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Apparent Doubling of Kikuchi Lines Inside Strong Bands

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Doubling of Kikuchi lines inside strong bands has been reported previously in electron diffraction patterns from MgO. The 'doubling' is now explained as being due to two different lines, which at the particular wavelength employed in the experiment are very close. Owing to strong enhancement from multiple beam interactions inside the band, one of the lines is visible only in this region. Further examples of such doubling are shown in patterns from MgO and natural spinel. The observed patterns are compared with theoretical calculations.

In a recent paper on dynamic effects in diffuse scattering from MgO, doubling of the deficient (820) Kikuchi line inside the (002) band was reported by two of us (Gjønnes & Watanabe, 1966). A pattern showing the doublet is reproduced in Fig. 1. The doubling was not theoretically explained; it was pointed out, however, that 4-beam calculations revealed an appreciable enhancement of contrast inside the band for Kikuchi lines crossing the band at right angles. It is the purpose of this note to present an explanation of the reported 'doubling' as being due to two different lines, one of which is visible only inside the band because of enhancement from multiple beam interactions in this region.

This explanation occurred to us during further experimental and theoretical studies on Kikuchi lines from other crystals. Effects reminiscent of the doubling were occasionally observed, as in the pattern reproduced in Fig. 2, taken from a small chip of natural spinel, $MgAl_2O_4$. Inside the (400) band a double line is clearly seen. Detailed analysis of this pattern and comparison with a pattern taken at a different voltage revealed that this particular doublet was composed of the line (084) and the central part of the $(2n+1,\bar{9},\bar{5})$ envelope. On changing the voltage from 100 kV to 80 kV, the (084) line and the envelope were moved apart and there was no appearance of a doublet.

In view of this, we re-examined the MgO pattern (Fig. 1) and found that at wavelengths close to 0·044 Å (corresponding to 72·5 kV) there would be near overlap of the deficient lines (820) and (14,4,0). An independent determination of the wavelength using the Kikuchi lines $(\bar{2}0\bar{8})$, $(\bar{2}08)$ and (820), (see Fig. 1) gave $\lambda = 0{\cdot}04393 \pm 0{\cdot}00007$ Å assuming the value $a = 4{\cdot}2119$ Å (Brown, 1965) for the lattice constant of MgO. Assuming the weaker line in the doublet to be (14,4,0), we

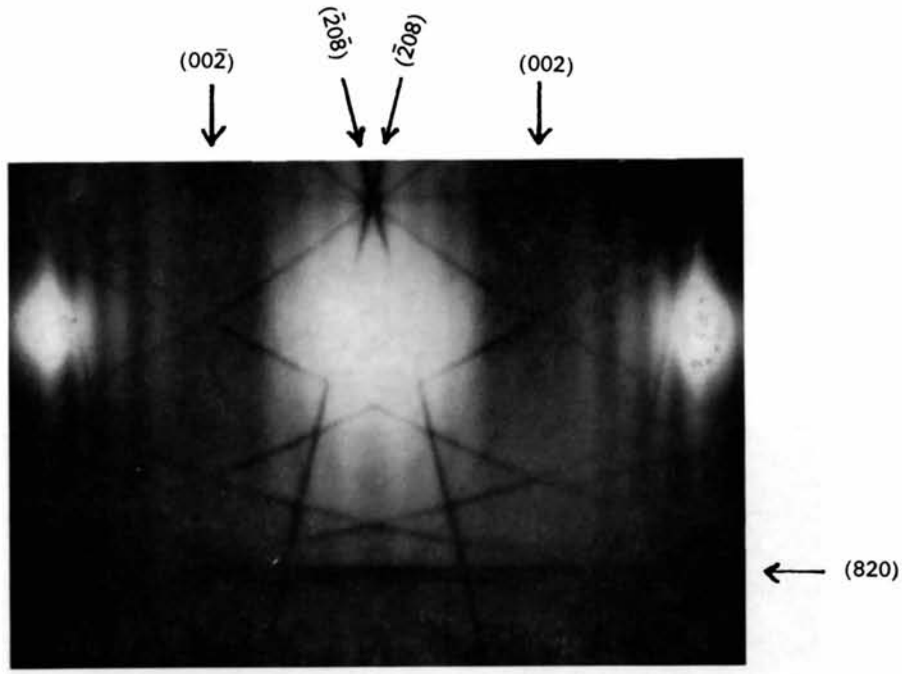

Fig. 1. Transmission Kikuchi pattern from MgO, showing apparent doubling of (820) deficient line inside the (002) band. Nominal voltage 80 kV.

