between the heavy lines corresponds to a possible combination of $U_{H+H'}$ and $U_{H-H'}$.

The square, defined by (7) and (8), the inequalities of Karle & Hauptman, and the set of lines defined by (1) and (2) include the allowed region entirely. The corners of the square coincide with the intersections of the hyperbolas. This is to be seen immediately from (7a) and (8a), (3a) and (4a). For these points $G_1 = 0$. So these inequalities do not belong to the fundamental set. The inequality of Karle & Hauptman, however, is important for asymmetric structures, as will be shown in the next section.

6. Asymmetric structures

If we consider

$$g_+ = U_{H+H'} - U_H U_{H'} ,$$

we find that it may be written

$$g_+ = \tfrac{1}{2} \sum_{i,j} n_i n_j \left[\exp 2\pi i(\mathbf{h}, \mathbf{r}_j) - \exp 2\pi i(\mathbf{h}, \mathbf{r}_i)\right] \times \left[\exp 2\pi i(\mathbf{h}', \mathbf{r}_j) - \exp 2\pi i(\mathbf{h}', \mathbf{r}_i)\right] .$$

If we apply the inequality of Cauchy in the same way as we did in the proof of (9), we find

$$|U_{H+H'} - U_H U_{H'}|^2 \leqslant (1-|U_H|^2)(1-|U_{H'}|^2) , \quad (10)$$

the relation of Karle & Hauptman. If we write

$$g_1 = 1-|U_H|^2, \; g_2 = 1-|U_{H'}|^2$$

then (10) may be written

$$|g_+| \leqslant \sqrt{(g_1 g_2)} . \quad (10a)$$

The same relation obtains for g_-, which is g_+ after replacing H' by $-H'$.

The relation (10) plays the same part here as does the new inequality (9) for centrosymmetrical structures. We mention without proof, that the inequalities of Harker & Kasper, valid for asymmetric structures, namely

$$|U_H \pm U_{H'}|^2 \leqslant 2(1+\mathrm{Re}\, U_{H-H'}) ,$$

can be derived from (10). Hence the latter implies all known inequalities for asymmetric structures. Combined with its transcription for $U_{-H'}$, it constitutes the fundamental set for U_H, $U_{H'}$, $U_{H+H'}$ and $U_{H-H'}$.

For centrosymmetric structures, however, application of these inequalities leads to the rather poor results (7, 8) in comparison with (3) and (4), which form the fundamental set in this special case (cf. Fig. 1).

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'Mean Strains' in Worked Aluminium

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Experiments have been carried out to investigate the cause of the relative radial displacements of adjacent diffraction spots on some X-ray microbeam back-reflexion photographs of rolled polycrystalline aluminium. Among other causes, it is possible that the displacements are due to the existence, within the material, of particles in which the lattice spacing is different from the average value. From the present experiments it is concluded that a few reflexions from such particles have been found. The stresses required to produce strains of the observed magnitude are of the order of the yield stress of the material.

1. Introduction

It is possible to resolve the continuous Debye–Scherrer rings on normal X-ray back-reflexion photographs of deformed polycrystalline aluminium into discrete reflexions by the use of the X-ray microbeam technique (Kellar, Hirsch & Thorp, 1950). A feature of the microbeam photographs is that not all the reflexions of given indices lie on a ring of definite radius: adjacent reflexions are often displaced radially from one another, and variations in the magnitude of the displacements from point to point give an appearance of waviness around the ring. The effect is very often most marked on photographs of lightly deformed specimens taken with relatively large beam diameters ($\sim 100\,\mu$) (see Hirsch & Kellar, 1952). When smaller X-ray beam

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diameters ($\sim 30\,\mu$) are used to examine more heavily deformed material, this radial displacement of spots is less marked but is still frequently observed. Various possible causes will be considered below; the most important of these is that after deformation the average lattice spacing in different particles may vary, i.e. different particles are subjected to different mean strains. The present experiments have sought to elucidate the causes of the displacements and, in particular, to see whether particles with changed lattice spacings exist.

