

# THE OUTER FRINGE OF A STACKING FAULT

By A. K. HEAD\*

[Manuscript received May 26, 1969]

## Summary

The rule of Hashimoto, Howie, and Whelan, much used in electron microscopy for determining the nature of stacking faults, is known to be true when the specimen thickness  $t$  is sufficiently great. It is shown that sufficiently great means that the product  $(t/\xi_g)(\xi_g/\xi'_g)$  must be greater than 0.2 for bright field or greater than 0.25 for dark field, these values being for reasonable deviations from the Bragg condition.

## INTRODUCTION

In electron microscopy the nature of stacking faults in face-centred cubic crystals is usually determined by using the rule introduced by Hashimoto, Howie, and Whelan (1962). This states that if  $g$  is the diffracting vector and  $R$  the displacement vector of the fault, then the outer fringe of the bright field stacking fault image on a positive print is white if  $g \cdot R = +\frac{1}{3} \bmod(1)$  and black if  $g \cdot R = -\frac{1}{3} \bmod(1)$ . White and black are used as convenient descriptions of intensities which are greater than or less than the background intensity of nearby perfect crystal. For the dark field image, the outer fringe at the top surface is given by the same rule as for a bright field, and the outer fringe at the bottom surface is reversed, i.e. black for  $g \cdot R = +\frac{1}{3}$  and white for  $g \cdot R = -\frac{1}{3}$ .

It is known that this rule is true when the specimen is sufficiently thick but there is little information available as to what is the minimum thickness that is sufficient. This question is examined in this paper and a convenient criterion is established.

## RESULTS AND DISCUSSION

At the edge of a stacking fault image there is a jump in intensity gradient on passing from the constant intensity of background outside the fault into the fault itself. This jump in intensity gradient for a bright field image is given by (Head 1969)

$$\Delta I' = Q P_{00}^* P_{g0} \{ \exp(2\pi i g \cdot R) - 1 \} + \text{c.c.}, \quad (1)$$

where  $Q = i - \xi_g/\xi'_g$ ,  $P_{00}$  and  $P_{g0}$  are elements of the scattering matrix for a perfect crystal of thickness  $t$ , and c.c. indicates complex conjugates. The bright field rule of Hashimoto, Howie, and Whelan is then that  $\Delta I'$  is positive or negative according as  $g \cdot R$  is  $+\frac{1}{3}$  or  $-\frac{1}{3}$ .

The jump in intensity gradient given by (1) has been calculated for four values of the anomalous absorption  $\xi_g/\xi'_g$  and the results are given in Figures 1(a)–1(d) for a range of thickness  $t$  and deviation from the Bragg condition  $w$ . A dot indicates where the rule of Hashimoto, Howie, and Whelan is correct and the letters B, W, and

\* Division of Tribophysics, CSIRO, University of Melbourne, Parkville, Vic. 3052.

R where it is incorrect. The letter B indicates that the outer fringe is black for  $g.R$  both  $+\frac{1}{3}$  and  $-\frac{1}{3}$ , the letter W that the outer fringe is white in both cases, and the letter R that the rule of Hashimoto, Howie, and Whelan is reversed.