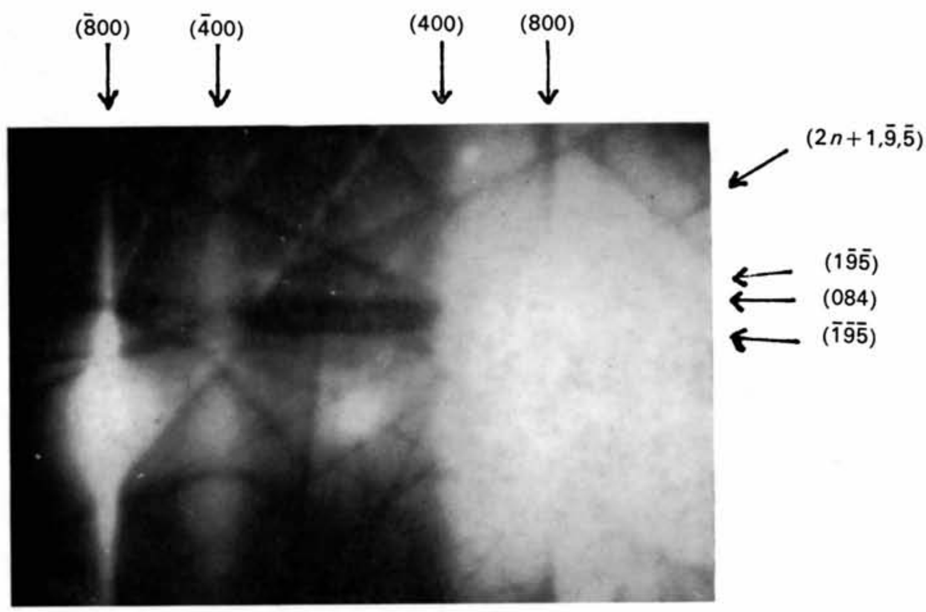

Fig. 2. Transmission Kikuchi pattern from $MgAl_2O_4$ showing apparent doubling of the (084) line inside the (400) band (100 kV).

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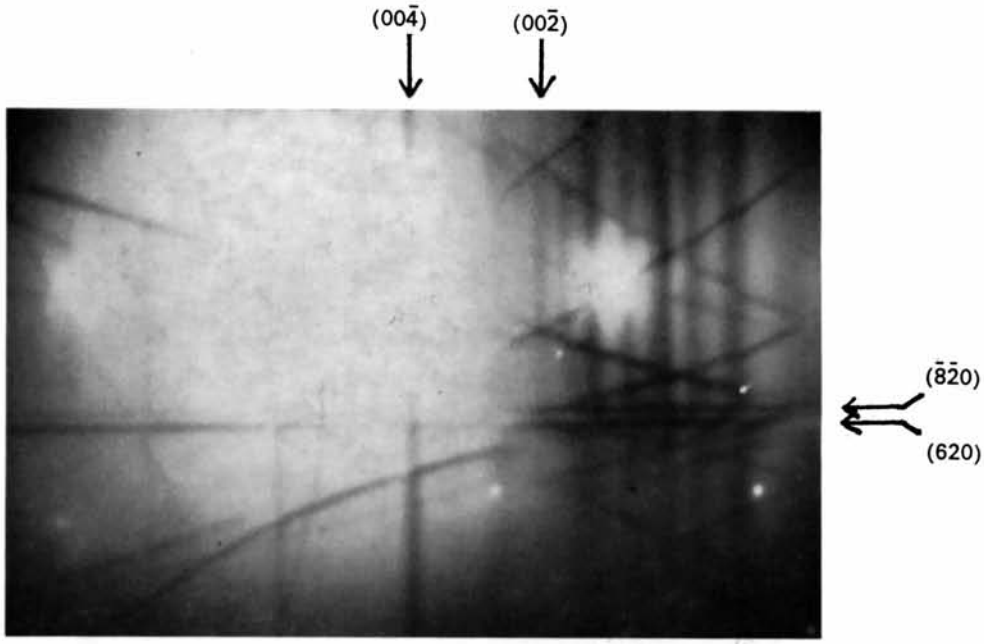

Fig. 3. Transmission Kikuchi pattern from MgO showing $(\bar{8}\bar{2}0)$ and (620) lines at right angles to the (002) band. Nominal voltage 80 kV.

