

THE PLASTIC DEFORMATION OF BICRYSTALS OF F. C. C. METALS *

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An analysis is given of the conditions that govern the compatibility of the deformation of the two crystals of a bicrystal and the interaction of adjacent crystals is discussed in terms of macroscopic and microscopic effects. A technique is described for the production of bicrystals and for the preparation of a new type of bicrystal in which one crystal totally surrounds the other; also a technique for the preparation of specimens of silver consisting of a single crystal surrounded by a layer of polycrystalline metal. The results of tensile tests on such specimens are reported and discussed in terms of the conditions of microscopic and macroscopic compatibility.

DEFORMATION PLASTIQUE DE BICRISTAUX DE METAUX C.F.C.

Les auteurs analysent les conditions qui gouvernent la compatibilité de déformation des deux cristaux qui constituent un bicristal, et discutent les effets macroscopiques et microscopiques de l'interaction de cristaux adjacents. Ils décrivent une technique de préparation des bicristaux, une technique de préparation d'un nouveau type de bicristal dans lequel l'un des cristaux entoure entièrement l'autre, ainsi qu'une technique de préparation d'éprouvettes d'argent comportant un monocristal entouré par une couche de métal polycristallin. Les auteurs donnent des résultats d'essais de traction exécutés sur de tels échantillons et discutent les conditions de compatibilité microscopique et macroscopique, telles qu'elles apparaissent à partir de ces essais.

DIE PLASTISCHE VERFORMUNG VON BIKRISTALLEN AUS K.F.Z. METALLEN

Die Bedingungen, welche die Kompatibilität der Verformung eines Bikristalls gewährleisten, werden analysiert und die Wechselwirkung benachbarter Kristalle wird mit Hilfe von makroskopischen und mikroskopischen Effekten diskutiert. Ein Verfahren zur Herstellung von Bikristallen und zur Präparation eines neuen Typs von Bikristallen, bei dem der eine Kristall den anderen vollkommen umgibt, wird beschrieben, ferner wird ein Verfahren zur Herstellung von Silberproben beschrieben, welche aus einem Einkristall bestehen, der vollkommen von einer Schicht polykristallinen Materials umgeben ist. Die Ergebnisse von Zugversuchen an solchen Proben werden mitgeteilt und an Hand der Bedingungen für makroskopische und mikroskopische Kompatibilität besprochen.

1. INTRODUCTION

The effects of crystal boundaries on plastic deformation have been the subject of numerous investigations.⁽¹⁻¹¹⁾ Most of the experimental studies have been concerned with the comparison between the behavior of a single crystal with that of a specimen consisting of two crystals and one boundary that is, a bicrystal. The earlier experiments^(1,2,4,5,6) were mainly restricted to establishing the existence of an effect and to semi-quantative studies of the effects of various parameters such as orientation and size. In the more recent experiments^(3,9,12) attempts were made to examine the effect in terms of the dislocation mechanism of plastic deformation. This earlier work led to the formulation of the concept of "ma-

croscopic compatibility" as a necessary condition for the deformation of a bicrystal. This is the requirement that the two crystals deform identically in respect to those components of strain that control the deformation of the boundary plane. It was shown⁽¹⁰⁾ that the application of this criterion led to the prediction of secondary slip near the boundary under stress conditions that would cause only primary slip in the single crystal.

One objective of these studies has been the prediction of the stress-strain behavior of polycrystals in terms of the properties of single crystals. The bicrystal consisting of two rectangular single crystals with a planar boundary is only the first step from the single crystal to the polycrystal; the interaction at the single planar boundary is less severe than for the crystals of the polycrystal, where each surface of each crystal is expected to demand compatible deformation. For this reason, two further stages towards the polycrystal have been studied; these are

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- (1) bicrystals in which one crystal is totally surrounded by the other crystal;
- (2) specimens in which a single crystal is totally surrounded by a thin layer of polycrystalline metal.

2. THEORY OF GRAIN BOUNDARY EFFECTS

2.1 Cases of compatibility

Consider the bicrystal described in Fig. 1, with the three orthogonal axes x , y , z , such that y is normal to the grain boundary, x is in the boundary and z is the axis of the specimen but not necessarily the tension axis. It will be assumed that the single crystals

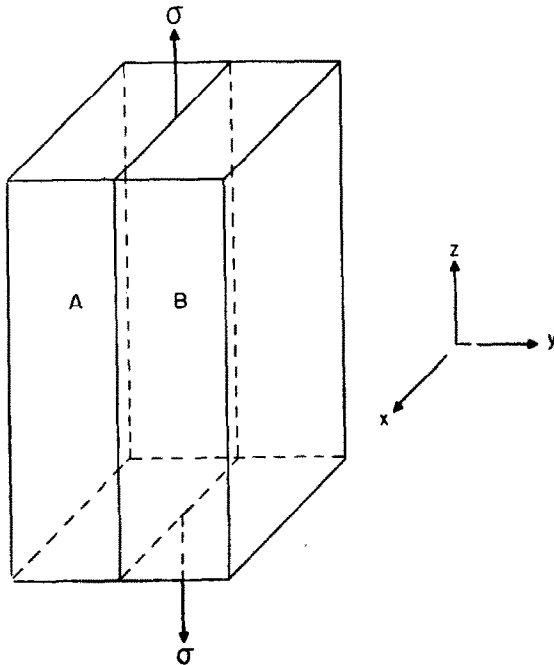


FIG. 1. Conventional bicrystal.