Müller (1937) observed similar effects on back-reflexion X-ray photographs of annealed metals; he attributed them to variations in lattice spacings amongst the individual grains. The conclusion was criticized by various authors (Bragg & Lipson, 1938; Stephen, 1938). More recently very accurate experiments have been carried out by Frohnmeyer (1951), who concludes that the lattice spacing in annealed high-purity aluminium is constant to $\pm 0{\cdot}05$ X. In their paper, Bragg & Lipson suggested that some of the ambiguities in the interpretation of the earlier work could be removed if the specimen was oscillated over a small angle about the incident beam; this suggestion has been adopted in one of the experiments to be described.

2. Possible causes of the relative radial displacement of spots

In a polycrystalline specimen consisting of perfect crystals of identical lattice parameter, giving no broadening of the X-ray reflexions due to small size, three factors can contribute to a radial scatter of the discrete spots on a back-reflexion Debye–Scherrer ring received on a flat film. First, crystals situated at different parts of the irradiated volume will give reflexions at different distances from the centre of the ring; then, since the divergence of the X-ray beam is finite, crystals can reflect at slightly different angles to the axis of the camera. In practice these two causes are closely connected; estimates of the magnitude of the effects can be obtained from a consideration of the particular experimental arrangement. Thirdly, the wavelength spread of the incident radiation can cause a scatter of the diffraction spots. This effect can be very large as θ approaches 90°.

If the crystals in the specimen are not perfect but give rise to broadened reflexions, owing to their physical state or small size, a further effect must be considered. Crystals of this kind can reflect X-rays over a range of angles; under particular experimental conditions some particles may have the opportunity of reflecting over only a part of their total range. The spots on the X-ray photographs will then vary in size and their centres will not necessarily lie on a ring of definite radius.

Finally, if different crystals in the specimen have different values of the lattice parameter, the individual reflexions will occur at slightly different Bragg angles and hence the centres of the spots will be radially displaced from each other.

It should be noted that the radial scatter can be clearly seen only if diffraction spots occurring near to each other on the ring show large relative displacements; a slow variation in the radius of the ring is difficult to observe.

3. Experimental methods

Two experiments have been carried out to investigate the causes of the relative radial displacements of diffraction spots.

In the first an X-ray back-reflexion photograph of lightly deformed polycrystalline aluminium was taken using a relatively large beam diameter ($\sim 100\,\mu$) but with the incident beam divergence as small as possible. Two exposures of the same Debye–Scherrer ring from the same irradiated volumes were taken at different specimen–film distances, other experimental conditions being left unchanged. These experiments show (*a*) whether the waviness of the ring can be eliminated from a photograph taken under carefully controlled conditions, and (*b*) whether the diffracted rays giving rise to the displaced spots are divergent or parallel.

In the second experiment a heavily rolled specimen was oscillated during the exposure about a vertical axis accurately perpendicular to the incident beam of small diameter ($\sim 30\,\mu$). Under these conditions the effects of the wavelength spread of the incident radiation and the ability of a particle to reflect X-rays over a range of angles are as follows. Since each particle is now able to reflect the complete characteristic spectral distribution in the incident beam, the reflexion spot is drawn out into a streak. The position of maximum intensity of the streak corresponds to the reflexion of the component of maximum intensity and thus, in the absence of factors other than wavelength spread, the centres of gravity of all reflexions will lie on a ring of definite radius. Similarly, during the oscillation the particle has the opportunity of reflexion over the whole of its reflecting range and so the centre of gravity of the reflexion will correspond in position to a reflexion by a perfect crystal of large size.

However, apart from any effect of different mean strains within the particles, in this experiment there is still a possible shift in the positions of the intensity maxima of the streaks due to the different positions of the reflecting particles within the irradiated volume. The magnitude of this shift can be evaluated from the geometry of the experimental arrangement. It is necessary to determine the largest distance between the maxima of streaks on the film due to particles situated anywhere within the irradiated volume. In the geometrical treatment the irradiated area must be divided into two parts, in one of which particles receive radiation from the whole of the focus whilst in the other radiation is received from only part of the focus. For each of these areas, an expression for the largest distance between intensity maxima on the streaks is found. Which is the greater of the two expressions depends on the particular experimental arrangement. The maximum possible separation for the 422 ring used in this work is typically 15 μ; there can however be a large scatter of the streaks if θ is much less than 67°. A detailed account of the derivation of the expressions may be found elsewhere (Kelly, 1953).

