DIFFRACTION OF X-RAYS BY THE ALLOY $AuCu_3$

THE alloy $AuCu_3$ has an ordered structure below 391° C. If a disordered alloy is heat-treated below this temperature, superlattice lines appear on X-ray powder photographs, and the development of the perfectly ordered structure can be followed by observation of these superlattice lines; they are diffuse at first and increase in sharpness as the heat-treatment progresses, until they become as sharp as the main lines.

A simple explanation of this phenomenon is that the domains of similar order (anti-phase domains) are initially much smaller than the crystal grains in which they exist; on this basis, Jones and Sykes[1] showed that it should be possible to derive the sizes of the anti-phase domains from the breadths of the superlattice lines. Detailed investigation showed, however, that different lines gave different results, and the problem remained unsolved.

Wilson[2] has produced a method of calculating the diffraction effects given by such an alloy, and has shown that the breadths of the various superlattice lines will be dependent upon the way in which one domain is bounded by its neighbours; he tried the effect of imposing certain conditions on the boundaries and found one model that gave fair agreement with Jones and Sykes' results. He pointed out, however, that it was possible that other models may give as good agreement or even better.

We have attempted to test Wilson's theory by taking X-ray oscillation photographs of a single crystal; such photographs contain much more evidence than powder photographs and so should provide a much more stringent test of the theory. Similar considerations have led Strijk and MacGillavry[3] also to carry out experimental work on a single crystal to test a theory of their own[4]. Their theory is rather different from Wilson's, and their experimental results do not fit in perfectly with either. We believe, however, that their experimental methods are not well suited to differentiate between the two theories, as the following considerations show. MacGillavry and Strijk's theory would lead to sharp reciprocal points for the main reflexions and diffuse spots all of the same shape and with cubic symmetry for the superlattice reflexions; Wilson's theory leads to a more complicated representation which is shown in Fig. 1. MacGillavry and Strijk used a rod-like crystal with its length approximately in the [110] direction, and they investigated the distribution of intensity only in the plane perpendicular to [110]. Therefore, they have not checked that the spots have cubic symmetry, as their theory demands; nor have they disproved Wilson's theory, since this leads to similar shapes for all spots with $h + k = 0$.

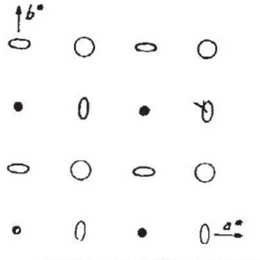
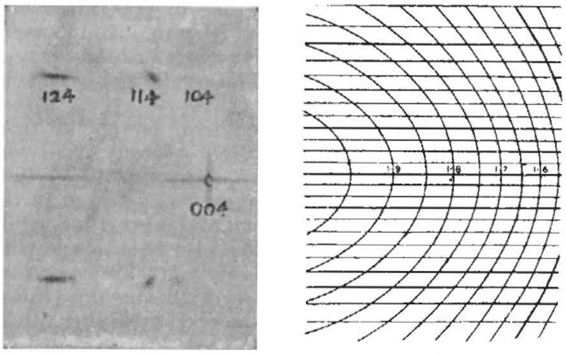


Fig. 1. RECIPROCAL LATTICE OF $AuCu_3$ ACCORDING TO WILSON'S THEORY



a b

Fig. 2 *a* and *b*. PORTION OF OSCILLATION PHOTOGRAPH OF $AuCu_3$ AND CORRESPONDING PORTION OF BERNAL CHART

Our crystal is smaller than that used by MacGillavry and Strijk; it gives main reflexions that are quite small, and so the shapes of the superlattice reflexions stand out clearly. Preliminary results show qualitative agreement with Wilson's theory; this is shown by Fig. 2, which is part of an oscillation photograph about the [100] axis.

It will be seen that the spots are not all of the same shape; for example, 114 is elongated at an angle to the layer line and 124 is elongated along the layer line. Such an effect cannot be produced by differences in the geometrical conditions for reflexion due to difference in θ. Moreover, the slope of the spot 114 is about the same as that of the curves on the Bernal chart (Fig. 2*b*) at the same point, which means that the elongation is parallel to one of the reciprocal axes. In this respect, the results are in accordance with the reciprocal lattice shown in Fig. 1.

Oscillation photographs do not provide a complete test, as the spots recorded represent projections of the reciprocal-lattice spots on to a plane. We are, therefore, undertaking a more detailed investigation of sections of the spots, and this should provide quantitative evidence by means of which the two theories can be adequately tested.

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[1] Jones and Sykes, *Proc. Roy. Soc.*, A, **166**, 376 (1938).

[2] Wilson, *Proc. Roy. Soc.*, A, **181**, 360 (1943).

[3] Strijk and MacGillavry, *Physica*, **12**, 129 (1946).

[4] MacGillavry and Strijk, *Physica*, **11**, 369 (1946).

IN treating the integral breadths of the lines in the powder photographs of $AuCu_3$ obtained by Jones and Sykes[1], it was not necessary to consider the actual shapes of the regions of high intensity in the reciprocal lattice, the apparent particle-size of the *hkl* reflexion being given directly by

$$\varepsilon = (J_0 V_0)^{-1} \int V_t J_t dt, \qquad (1)$$

where V_t is the volume common to the crystal and its 'ghost' shifted a distance t in the *hkl* direction, and J_t is the mean value of the product FF^* for two cells separated by a distance t in the *hkl* direction[2]. The distribution of intensity in the reciprocal lattice may be obtained from the same functions. If a, b, c