A and B are oriented in such a manner that the resolved shear stress is greater on one slip plane than on any other. The point of interest is to find how the boundary perturbs the deformation of the single crystals. It will be assumed during this analysis that slip can be regarded as homogeneous shear deformation and the microscopic inhomogeneities that can arise at the grain boundary will be ignored. The deformation of the bicrystal can be described in terms of the six strain components: ϵ_{xx} , ϵ_{yy} , ϵ_{zz} , ϵ_{xy} , ϵ_{yz} and ϵ_{zx} . The stress situation will not be considered for the moment, and consequently the analysis is similar to the one used by Taylor for the polycrystalline material.⁽¹³⁾

If crystal A shears by an amount s_1^A , on its primary slip system, the strain components mentioned above, can be expressed in terms of s_1^A . If it is further assumed that s_1^A is small, and second order terms in s_1^A can be ignored, then the strain components are simply proportional to s_1^A . The three strain components of importance at the grain boundary are related to s_1^A as follows:

$$\epsilon_{zz}^A = m_1^A s_1^A \quad \epsilon_{xx}^A = n_1^A s_1^A \quad \epsilon_{xy}^A = p_1^A s_1^A.$$

If \mathbf{e} is a unit vector normal to the slip plane, \mathbf{g} a unit vector parallel to the slip direction, the three geometrical factors m_1^A , n_1^A , p_1^A are defined by the following relations

$$m_1^A = (\mathbf{z} \cdot \mathbf{e})(\mathbf{z} \cdot \mathbf{g}) \quad n_1^A = (\mathbf{x} \cdot \mathbf{e})(\mathbf{x} \cdot \mathbf{g})$$

$$p_1^A = \frac{1}{2}[(\mathbf{z} \cdot \mathbf{e})(\mathbf{x} \cdot \mathbf{g}) + (\mathbf{x} \cdot \mathbf{e})(\mathbf{z} \cdot \mathbf{g})] \quad (2)$$

where \mathbf{z} for example, represents a unit vector along the z axis. If single crystal A deforms on N slip systems by shearing by a small amount s_i^A on each one of them, then

$$\begin{aligned} \epsilon_{zz}^A &= \sum_{i=1}^N m_i^A s_i^A \\ \epsilon_{xx}^A &= \sum_{i=1}^N n_i^A s_i^A \\ \epsilon_{xy}^A &= \sum_{i=1}^N p_i^A s_i^A. \end{aligned} \quad (3)$$

The presence of the boundary requires continuity of strain across it, which can be represented by the relations:

$$\epsilon_{zz}^A = \epsilon_{zz}^B, \quad \epsilon_{xx}^A = \epsilon_{xx}^B, \quad \epsilon_{xy}^A = \epsilon_{xy}^B. \quad (4)$$

If crystal B deforms by a small amount s_1^B on its primary slip system a relation similar to expression (1) can be written for crystal B . Substituting (1) and the similar expression for B into relation (4) yields

$$m_1^A = c m_1^B, \quad n_1^A = c n_1^B, \quad p_1^A = c p_1^B. \quad (5)$$

Where $c = \frac{s_1^B}{s_1^A}$ and $c = 1$ does not imply isoaxiality because the tensile axis does not necessarily lie along the z axis. However, if the bicrystal is isoaxial and the tensile axis is along the z axis, then the m factor defined by relation (2) is identical to the Schmid factor, and for such a bicrystal $m_1^A = m_1^B$ and $c = 1$.

A compatible bicrystal satisfies the conditions (4), and deforms on two slip systems, one system in each single crystal. A bicrystal which does not satisfy

these relations is called incompatible. As expression (4) represents three independent relations and in addition there exists a fourth relation fixing the value of ϵ_{zz} (if the tensile axis is assumed to be along the z axis), the most incompatible bicrystal will therefore, in general, deform on a total of four slip systems. These four slip systems can be distributed in such a way that there is one slip system in A and three in B or vice versa, or two in A and two in B .

As the compatible bicrystals, from a macroscopic point of view, should have the same stress-strain curve as the component single crystals, it is of interest to know all the types of compatible bicrystals.

For each single crystal, e and g refer to the primary slip system. By inspection of the relations, (2) it is obvious that y can be changed into $-y$, or e into g without altering any of the relations. Thus if crystal B is obtained from crystal A by one of these operations, the result will be a compatible bicrystal (at least compatible at the onset of deformation before appreciable lattice rotation has occurred).

So far, the tensile axis t has not been specified. However, it will be apparent that in certain special cases of compatibility the tensile axis can only have one specific orientation or at most can only vary within specified limits. Furthermore, for any compatible case satisfying the relations (5), the tensile axis must be such that the slip systems under consideration are really activated. Consequently, certain solutions which satisfy the relations (5) might be unacceptable because no tensile axis can be chosen that will activate that combination of slip systems. From another point of view, lattice rotation occurs during deformation. This gives rise to a group of bicrystals which shall be called transiently compatible. This group satisfies the relations (5) before deformation takes place, but subsequently as deformation takes place and lattice rotation ensues, the relations (5) are no longer satisfied and the bicrystal becomes more and more incompatible.

A *symmetric* bicrystal, in which single crystal B is the mirror image of single crystal A with respect to the grain boundary plane xz is compatible. As described by Schmid and Boas,⁽¹⁴⁾ after a tensile strain of ϵ , the angle λ_0 between the tensile axis and the slip direction in a single crystal decreases to a value λ given by

$$\frac{\sin \lambda_0}{\sin \lambda} = 1 + \epsilon. \quad (6)$$

Consequently, the rate of rotation is

$$\omega = \Delta\lambda/\epsilon = \tan \lambda. \quad (7)$$

Therefore unless the tensile axis is in the grain boundary plane, $\lambda_A \neq \lambda_B$ and consequently $\omega_A \neq \omega_B$ and this is a case of transient compatibility. The same conclusion follows from the fact that in this symmetric case, c in relations (5) is unity, which, means that $s_1^A = s_1^B$. Thus the only type of symmetric bicrystal which is compatible is isoaxial; a non-isoaxial symmetric bicrystal is only transiently compatible.

A second case of compatibility arises when single crystal B is the mirror image of A with respect to the slip plane. Therefore, both A and B have the same slip plane and the same slip direction. This bicrystal has the lowest easy glide slope as demonstrated by Livingston⁽⁹⁾ because even the microscopic incompatibilities, that will be discussed later, are minimized when the slip system is continuous across the grain boundary. This type of bicrystal will be called *pseudo-identical* because the two single crystals are identical as far as the primary slip systems are concerned. Here again, the constant c in relations (5) is unity and $s_1^A = s_1^B$; however, as the slip plane and slip direction are continuous across the boundary, this does not restrict the position of the tensile axis. Thus in general, although $c = 1$, the pseudo-identical bicrystal is not isoaxial.

