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On the structure of CuAu II revealed by electron diffraction.

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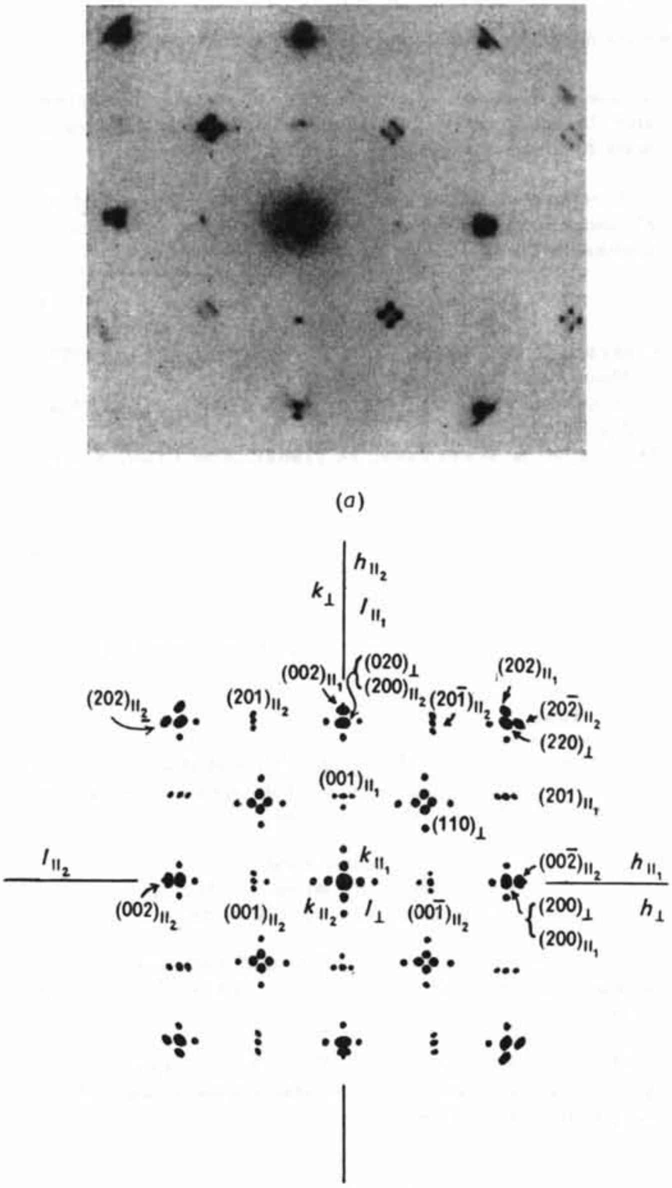
Since the previous short communication (Ogawa & Watanabe, 1952) we have obtained the electron-diffraction pattern shown in Fig. 1(*a*) from a well orientated alloy film of CuAu II containing 50 atomic % gold, quenched at 380° C. In this pattern sharp crosses consisting of four spots appear at some of the positions of superlattice reflexion, being accompanied by subsidiary maxima, and regularly spaced satellites occur around the positions of normal reflexion, especially conspicuously around the direct spot. The former phenomenon arises from the manner of ordering of the alloy and can be clearly interpreted by the orthorhombic structure of CuAu II in which antiphase domains 5*a* thick are lined up in the direction of one of the *a* axes in the tetragonal lattice, as concluded by Johansson & Linde (1936). The latter phenomenon, which was first found in this experiment, means, on the other hand, that an actual defect exists periodically in the crystal lattice.


(*a*)

(*b*)

Fig. 1. (*a*) The electron-diffraction pattern of the orientated CuAu II film quenched at 380° C. Crosses consisting of four spots are sharp and distinct, accompanied by satellites. These are visible also around the normal spots, especially clearly around the direct spot. (*b*) The explanation of the photograph shown in (*a*).

At each boundary between antiphase domains in CuAu II the distribution of gold and copper atoms is asymmetrical (Fig. 2). Owing to this and the tetragonality ($c/a \sim 0{\cdot}92$), a repulsive force is considered to act between the two neighbouring planes *A* and *B*. Thus an elongation $\delta . a$ of the distance *AB* may arise. The Laue function for a lattice such that 'out-of-step' occurs at each distance *Ma* along the *x* direction, and that the total extent of the lattice in this direction is *NMa*, is

$$G = G_1 . G_2 = \frac{\sin \pi M A_x}{\sin \pi A_x} \cdot \frac{\sin \pi N\{(M+\delta)A_x - \frac{1}{2}(A_y+A_z)\}}{\sin \pi\{(M+\delta)A_x - \frac{1}{2}(A_y+A_z)\}} ,$$