Table 1. *Observed and calculated separations between the* (820), (14,4,0) *and the* ($\bar{8}\bar{2}0$), (620) *lines*

Wavelength (Å)	0·04437	0·04390	0·04369	
Calculated line separation (mm on plate)				
(820) (14,4,0), geometrical	0	0·17	0·24	
(820) (14,4,0), dynamical	0·15	0·23	0·28	
($\bar{8}\bar{2}0$) (620), geometrical	0	0·39	0·55	
Observed line separations (mm)				
(820) (14,4,0)				0·25 ± 0·02
($\bar{8}\bar{2}0$) (620)				0·56 ± 0·02

obtained $\lambda = 0{\cdot}04389$ Å from the three lines ($\bar{2}0\bar{8}$), ($\bar{2}08$) and (14,4,0).* From simple geometrical considerations one finds that other lines also are expected to be very close at this particular wavelength, *viz.* ($\bar{8}\bar{2}0$) and (620) as well as ($1\bar{4},\bar{4},0$) and ($\bar{6}\bar{2}0$). Incidentally, a plate taken at the same time, (Fig. 3) does show the ($\bar{8}\bar{2}0$) and (620) lines with very nearly the predicted separation. Here both lines can be seen also outside the band, although with considerably diminished contrast.

We then calculated the deficient contrast profile across (820) and (14,4,0) inside and outside the (002) band, using different wavelengths and including the 9 beams (000); (002); (00$\bar{2}$); (820); (822); (82$\bar{2}$); (14,4,0); (14,4,2); (14,4,$\bar{2}$), (the results are summarized in Table 1); by interpolation the best agreement with the observed separation of the doublet was found for $\lambda = 0{\cdot}0438 \pm 0{\cdot}0001$ Å, in good agreement with the other determination of the wavelength. The corresponding theoretical profiles, inside and outside the (002) band are shown in Fig. 4; it is seen that the (14,4,0) line is very narrow outside the band and hence not expected to be visible in this region. Inside the band the lines are displaced slightly away from their kinematical positions – the order of magnitude of the displacement of (820) agrees with what can be seen on the plate.

* Details on the determination of wavelength from Kikuchi patterns will be discussed elsewhere; see however Uyeda, Nonoyama & Kogiso (1965).

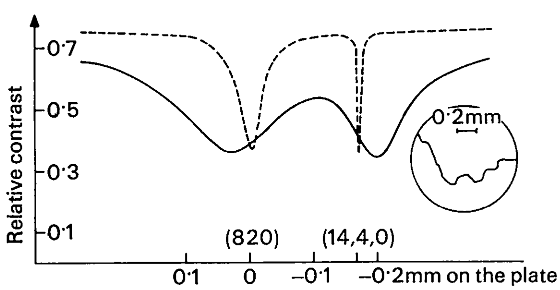

Fig. 4. Calculated contrast profiles across the (820) and (14,4,0) deficient lines. Full line: inside the (002) band; dotted line: outside the (002) band. Distances in mm on the plate are referred to the kinematical (820) position, negative distances correspond to negative (820) excitation errors ($\lambda = 0{\cdot}04390$ Å). Inset: Photometer trace (not to scale) of the observed doublet, inside the (002) band.

Calculated and measured ($\bar{8}\bar{2}0$), (620) line separations are also given in Table 1; here the separation was measured outside the band, where dynamical corrections to line positions are negligible. There is a slight discrepancy, of about 0·0002 Å, between the wavelength which can be determined from these lines (Fig. 3) and the two determinations from Fig. 1, indicating, perhaps, a slight drift in the high tension between these exposures.

A photometer trace of the observed pattern was used to measure the (820), (14,4,0) line separation on the plate (see inset of Fig. 4). The two lines do not appear so well resolved in the experimental as in the calculated curve. This may be due to insufficient resolution; in view of the very small angles and plate distances involved, the resolution would have to be extremely good in order to reproduce all details.

It should be mentioned that we have not been able to explain the double Kikuchi lines reported by Menzel-Kopp & Menzel (1962) in the same way.

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