Finally the two symmetry operations, one with respect to the grain boundary and one with respect to the slip plane can be combined to yield a *pseudo-symmetrical* bicrystal. This bicrystal is such that the primary slip systems of A and B are symmetrical with respect to the grain boundary but the lattices of A and B are not. As in the symmetric case, the tensile axis must lie in the grain boundary plane because $c = 1$. But, because of the symmetry operation with respect to the slip plane, this bicrystal is not necessarily isoaxial.

The cases that will be considered now are special cases, in the sense that the boundary has been chosen in such a way that at least one of the three geometrical factors m , n or p be zero. The case where both m and n are zero is impossible as this would imply that no deformation at all is taking place.

From the definition of c , it is obvious that if the cases of symmetry, pseudo-symmetry, pseudo-identity and the case where e and g are interchanged, are left

aside, c must in general be different from unity. It will now be shown that when c is different from unity, permanent compatibility can only be attained if the tensile axis is along the z axis. For a certain bicrystal m_1^A and m_1^B are fixed, and consequently c is fixed through relations (5). If the axis of tension is parallel to t and $t \neq z$

$$s_1^A = \frac{\epsilon_{tt}}{m_1^A} \quad \text{and} \quad s_1^B = \frac{\epsilon_{tt}}{m_1^B} \quad (8)$$

$$c = s_1^B/s_1^A = m_1^A/m_1^B \quad (9)$$

where

$$m_1^A = (\hat{t} \cdot \hat{e}_A)(\hat{t} \cdot \hat{g}_A) \quad \text{and} \quad m_1^B = (\hat{t} \cdot \hat{e}_B)(\hat{t} \cdot \hat{g}_B). \quad (10)$$

Thus, in general when $t \neq z$, $m_1^A/m_1^B \neq m_1^A/m_1^B$, if one ignores the special cases treated before, and the case where e and g are interchanged (which will be treated later), where $m_1^A/m_1^B = 1$. Therefore, after an infinitesimal amount of deformation $s_1^B/s_1^A = m_1^A/m_1^B$ which is different from $c = m_1^A/m_1^B$, and consequently, this can be at best a case of transient compatibility. The analysis will therefore be pursued, assuming the tensile axis to be along the z axis.

$$n = p = 0$$

The only solution is $(x \cdot e) = (x \cdot g) = 0$.

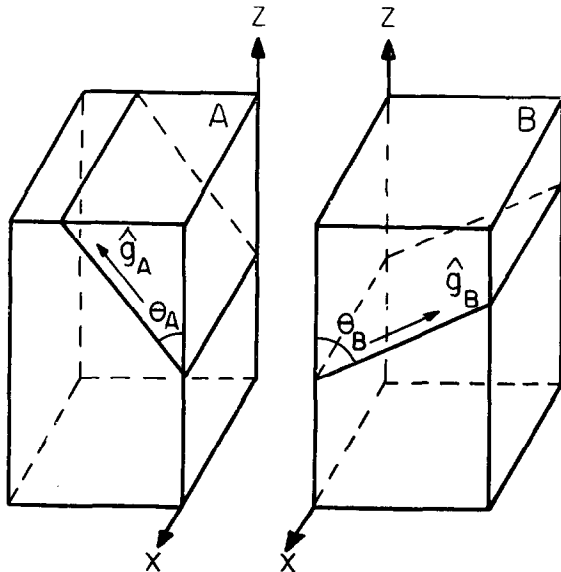


FIG. 2. Compatible bicrystal with $n = p = 0$.

A compatible bicrystal of this type is shown in Fig. 2 for $0 < \theta_A < 90^\circ$. In general $\theta_A \neq \theta_B$, be-

cause $\theta_A = \theta_B$ is the symmetric case treated before. The relations (5) for such a bicrystal become,

$$m_1^A = cm_1^B \quad 0 = c \cdot 0 \quad 0 = c \cdot 0. \quad (11)$$

The last two relations in (11) are satisfied regardless of the value of c and the first relation will be satisfied even during deformation.

$$m = p = 0$$

This case can be obtained from the previous one by a simple interchange of z and x . However, as the tensile axis is assumed to be along the z axis, any case with $m = 0$ is impossible.

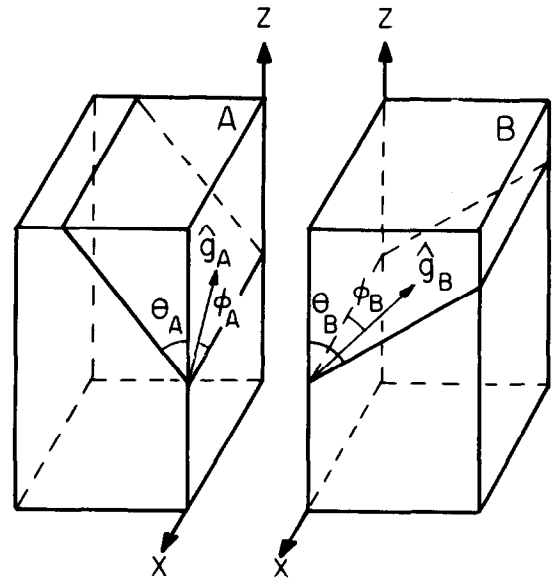


FIG. 3. Transiently compatible bicrystal with $n = 0$ ($x \cdot e) = 0$.

$$n = 0 \quad m \neq 0 \quad p \neq 0$$

$n = 0$ if either $(x \cdot e) = 0$ or $(x \cdot g) = 0$. If $(x \cdot e) = 0$ a bicrystal can be produced with single crystals of the type shown in Fig. 3 with $0 < \theta_A < 90^\circ$. For such a bicrystal the relations (5) become

$$\begin{aligned} (x \cdot e_A)(z \cdot g_A) &= c(z \cdot e_B)(z \cdot g_B) \quad 0 = c \cdot 0 \\ \frac{1}{2} (z \cdot e_A)(x \cdot g_A) &= c \frac{1}{2} (z \cdot e_B)(x \cdot g_B). \end{aligned} \quad (12)$$