where A_x, A_y and A_z are continuous variables in the reciprocal lattice corresponding to the tetragonal lattice and where *M* is 5 in the present case, if the parts in the function, independent of the existence of 'out-of-step', are neglected. If *N* is far greater than *M*, the positions of maxima of *G* are determined by those of G_2, and this function corresponds to the lattice which behaves as if it has an elongated lattice constant $a(1+\delta/M)$ in the *x* direction. For this reason δ can be determined from the pattern of electron diffraction and more precisely from that of X-ray diffraction; from the data which Johansson & Linde have already reported δ is estimated to be 0·015. At the positions of normal reflexion the function G_2 becomes

$$\frac{\sin \pi N(M+\delta)A_x}{\sin \pi(M+\delta)A_x} ,$$

which has its maxima at $A_x = (Mh+n)/(M+\delta)$, where *h* and *n* are integers and $|n| < M$. Intensities of satellites around normal spots can be deduced from values of the function G_1,

$$\frac{\sin \pi(h+n/M)\delta}{\sin \pi n/M} ,$$

and the crystal structure factor. Around the direct spot their strong intensities can be qualitatively explained by the fact that the atomic scattering factor for electrons becomes abnormally large in the range of very small $\sin\theta/\lambda$ (this value is 0·026 at a position of the first satellite around the direct spot) owing to the ionized state of gold and copper atoms, characteristic of the alloy.

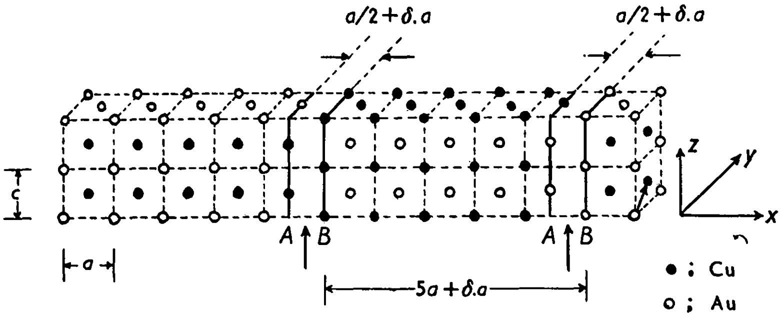


Fig. 2. The ordered structure of CuAu containing antiphase domains in the x direction.

Around the other normal spots, however, the calculated intensities for satellites are far smaller than those actually observed. For this and other reasons we consider satellites actually observed around the normal spots to be the mere repetition of those around the direct spot, i.e. the secondary elastic scattering effect occurs in our film (owing to the small angle of Bragg reflexion in electron diffraction and to the mosaic structure in an evaporated film) as Cowley, Rees & Spink (1951) observed in films of long-chain paraffins.

Thus, the satellites around the direct spot and the other normal spots can be explained by the existence of the elongation $\delta.a$ at each boundary between antiphase domains and by the characteristics of electron diffraction. It is exceedingly difficult to observe these satellites by means of X-rays, owing to their depressed intensities, and the inherent lattice defect in CuAu II has therefore been hitherto overlooked.

A report in detail will appear in the *Journal of the Physical Society of Japan*. We wish to express our sincere thanks to Dr G. Honjo for his kind discussions.

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Space group of fluoranthene.

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The molecular formula of fluoranthene, first given as $C_{15}H_{10}$ by Fittig & Gebhard (1877), was later established unambiguously by Braun & Anton (1929) as $C_{16}H_{10}$. Groth (1906–19) gave the following data for the monoclinic crystals:

$$a:b:c = 1{\cdot}495:1:1{\cdot}025,\ \beta = 97^\circ\ 10'\ .$$

Single crystals obtained from a concentrated solution in ethanol have been studied by the author.

Goniometric study as well as rotation photographs about different axes gave a different c direction as fundamental, and the following values of the axial lengths and axial angle were obtained:

$$a = 18{\cdot}46,\ b = 6{\cdot}205,\ c = 22{\cdot}11\ \text{Å},\ \beta = 121^\circ\ 45',$$

whence $$a:b:c = 2{\cdot}975:1:3{\cdot}563\ .$$

The density was found by the flotation method to be $1{\cdot}238 \pm 0{\cdot}01$ g.cm.$^{-3}$, whence the number of formula weights $C_{16}H_{10}$ per unit cell is 8. Over-exposed zero-level Weissenberg photographs were taken about the b and a axes by the normal-beam method, giving ($h0l$) and ($0kl$) reflexions respectively. First- and second-level Weissenberg pictures about the b axis were also taken by the equi-inclination method, giving ($h1l$) and ($h2l$) reflexions respectively. The indexing of the spots showed the following conditions of extinctions:

hkl: no systematic extinctions;
$h0l$: present only when $l = 2n$;
$0k0$: present only when $k = 2n$.

Thus the space group is $P2_1/c$ and two molecules of fluoranthene form one asymmetric unit in the unit cell of the crystal.

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