Thus if after oscillation of the specimen the positions of the maximum blackening of the streaks on microbeam photographs of the 422 ring of worked aluminium have a radial separation which exceeds the value given above, it must be concluded that particles with different mean strains exist within the metal.

4. Experimental results

The experiments were carried out on spectroscopically pure aluminium (purity 99·99%, Johnson, Matthey Ltd, J. M. 340) deformed by rolling. After deformation, the specimens were etched in a mixture of hydrofluoric acid, hydrochloric acid, nitric acid and water to remove any surface contamination effects.

The X-ray pattern obtained from a lightly rolled specimen ($\sim$4% reduction in thickness), using an X-ray beam of diameter 110 μ, is shown in Fig. 1. Two exposures of the 422 ring are shown at specimen–film distances of 10 mm. and 16 mm. The angular divergence of the incident beam was minimized; an average value of $1{\cdot}6 \times 10^{-3}$ rad. was found, using the method of Hirsch & Kellar (1951). No marked waviness of the ring is apparent although the diameter of the area of specimen irradiated was $\sim$130 μ. Thus, with well collimated beams the radial scatter of the diffraction spots can be reduced even if the volume irradiated is large. However, a closer microscopic examination of the photograph revealed positions around the ring where the centres of adjacent spots are radially displaced with respect to one another. Corresponding measurements of these displacements on the two rings are compared in Table 1.

If these relative displacements are due solely to a positional effect they should be the same on both

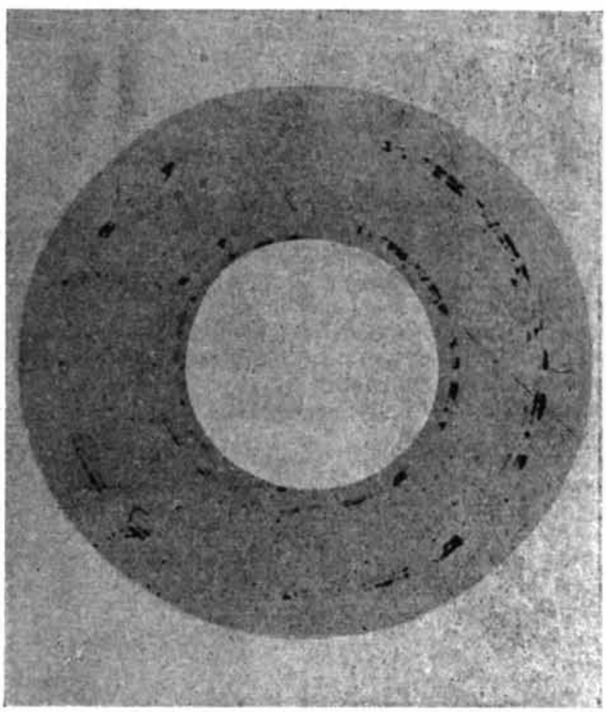

Fig. 1. X-ray microbeam back-reflexion photograph of lightly rolled aluminium. Beam diameter 110 μ; the two prominent rings are the 422 reflexion, Cu $K\alpha$ radiation; specimen–film distances of 16 mm. (outer ring) and 10 mm. (inner ring).