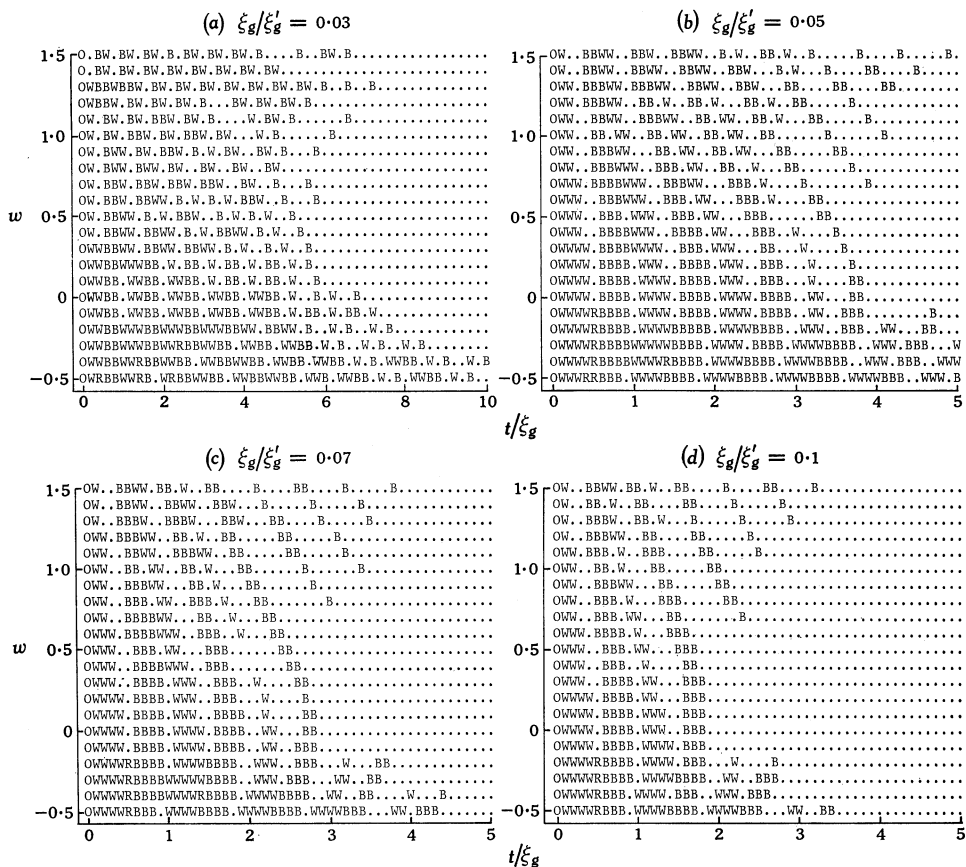


Fig. 1.—Validity of bright field rule of Hashimoto, Howie, and Whelan (1962) tested for a range of values of  $t$  and  $w$  and four values of  $\xi_g/\xi'_g$ :

- bright field rule correct,
- B outer fringe black for  $g.R = +\frac{1}{3}$  and  $-\frac{1}{3}$ ,
- W outer fringe white for  $g.R = +\frac{1}{3}$  and  $-\frac{1}{3}$ ,
- R bright field rule reversed.

For the dark field image the jump in intensity gradient is given by

$$\Delta J' = -Q P_{gg} P_{g0}^* \{\exp(2\pi i g.R) - 1\} + \text{c.c.} \quad (2)$$

at the top surface and by

$$\Delta J' = Q^* P_{00}^* P_{g0} \{\exp(2\pi i g.R) - 1\} + \text{c.c.} \quad (3)$$

at the bottom surface. Figures 2(a) and 2(b) follow from (2) and (3) and are for two values of anomalous absorption. A dot indicates where the dark field rule of

Hashimoto, Howie, and Whelan is correct at both surfaces and the letter X that it is incorrect at one or other or both surfaces. The cases of failure are not categorized as for bright field since there are now 15 possibilities.

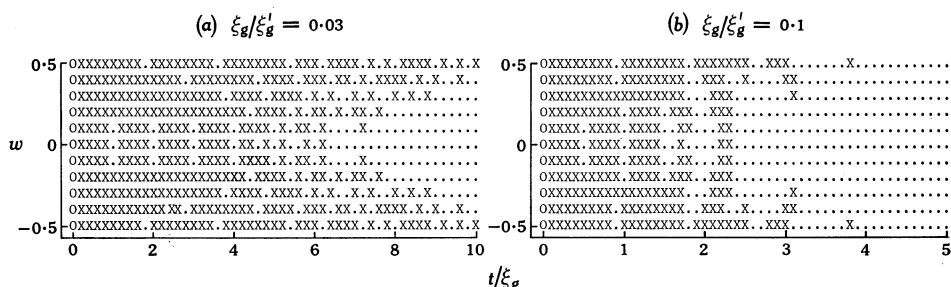


Fig. 2.—Validity of dark field rule of Hashimoto, Howie, and Whelan (1962) tested for a range of values of  $t$  and  $w$  and two values of  $\xi_g/\xi'_g$ :

- dark field rule correct,
- X dark field rule incorrect.

The rule of Hashimoto, Howie, and Whelan is certainly true in the asymptotic limit of large thickness when one Bloch wave is effectively completely absorbed. The differential absorption between Bloch waves depends on the product  $(t/\xi_g)(\xi_g/\xi'_g)$  which suggests that the start of the asymptotic region may also depend on this product. Restricting attention to those values of  $w$  for which there is high anomalous transmission, that is,  $w$  small and positive for bright field and near zero for dark field, it will be seen from Figures 1 and 2 that the asymptotic region is given by:

$$\text{bright field} \quad (t/\xi_g)(\xi_g/\xi'_g) > 0.2,$$

$$\text{dark field} \quad (t/\xi_g)(\xi_g/\xi'_g) > 0.25.$$

An example of the failure of the rule of Hashimoto, Howie, and Whelan is shown in Figure 1(b) of the preceding paper by L. M. Clarebrough (present issue, pp. 559–67). This shows the bright field image of a stacking fault for 18 different values of parameters. For all cases  $g \cdot R = -\frac{1}{2}$  so the outer fringe would be expected to be black, but in one case it is obviously white. This case ( $t = 3.2\xi_g$ ,  $\xi_g/\xi'_g = 0.03$ ,  $w = 0.15$ ) is correctly predicted by Figure 1(a). Another case ( $t = 3.2$ ,  $\xi_g/\xi'_g = 0.05$ ,  $w = 0.15$ ) is predicted by Figure 1(b) also to have a white outer fringe but it is not visible in the micrograph of Clarebrough's paper. In this case the amplitude of the fringe is not sufficiently different from background to register and the net effect is that the fault appears to have a black outer fringe but the overall width of the fault appears significantly smaller than its true size.

#### ACKNOWLEDGMENT

The author would like to thank Dr. L. M. Clarebrough for discussions and a preview of his paper.

#### REFERENCES

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