Taking the ratio of the first and last relations in (12) one obtains the condition of compatibility:

$$(z \cdot g_A)/(x \cdot g_A) = (z \cdot g_B)/(x \cdot g_B). \quad (13)$$

Consequently, the locus of g_A and g_B is a plane going through the y axis and making the x - z plane an angle $\tan^{-1} (z \cdot g_A)/(x \cdot g_A)$. In general when $\theta_A \neq \theta_B$ and

$\varphi_A \neq \varphi_B$ this will be a case of transient compatibility. If $n = 0$ were obtained by $(\mathbf{x} \cdot \mathbf{g}) = 0$, this case would only differ from the previous one by an interchange of \mathbf{e} and \mathbf{g} and consequently would yield the same result, namely: transiently compatible bicrystals.

$$m = 0 \quad n \neq 0 \quad p \neq 0$$

This case is impossible when the tensile axis is along the z axis.

$$p = 0 \quad m \neq 0 \quad n \neq 0$$

$$p = \frac{1}{2} [(\mathbf{z} \cdot \mathbf{e})(\mathbf{x} \cdot \mathbf{g}) + (\mathbf{z} \cdot \mathbf{g})(\mathbf{x} \cdot \mathbf{e})] = 0$$

therefore

$$(\mathbf{z} \cdot \mathbf{e})(\mathbf{x} \cdot \mathbf{g}) = -(\mathbf{z} \cdot \mathbf{g})(\mathbf{x} \cdot \mathbf{e}). \quad (14)$$

Definition (14) will be satisfied if \mathbf{e} and \mathbf{g} are at 45° to the z axis that is for any isoaxial "0.5" bicrystal. For all bicrystals with $p = 0$, $m_1^A = m_1^B = \frac{1}{2}$ and consequently $c = 1$.

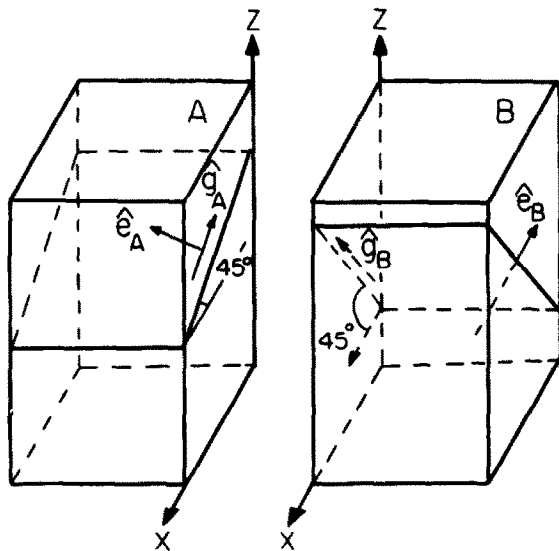


FIG. 4. Transiently compatible bicrystal with $p = 0$.

In conformity with Livingston's notation let the angle between the \mathbf{e} - \mathbf{g} plane and the x - z plane be called θ . As deformation takes place \mathbf{g}_A and \mathbf{g}_B rotate towards the tensile axis and make an angle $\lambda \neq 45^\circ$ with the z axis. Then $m_1^A = m_1^B = \cos \lambda \sin \lambda$. Thus

$$|\Delta p| = \frac{1}{2} \cos \lambda |\cos \theta_A - \cos \theta_B| \quad (15)$$

One of these cases is shown in Fig. 4. For this bicrystal, as initially $\lambda = 45^\circ$, $\Delta m = 0$ and $\Delta n = 0$ and from relation (15) $|\Delta p| = 0$. However, when deformation takes place, Δn and Δm are still zero, but

$|\Delta p| = \cos 2\lambda$ and consequently this is a case of transient compatibility.

Livingston considered that as the bicrystals with $\theta_A = 0^\circ$, $\theta_B = 180^\circ$, on one side and the bicrystal with $\theta_A = -90^\circ$, $\theta_B = 90^\circ$ on the other side had the same $\Delta\theta = 180^\circ$, the same m 's, the same $\Delta n = 0$ but differed only in the $\Delta\omega_y$ which was two for the first bicrystal and zero for the second, the comparison of these bicrystals was an excellent test of the importance of $\Delta\omega_y$. However, the validity of this comparison is debatable for the following reasons: first of all, whenever $\Delta\omega_y = 0$ the bicrystal is permanently compatible and whenever $\Delta\omega_y \neq 0$ the bicrystal is transiently compatible only; furthermore, referring to formula (7)

$$\omega_y = \tan \lambda \cos \theta.$$

Thus for $\lambda = 45^\circ$

$$|\Delta p| = \frac{\cos 2\lambda}{2} \Delta\omega_y. \quad (16)$$

Consequently, the fact that for a given $\Delta\theta$, it is found that the higher $\Delta\omega_y$ the harder the bicrystal, could be explained by the fact that the higher $\Delta\omega_y$, the higher $|\Delta p|$, and hence the faster the departure from compatibility. Although it is true that the lattice rotation is very small, and that consequently the departure from compatibility will also be very small, it is possible that $\Delta\omega_y$ is only important through its effect in equation (16).

$$m \neq 0 \quad n \neq 0 \quad p \neq 0$$

It is obvious, without any analysis, that in this most general case there is no permanently compatible bicrystal. Even when \mathbf{g}_A , \mathbf{g}_B and \mathbf{t} were coplanar, and \mathbf{g}_A and \mathbf{g}_B made equal angles with \mathbf{t} in the case $p = 0$, there is no permanently compatible bicrystal other than the four special cases mentioned before. A completely general analysis of the relations (5) is very lengthy and does not make any contribution.

So far, the state of stress has not been mentioned at all, although it is quite possible that satisfactory solutions to relations (5) require an impossible state of stress. However, the stress analysis is very complicated and should be studied for each case separately. The only approach to the calculation of the state of stress is that of Budiansky,⁽¹⁵⁾ on very thin, plate-like bicrystals, but this method cannot yet be applied to the type of bicrystals used in this investigation.

2.2 Factors affecting the stress-strain curve of a bicrystal

It has not been possible to establish a theory that would predict the stress-strain curve of a bicrystal from the stress-strain curves of its component single crystals. However, certain factors are found to be important in affecting the stress-strain curve of the bicrystal, and these factors can in certain cases help to predict the relative level of two or more bicrystals.

