc phase, a=0.354 nm) with the thickness, t=185 nm was considered. The common data given in simulations was follows: the energy of electron beam, 200 kev; the orientation of specimen to the beam, (-1 3 4) and the tie point for central beam direction, Kx, 1.68**g**(1 1 1)+ 0.22[7 5 2]; the convergent angle of the beam, 0.615º and the specimen height from the convergent point, 0.0586 mm; the **ns** and **nd** directions were assumed to be [-1 3 4] and [1 1 1] respectively. That is, the slip plane is (1 1 1) with the inclination angle, 44.7° to the beam direction.

Fig. 2 shows the bright field LACBED pattern for an edge type of dislocation. In this calculation the dislocation depth, y=92.5 nm, the Burger vector, **b**= [0 -½ ½] and 11 beams with **g**=(1 -1 1) systematic row of reflections were given. Also the assumption of **ns**//**nd** was given to get the same pattern as calculated with HW equations. The vector of the dislocation line was assumed to be [3 1 0] to see the case as an edge type of dislocation, where the angle between **b** and dislocation line is about 77. In fig. 3a and b, the Burger vector, **b**= [0 -½ ½], y=92.5 nm, and 8 beams are given in calculations. In this case the vector of dislocation line was assumed to be [1 -1 1], and the angle between **b** and the dislocation is about 35, which may mean a screw type of dislocation. In fig. 3a, the assumption of **ns**//**nd** was also given, but in b the **nd**=[111] unit vector was input in calculations.

Discussion: As seen in fig. 2 and 3, Cherns and Prestons rule generally holds. But calculations also showed that if dislocations lied near specimen surface (in this case, y is less than 40 nm or greater than 145 nm), the contrast of n-fringes of splitting **g** reflection line became weaker. Also the inclination of the slip plane of dislocation causes contrast weak as seen in fig. 3b. The experimental proof for this theoretical prediction would be interested. Finally one must note that to see n-fringes clearly, the separation between dislocations or the projected length of dislocations to the micrograph must be greater than an order of 50 nm.

References

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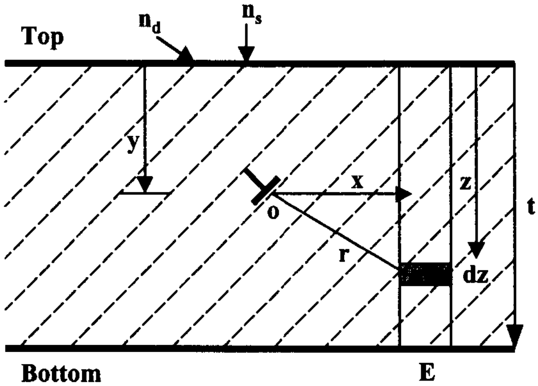

Fig. 1. Schematic diagram of a dislocation at the **o** and slip planes (dot lines), lying perpendicularly to the paper plane.

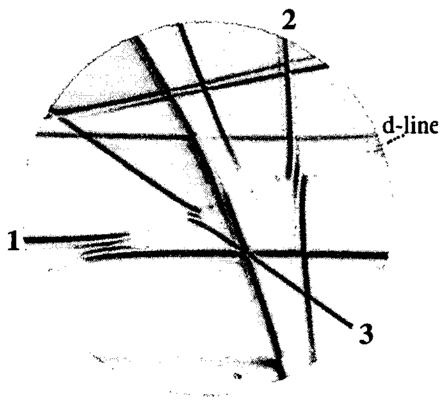

Fig. 2

The bright field LACBED pattern for an edge type of dislocation. The radius of the pattern is 629 nm. The lines of 1, 2 and 3 are for reflections of **g**=3 -3 3 (**g.b**=3), **g**=5 3 -1 (**g.b**=-2) and **g**=-7 1 -3 (**g.b**=-2), respectively. The effect of the inclination of the slip plane containing dislocation line(d-line) on diffraction is ignored.

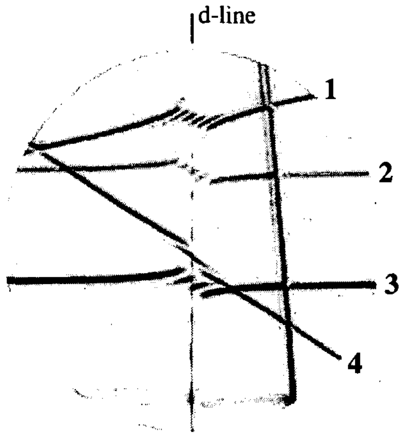

Fig. 3a

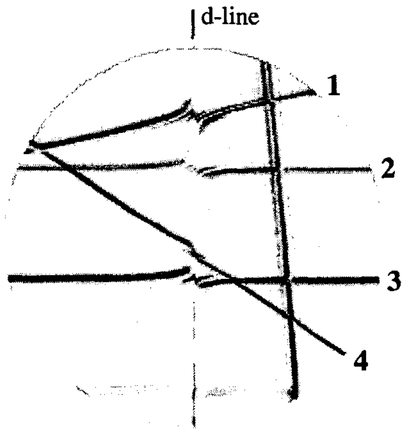

Fig. 3b

The bright field LANCED pattern for a screw type of dislocation. The lines of 1, 2, 3 and 4 are for reflections of g=-3 5 -5 (g.b=-5), g=4, -4, 4 (g.b=4), g=3 -3 3 (g.b=3) and g=-7 1 -3 (g.b=-2), respectively in order. In the fig.3a the effect of the inclination of the slip plane is ignored, but in b the effect is included.