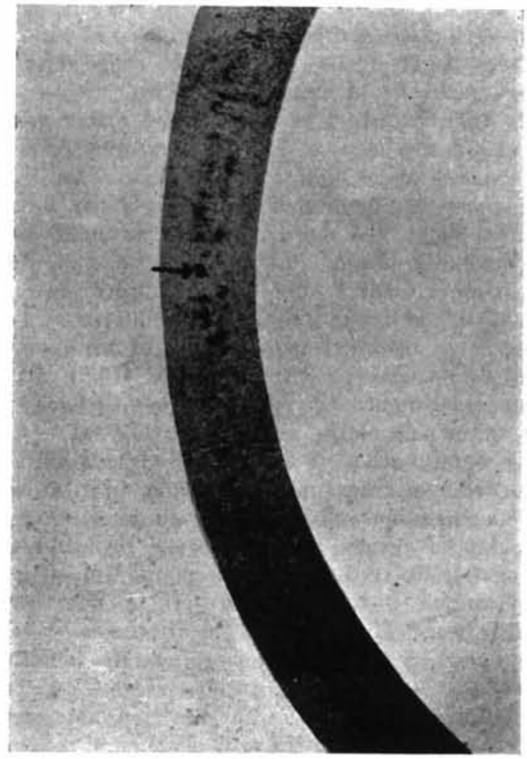

Fig. 2. Part of an X-ray microbeam back-reflexion photograph from an oscillated specimen of heavily rolled aluminium. The arrow indicates diffraction spots with radially displaced central regions. Beam diameter 30 μ; 422 reflexion, Cu $K\alpha$ radiation.

Table 1. *Measurements of the relative displacement of spots on the 422 ring of 4% reduced aluminium*

Beam diameter 110 μ; Cu $K\alpha$ radiation.

Inner ring (R=10 mm.)	Outer ring (R=16 mm.)	Ratio of displacements
68 μ	119 μ	0·57
85 μ	136 μ	0·63
85 μ	153 μ	0·55
68 μ	153 μ	0·45

rings. If each pencil of diffracted rays is diverging from an effective point source, then the ratios of the corresponding displacements on the two rings should be $10/16 = 0{\cdot}625$. From Table 1, therefore, it is seen that in this case the effect is angular and hence position alone is not the cause of the observed displacements.

In the second experiment a specimen reduced 30% in thickness was examined, using an X-ray beam of diameter 30 μ. The specimen was mounted on the specimen holder designed for use with the X-ray microbeam camera; this holder (which allows oscillation of the specimen about the point of incidence of a very narrow X-ray beam) and the method of use have been described elsewhere (Gay & Kelly, 1952). In the present experiments, the specimen was oscillated over $\frac{3}{4}°$ on either side of the normal position.

Close examination of the resulting streaks on the Debye–Scherrer rings on photographs from an oscillated specimen showed that the regions of maximum blackening of nearly all the streaks lay closely on rings of definite radii. As has been mentioned in § 3, the maximum possible spread on the 422 ring is typically 15 μ.* The length of the streaks is 50–100 μ.

Some pairs of streaks occurring near the equator of the 422 ring have the most intense regions separated by a distance $\sim 50\,\mu$ in a radial direction; an example is shown in Fig. 2. It is thought that these reflexions are due to particles having different mean strains. The 420 and 331 rings, occurring on some photographs, showed larger separations for some streaks; however, these may be accounted for by the effects dealt with in § 3 since the θ values for these are less than that for the 422 ring, and the maximum separation due to the effects dealt with in § 3 is critically dependent on θ.

5. Conclusions

It appears, therefore, that the large radial separations of diffraction spots on resolved microbeam photographs of deformed aluminium are due, in the main, to the geometrical conditions under which the photographs are taken. A small number of reflexions, however, show displacements which cannot be accounted for by the geometry of the arrangement; these are interpreted as being due to reflexions from particles having slightly different lattice parameters. In this case, it is possible to calculate the difference in mean strain between two particles giving rise to two adjacent radially displaced diffraction spots. It is found that this difference is $\sim 10^{-3}$, which is of the order of the yield stress of the material. Thus the present experiments indicate that in some of the distorted particles in worked aluminium the internal stresses are sufficient to lead to a change of the average lattice parameter. It is interesting to note that in previous X-ray microbeam work examination of the breadths of the X-ray reflexions from individual particles has shown that the distorted particles in heavily worked aluminium are subject to stresses of the order of the yield stress (Hirsch, 1952).

The existence of mean strains in worked aluminium has been deduced by a process of eliminating other possible causes of displaced spots. If any cause of this displacement has been neglected in the above analysis the conclusion may be invalidated.

* It should be noted that the geometrical treatment from which this figure is derived applies strictly only to those reflexions occurring near the equator of the diffraction ring, i.e. where the diffracted beam is approximately perpendicular to the axis of oscillation.

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