The first factor of importance is the Schmid factors of the component single crystals as it controls the value of the resolved shear stress on the primary and the secondary slip systems. This makes the analysis of a non-isoaxial bicrystal very hard as the two component single crystals have completely different stress-strain curves. The resolved shear stress on the secondary slip systems is very important, because no matter what mechanism prevails in the bicrystal deformation, it is only necessary to raise the shear stress from the tensile resolved shear stress up to the critical resolved shear stress to make that secondary system operative.

The comparison of an isoaxial bicrystal with its component single crystals can be ambiguous too, because of the size effects encountered with single crystals. Gilman⁽³⁾ and Livingston⁽¹⁰⁾ chose to compare their bicrystals with single crystals of the same cross-sectional shape. Livingston justified this comparison on the basis that the difference between the single crystal curves could be due to grip constraints. However, the grip effect discussed by Jackson and Hauser⁽¹⁶⁾ is zero for the 0.5 orientation, and the grip effect due to lattice rotation could be less for a bicrystal than for a single crystal of the same cross section. Therefore, it might be better to compare the bicrystals with single crystals that have the same geometry as those composing the bicrystal.

The most important factor controlling the stress-strain curve of a bicrystal is its degree of compatibility which is represented by the relations (5). Actually, if the bicrystal is incompatible, its stress-strain curve will depend on the solutions of equations (4).

When the incompatibility is of a macroscopic nature, the multiple slip layer can extend up to two or three millimeters. The volume of bicrystal affected by this multiple slip layer will affect the level of the stress-strain curve in a proportional manner. When the incompatible bicrystal deforms on its two primary slip systems, very high elastic stresses are built up at

the grain boundary. In order to relieve these very high stresses, secondary slip systems are activated. Single crystal *A* of bicrystal *A-B* is assumed to have the same resolved shear stress due to tension as it would have if it were to be pulled in tension separately on each of its slip systems. In addition, single crystal *B* superimposes on single crystal *A* the shear taking place on its primary slip system. This means that the extensions of the slip planes of crystal *B* in crystal *A* have a shear which is the continuation of the applied shear on the primary slip planes in *B*. This "transferred" shear decreases away from the boundary in a manner which is controlled by the relative sizes of the neighboring single crystals and the degree of incompatibility. The superimposed shear of crystal *B* on crystal *A* can be resolved on all the systems of crystal *A*. If *P* is the shear on the primary system ($\mathbf{e}_1, \mathbf{g}_1$) of crystal *B*, the resolved shear P_i on system ($\mathbf{e}_i, \mathbf{g}_i$) of crystal *A* is

$$P_i = PN_{i1} = P[(\mathbf{e}_1 \cdot \mathbf{e}_i)(\mathbf{g}_1 \cdot \mathbf{g}_i) + (\mathbf{e}_1 \cdot \mathbf{g}_i)(\mathbf{e}_i \cdot \mathbf{g}_1)]. \quad (17)$$

Similarly the shear on the primary system of *A* can be superimposed on crystal *B* by the use of N_{1j} . As the transferred shear is produced by the action of one crystal on its neighbor, such macroscopic consideration will not lead to a grain size effect in polycrystals.

Therefore, although secondary slip systems can be predicted by the N_{ij} factors, the major effect on the stress-strain curve is obtained by checking how well the slip systems satisfy the relations (4), i.e. how well these slip systems help to maintain the continuity of strain across the grain boundary.

Another important consideration is the type of secondary slip system that is activated, and the type of dislocation reaction that it makes with the primary slip system. If, because of grain boundary interaction, a system forming Cottrell-Lomer locks with the primary system is generated, this will shorten easy glide considerably and lead to a very high stress-strain curve. For a given type of secondary slip system, the amount of secondary slip relative to primary slip will also be of importance as it is a measure of the amount of interaction. If in the vicinity of the grain boundary, the conditions are such that the secondary slip system is activated so strongly as to obliterate the primary slip system, this will produce a weak interaction, because the secondary slip sys-

tem has no primary slip system with which to interact.

These various factors were applied successfully to the isoaxial bicrystals investigated by Livingston.⁽¹⁰⁾ For example the bicrystal with $\theta_A = 0^\circ$ and $\theta_B = 45^\circ$ and the one with $\theta_A = 45^\circ$ and $\theta_B = 90^\circ$ both have the same $\Delta\theta$ of 45° . Consequently the N_{ij} factors are the same for both and predict secondary slip in B only. However, the solution of (4) requires no secondary slip in A for the first bicrystal but requires secondary slip in A for the second bicrystal. Therefore, the second bicrystal should be harder than the first because the compatibility requirements are not satisfied. This is in agreement with experiment. The relative stress level of other bicrystal stress-strain curves can be rationalized in the same manner.

2.3 Microscopic considerations

So far it has been established that when a bicrystal is incompatible, i.e. when its primary slip systems do not satisfy the relations (5), an additional number of slip systems must be introduced. Livingston proposed, as a model for the selection of these slip systems, the stress concentration arising ahead of dislocations "piling-up" at the grain boundary. Frank⁽¹⁷⁾ has pointed out that the stress concentration can be intense enough to activate sources in the neighboring crystal. However, aluminum or silver are not materials displaying a yield point and consequently the same stress is necessary to activate sources as to keep dislocations moving. Therefore, if the resolved shear stress was only large enough over the extent of a source, i.e. over the distances of the order of microns as was assumed by Livingston, the slip bands should only extend for a few microns. However, slip bands of the order of 0.1 mm to as much as 3 mm have been observed. Therefore, the stress concentration must raise the resolved shear stress on a secondary slip system above the critical resolved shear stress over such large distances, for dislocation pile-ups to be responsible for secondary slip system activation.

At the very beginning of plastic deformation, the slip bands in each individual crystal of the bicrystal are well separated and therefore it is possible to consider each pile-up separately. The boundary can act as an effective obstacle to moving dislocations. Therefore, in this stage, it is possible to assume, in agreement with Livingston's hypothesis, that the

pile-up leads to an effective shear stress acting in a plane parallel to the slip plane of the piled up dislocations and in a direction parallel to their slip direction. The resulting resolved shear stresses P_i in crystal A on the various possible slip systems is given in terms of the shear stress P due to the dislocations piled up in crystal B by the same formula (17) which gave the result of superimposing the shear of B on crystal A .

