Table 1.

Form	a (Å)	b (Å)	c (Å)	β	Z	Space group
α-Glycylglycylglycine	8·54	4·3	11·4	105·5°	2	Monoclinic
β-Glycylglycylglycine	14·6	4·80	11·69	105·5°	4	Monoclinic
Glycylglycylglycine dihydrate	22·0	9·8	4·7	90°	4	C_{2v}^5

Z = number of molecules per cell.

Table 2.

Form	a (Å)	b (Å)	c (Å)	β	Z	Density (g. cm.$^{-3}$)	Space group
α-Glycylglycylglycine	8·54	4·35	22·96	105°36′	4	1·57	C_{2h}^5
Glycylglycylglycine hemihydrate	16·04	4·64	24·99	112°43′	8	1·52	C_5^4 or C_{2h}^6

Several indications of the structure of the glycylglycylglycine molecules themselves can be deduced from the unit-cell dimensions in conjunction with data obtained with the polarizing microscope. In the case of α-glycylglycylglycine, it is likely that the peptide molecules are lying in an extended, or nearly extended, configuration parallel to the c axis. In the hydrated crystals, evidence seems to show that the peptide molecules are lying parallel to the $40\bar{6}$ plane. These elementary deductions are supported by Patterson projections for both modifications and although no entirely adequate trial structure for either crystal has been found as yet, the investigation is being continued.

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Crosses observed in the electron-diffraction pattern of an orientated CuAu film.

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In order to study the order–disorder problem of CuAu in the form of thin film, a film of orientated gold was first made by vacuum evaporation on a rocksalt cleavage surface heated at 400° C. Then copper was condensed on it at room temperature, the ratio of the thickness of the two films being so controlled that the double film was almost of the equi-atomic ratio of both atoms. After being detached from the rocksalt surface, this double film about 400 Å thick was homogenized at 350° C. for 1 hr., which was sufficient to complete the alloying of the two metals and to cause an ordering process; i.e. the electron-diffraction pattern showed an orientated f.c. tetragonal lattice after this treatment. When this alloy film was again annealed at a temperature immediately below the critical point, there appeared cross-like diffuse spots at some positions of superlattice reflexion in the diffraction pattern, as seen in Fig. 1(a). Patterns like this have been observed by several workers using X-ray methods; for instance, by Guinier & Griffoul (1948) in Cu₃Au and CuAu and by Newkirk et al. (1951) in the alloy CoPt. In the former case, the crosses appeared only at the superlattice reflexion positions, whereas in the latter the normal spots were converted into diffuse crosses. Therefore, our pattern belongs to the former type. Raether (1951) also observed the disc-like cross effect while studying Cu₃Au films by electron diffraction. In our case the crosses could be observed with comparative ease because of the greater intensity of the superlattice reflexion than in the case of Cu₃Au.

According to Guinier & Griffoul, the crosses can arise from the formation of anti-phase domains in the course of ordering, and the domain size can be calculated from the width of the cross. The thickness of an anti-phase domain thus calculated from our pattern was $4a$ in the direction of the a axis. According to Johansson & Linde (1936), such a lattice may be considered as orthorhombic. The ratio of the two axes perpendicular to the c axis, which could be determined with a polycrystalline alloy film* treated in the same way as the orientated film mentioned above, was 10, from which the thickness of an anti-phase domain of $5a$ resulted. The rough coincidence of the estimated values in both cases was thus obtained.

The condition of preparing the CuAu films was such that the (100) plane of an initially deposited orientated gold was parallel to the surface of the film, and in the homogenized alloy film the c axis was distributed in the directions of the three cubic axes of the gold. Therefore, in Fig. 1(a) a mixture of these orientations appears, which is illustrated by three kinds of marks in Fig. 1(b).

Fig. 2 shows a reciprocal lattice of CuAu containing anti-phase domains, cross-like platelets being indicated at the positions of superlattice reflexions as in the case of Cu₃Au (Guinier & Griffoul, 1948). In the ordered CuAu

* A break-up of a superlattice reflexion arising from anti-phase domains has previously been observed in the (110) ring of the polycrystalline Au₃Cu film (Ogawa & Watanabe, 1951) annealed at 200° C. for 150 hr. This fact, however, was overlooked at that time.
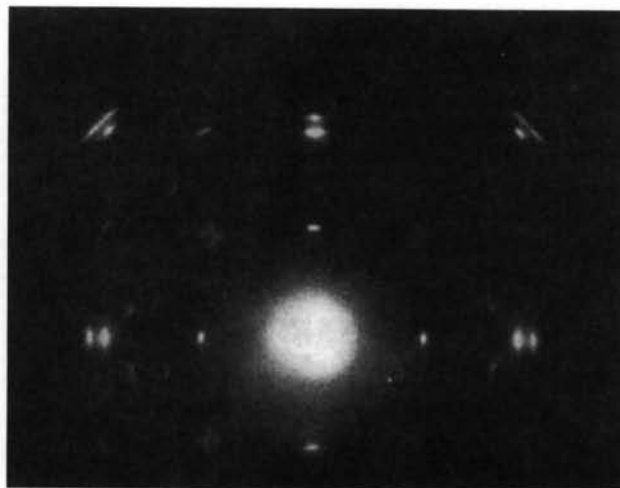
(a)
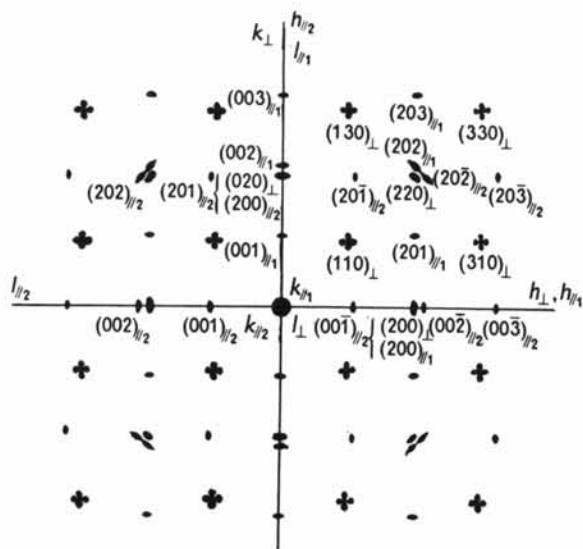
(b)