In the isoaxial bicrystals studied by Livingston,⁽¹⁰⁾ the secondary slip system predicted was always the one forming sessile jogs with the primary. The resolved shear stress on such a system is only 6 per cent lower than on the primary. The stress concentration factor is $q = [1 + (L/x)^{\frac{1}{2}}]$; thus in the case of a "0.5" aluminium bicrystal where one wants the shear stress to be raised by 6 per cent for a distance $x = 3$ mm, the length of the slip band will be $L = 0.001$ cm. The number of dislocations that can be packed into a length L of the slip plane is $n = \pi L \sigma k / \mu b$ ⁽¹⁸⁾ where

$$k = 1$$

$$\mu = 2.4 \times 10^6 \text{ g/mm}^2$$

$$b = 2.8 \times 10^{-8} \text{ cm}$$

$$\sigma = 50 \text{ g/mm}^2$$

therefore

$$n = 2$$

and consequently, in the early stages of deformation, when slip bands are well apart, it is very easy to produce by stress concentration very long slip bands of secondary slip system.

This type of slip activation has actually been observed in polycrystalline α -brass by Weinberg.⁽¹⁹⁾

However, as deformation proceeds, still during easy glide, the slip bands get very close, and it is not possible any longer to consider isolated pile-ups. Let the slip direction of a pile-up be the x axis, and the normal to the slip plane the y axis. A dislocation pile-up of n dislocations, with strength b , can be considered at fairly large distances as a large dislocation of strength nb situated at the center of gravity of the pile-up. Therefore, many pile-ups on a boundary can be thought of as a vertical array of dislocations. The shear stress due to an edge dislocation with a Burgers vector along the x axis in the $y = 0$ slip plane is

$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2 - y^2)}{(x^2 + y^2)^{\frac{3}{2}}} \quad (18)$$

If one considers an infinite wall of edge dislocations in the plane $x = 0$ separated by a distance h

$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\nu)} \sum_{n=-\infty}^{+\infty} \frac{x(x^2 - y_n^2)}{(x^2 + y_n^2)^2} \quad (19)$$

where

$$y_n = y + nh.$$

This sum has been evaluated by Burgers⁽¹⁸⁾ giving

$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\nu)} \frac{\pi^2 x}{h^2} \frac{(\cosh 2\pi x/h)(\cos 2\pi y/h) - 1}{2(\sinh^2 \pi x/h + \sin^2 \pi y/h)^2}. \quad (20)$$

At large distances, when $x \gg h$, equation (20) becomes

$$\sigma_{xy} \simeq \frac{\mu b}{2\pi(1-\nu)} \frac{\pi^2 x}{h^2} 4e^{(-2\pi x/h)} \cos 2\pi y/h. \quad (21)$$

Near one of the dislocations, where $x \ll h$ and $y \ll h$ equation (20) becomes identical to relation (18). When x is larger than h , the stress is given by relation (21) and is very small because of the exponential fall-off. Therefore, when pile-ups occur, the stress concentration is only present next to the head of one pile-up for a distance comparable to the separation h of the slip bands, which is of the order of a few microns. But at larger distances, the stress concentration produced by an individual pile-up is cancelled by the exponential decay.

So far the discussion has been restricted to pile-ups of edge dislocations, but pile-ups of screw dislocations should be considered as well. The shear stress of a screw dislocation lying along the z axis is

$$\sigma_{yz} = \frac{\mu b}{2\pi} \frac{x}{(x^2 + y^2)}. \quad (22)$$

For an array of such dislocations, using the techniques of Burgers, one finds:

$$\begin{aligned} \sigma_{yz} &= \frac{\mu b}{2\pi} x \sum_{n=-\infty}^{+\infty} \frac{1}{(x^2 + y_n^2)} \\ &= \frac{\mu b}{2h} \frac{\sinh 2\pi x/h}{\cosh 2\pi x/h - \cos 2\pi y/h}. \end{aligned} \quad (23)$$

Again when $x \ll h$ and $y \ll h$ equation (23) reduces to (22); but when $x \gg h$ one finds

$$\sigma_{yz} \simeq \frac{\mu b}{2h}. \quad (24)$$

This result is very different from the one found with edge dislocations. The stress levels off at an asymptotic value, which in aluminium for $h = 3 \times 10^{-4}$ cm is equal to about 100 g/mm². Therefore a single set of parallel screw dislocations will be unstable, because it produces a shear stress extending much too far from the boundary. This is why a crossed grid of screw dislocations must be introduced so as to eliminate these long range stresses. Thus, as screw dislocations are not limited to one slip plane, they will move out of the slip plane to avoid the pile-up.

Thus although at the very onset of deformation, dislocation pile-ups can activate a few fairly long but well separated slip bands of secondary slip, they cannot account for slip activation over a distance comparable with the separation of the slip bands, i.e. a few microns.

If a bicrystal is macroscopically compatible, it can still be harder than its component single crystals because of microscopic incompatibilities. In order to have a bicrystal which is not only compatible if considered as a continuum, but compatible everywhere, one would require a one to one correspondence of slip planes at the grain boundary. The lack of this 1:1 correspondence represents one form of microscopic incompatibility. Furthermore, because of the dislocation pile-ups and the superimposition of shear of one crystal on the other, secondary slip can be produced, even in cases where the bicrystal is macroscopically compatible and could therefore deform only on the primary slip systems. This secondary slip cannot exist in a pseudo-identical bicrystal. It can exist in a symmetric bicrystal, but as the bicrystal is symmetric even for the secondary slip systems, the effect will be negligible. However, when this secondary slip is present in a pseudosymmetric bicrystal, it destroys the compatibility of the bicrystal, because such a bicrystal is not compatible as far as its secondary slip systems are concerned. This explains why sometimes a pseudosymmetric bicrystal can be appreciably harder than the single crystals composing it.

It is by no means certain that there is a grain size effect in f.c.c. metals. The observed effects in polycrystals reported by many observers^(20, 21) could be due to substructure or preferred orientation. If a true size effect exists, it could be explained by the presence of this microscopic multiple slip layer

of constant thickness, but not by the compatibility analysis.

3. EXPERIMENTAL STUDY OF BICRYSTALS OF SILVER

3.1 Experimental procedure

All the single crystals used in this investigation had an axial orientation close to $\langle 210 \rangle$, called the "0.5" orientation. This is the orientation for which the tensile axis is 45° from both the slip plane and the slip direction. The two orientations used can be described by a θ of 27° (type B) and of 72° (type A) where θ is the angle between the e - g plane and the x - z plane. Fig. 4 shows on the left the reference orientation $\theta = 0^\circ$. The single crystals were grown from the melt in milled graphite boats at a rate of 8.6 mm/min under a helium atmosphere. The silver used in the experiment was 99.98 per cent pure. In order to obtain the proper cross-section, the free surface of any grown single crystal was machined by milling. The milling operation was carried out by taking off successively smaller amounts, starting at three thousandths and finishing at one thousandth, at a feed rate of 2 in/min. All the crystals had a length of 14 cm and an approximate cross-section of 1 cm \times 1 cm. Afterwards, the specimens were electro-polished in a solution of 9 per cent KCN in water and then annealed at $940^\circ\text{C} \pm 2^\circ\text{C}$ in a helium atmosphere for 24 hr and then furnace cooled over a period of 7 hr. The orientation of the specimen was determined within $\pm 2^\circ$ by the Laue back reflection method.

The specimens were tested in a soft-type tensile machine (the load is prescribed) up to 3 per cent strain. The stress was increased continuously at approximately 30 g/mm²/min. The strain was measured over a 5-cm gauge length with a mechanical extensometer employing an optical lever. The strain and stress were measured with accuracies of $\pm 2 \times 10^{-5}$ and ± 2 g/mm², respectively. The remainder of the stress-strain curve up to 20 per cent strain was obtained in a hard-type tensile machine (the strain rate is prescribed). The strain and the stress were measured in that machine with an accuracy of ± 2 per cent.

Bicrystals were grown from the melt, using seeds of predetermined orientation in milled graphite boats. The graphite boats had a longitudinal projection in the bottom, and another longitudinal projection in the cover, in order to prevent the boundary from wandering off the plane of symmetry.

A new technique was devised to produce the bicrystals with a longitudinal boundary, which previously had only been grown from the melt. Two single crystals about 14 cm long and with a cross section of $\frac{3}{8}$ in. \times $\frac{3}{16}$ in. were sintered together on their widest faces. The sintering was accomplished in very accurately milled graphite boats. The differential expansion of the graphite and the silver caused the crystals to be pressed together. Sintering was carried out at $940 \pm 2^\circ\text{C}$, under a helium atmosphere for a period of about 70 hr. The sintered surfaces were the flat surfaces in contact with the sides of the graphite boat and required no special preparation before sintering.

The amount of compression necessary for satisfactory sintering was determined by trial and error,

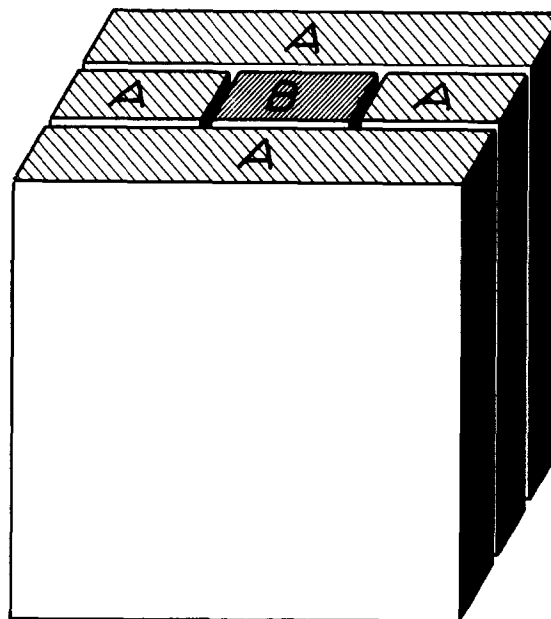


FIG. 5. Totally surrounded bicrystal.

as the expansion of the graphite is not very well known. Generally, it can be stated that the amount of compression should be large enough to bring the surfaces of the crystals into intimate contact, but not so large as to cause recrystallization to occur. After sintering, the specimens were always cooled in the furnace to avoid quenching stresses. As the sintering is never very good at the edges of the crystals, these bicrystals were machined by milling in order to remove the regions of poor sintering.

By means of this sintering technique it was possible to produce a "totally surrounded bicrystal" in which

one crystal *B* is completely surrounded by the other crystal *A*. Such a bicrystal is shown in the exploded view of Fig. 5. Crystal *B* had a cross section of $\frac{1}{16}$ in. \times $\frac{3}{8}$ in. and the two small adjoining *A* crystals had a cross section of $\frac{1}{8}$ in. \times $\frac{3}{8}$ in. These three crystals made contact on the $\frac{3}{8}$ in. wide faces. After sintering these three crystals, the resulting tricrystal was then milled to a width of $\frac{1}{4}$ in. measured parallel to the boundaries. After electropolishing and annealing, the resulting tricrystal was then sintered onto the large crystals *A* shown in Fig. 5. These large *A* crystals had a cross section of $\frac{1}{2}$ in. \times $\frac{1}{8}$ in. and were sintered on the previous tricrystal. The various *A* crystals shown in Fig. 5 form one continuous *A* crystal except for small misorientations.

Composite crystals in which a single crystal is completely surrounded by a polycrystalline layer were obtained by surface recrystallization. The four faces of an annealed single crystal were milled, and an amount of approximately ten thousandths was removed on each side. This resulting crystal was then subjected to the usual annealing treatment, thereby producing a fine polycrystalline layer about eighth thousandths thick.