Fig. 1. (a) The electron-diffraction pattern of the orientated CuAu film, showing the crosses at some positions of superlattice reflexion. (b) The explanation of the photographs shown in (a). The spots (hkl) belong to a set in which the c axis is perpendicular to the film surface; the spots $(hkl)_{//1}$ and $(hkl)_{//2}$ belong to the other two sets in which the c axes are lying in this surface.
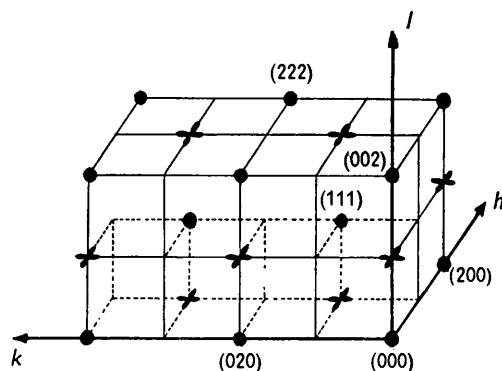
Fig. 2. The reciprocal lattice of the CuAu superlattice containing anti-phase domains. Circles: normal reflexion points; crosses: superlattice reflexion points.

the superlattice reflexions for which $h+k$ is odd must vanish (the c axis corresponds to l and is perpendicular to the alternate planes of gold and copper) and the crosses should remain only in those cases in which their planes are perpendicular to the c axis, as shown in Fig. 2. Consequently, the observed crosses belong only to such

a set in which the c axis is perpendicular to the film surface. The reflexion spots $(001)_{//1}$, $(00\bar{1})_{//1}$, $(001)_{//2}$ and $(00\bar{1})_{//2}$ in Fig. 1(b), corresponding to the other two sets, show the elongation in a perpendicular or in a horizontal direction, which arises from the intersection of platelets with the reflexion sphere.

When the film showing the crosses was heated above the transition point and, after quenching, was again annealed at about 400° C., the crosses disappeared; this might be due to the vanishing of the orientation in which the c axis was perpendicular to the film surface.

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A graphical method for the determination of the unit-cell dimensions of non-cubic materials from X-ray powder photographs.

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It is often necessary to determine the unit-cell dimensions of a non-cubic substance from powder photographs when there is an insufficiency or even an absence of suitable reflexions; and it is the purpose of the present note to describe a simple graphical method of doing this that is always applicable to tetragonal and hexagonal crystals, and may be applied to orthorhombic crystals in many instances. It requires that the measured spacings be first corrected for the usual errors, e. g. by reference to an internal standard. The method due to Cohen (1935) achieves, of course, both the correction of the spacings and the determination of the unit-cell dimensions, but it involves a considerable amount of computation. This is avoided in the present method by carrying out the correction of the spacings and the determination of the unit-cell dimensions in two stages. The method also avoids the danger of a systematic drift which is often inherent in methods of successive approximation.

For a tetragonal crystal we have

$$1/d_{hkl}^2 = (h^2 + k^2)a^{*2} + l^2 c^{*2} ,$$

where the symbols have their usual significance. This may be written

$$c^{*2} = \frac{1}{l^2 d_{hkl}^2} - \left(\frac{h^2 + k^2}{l^2}\right) a^{*2} . \quad (1)$$

A series of values for c^{*2} may be found from this expression by taking the observed spacings for a series of hkl reflexions and assuming a value for a^*. A good value for a^* may sometimes be obtained by one of the well known extrapolation techniques, or by a method such as that

described by Bacon (1948), using the $hk0$ reflexions; but if there is no $kh0$ reflexion, or if there are only one or two, perhaps at small angles, difficulties at once arise. However, let us accept the need for putting a poor value for a^* in equation (1). For a^* we must now put $(a^* + \delta a^*)$, where δa^* is the error in a^*, and (1) becomes

$$c_{obs.}^{*2} = \frac{1}{l^2 d_{hkl}^2} - \left(\frac{h^2 + k^2}{l^2}\right)(a^* + \delta a^*)^2 ,$$

or, neglecting δa^{*2},

$$c_{obs.}^{*2} = c^{*2} - \left(\frac{h^2 + k^2}{l^2}\right) . \; 2a^* \delta a^* . \quad (2)$$

But $2a^* \delta a^*$ is a constant, so that by plotting $c_{obs.}^{*2}$ against $\{(h^2 + k^2)/l^2\}$ a straight line is obtained which, at the value $\{(h^2 + k^2)/l^2\} = 0$, cuts the $c_{obs.}^{*2}$ ordinate at the correct value of c^{*2}. Moreover, the correct value of a^* may be obtained from the slope of the line. Alternatively, a value may be obtained by plotting the observed values of a^{*2} against $\{l^2/(h^2 + k^2)\}$.

The method is clearly applicable, mutatis mutandis, to the hexagonal system, and may be applied to the orthorhombic system as shown below.

For this system we have

$$1/d_{hkl}^2 = h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} .$$

Proceeding as before we may write, for example,

$$c_{obs.}^{*2} = c^{*2} - (2/l^2)(h^2 a^* \delta a^* + k^2 b^* \delta b^*) .$$