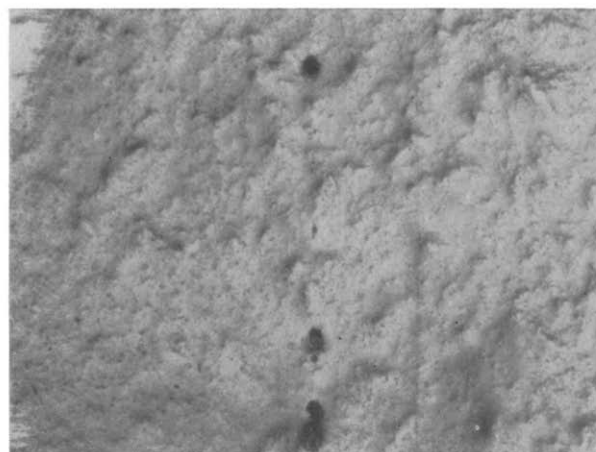
3.2 Experimental results

(a) *Bicrystals*. One single crystal was produced by sintering two identical single crystals, leaving a small misorientation of 2° or 3° at the grain boundary. Inside the bicrystal, about 90 per cent of the boundary is sintered. The rounded cavities left by the sintering process are shown in Figs. 6 and 7.

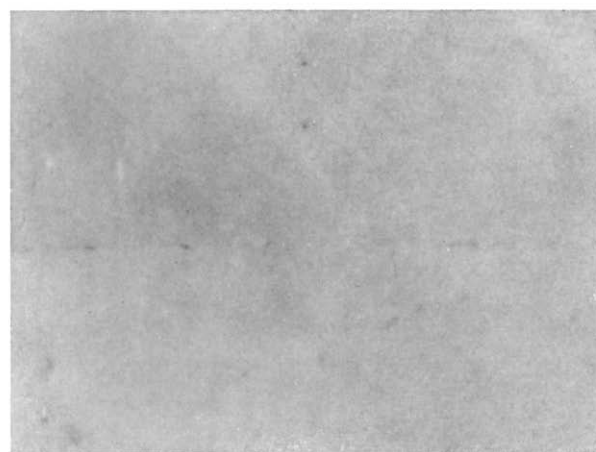
The cross section of the totally surrounded bicrystal is shown after 20 per cent elongation in Fig. 8. One can observe the continuity of slip lines across the boundaries in Fig. 9. The boundaries revealed in Fig. 9 are boundaries of the type *A-A* and hence, are not real boundaries or at most they may be small-angle boundaries.

The stress-strain curves for the various crystals investigated are shown up to 3 per cent elongation in Fig. 10 and up to 20 per cent elongation in Fig. 11. The two single crystals *A* and *B* have the same stress-strain curve. The single crystal which was obtained by sintering two single crystals with a slight misorientation, also has the same stress-strain curve as a regular single crystal.

The major difference between the single crystals and the bicrystals occurs during the early stages



(a)



(b)

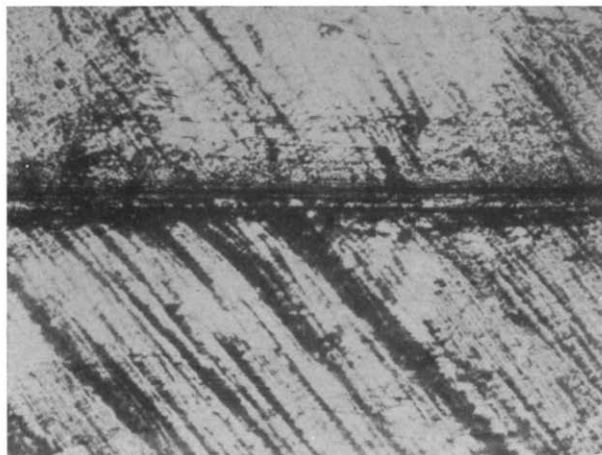
FIG. 6. Sintered boundary with cavities, top $\times 97$, bottom $\times 21,6$ as polished.



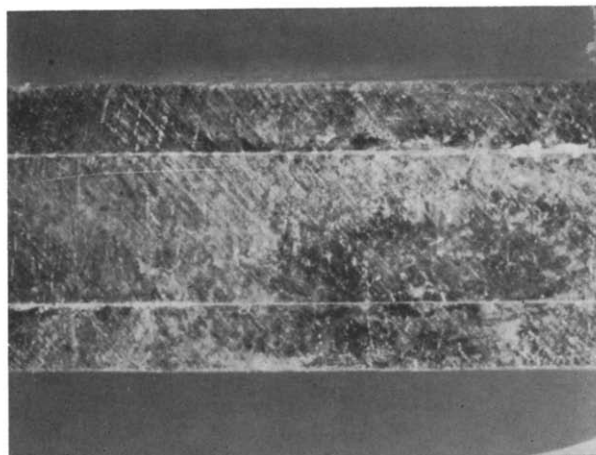
FIG. 7. Sintered boundary with cavity, $\times 97$, etched 20 per cent elongation.



FIG. 8. Cross section of totally surrounded bicrystal $\times 6.5$ 20 per cent elongation.



(a)



(b)

FIG. 9. Continuity of slip lines across boundaries of totally surrounded bicrystal, top $\times 54$, bottom $\times 4.3$

of deformation i.e. during easy glide; during the later stages of deformation, the stress-strain curves for the single crystals and the bicrystals run approximately parallel. The bicrystal which was obtained by the conventional technique of growing from the melt and the sintered bicrystal both have the same stress-strain curve.

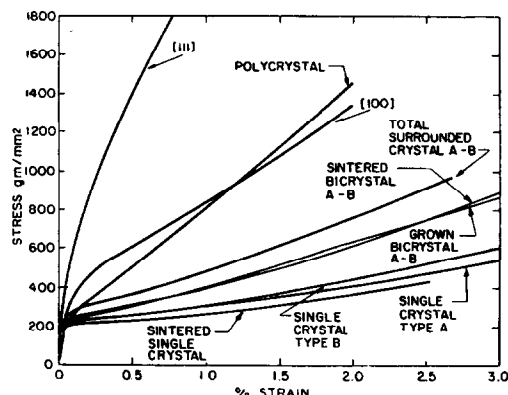


FIG. 10. Stress-strain curves up to 3 per cent elongation.

The totally surrounded bicrystal has a higher stress-strain curve than the conventional bicrystals. There is as much difference between the stress-strain curves of the totally surrounded bicrystal and the planar bicrystal, as there is between the bicrystal and the single crystal. In the later stages of deformation

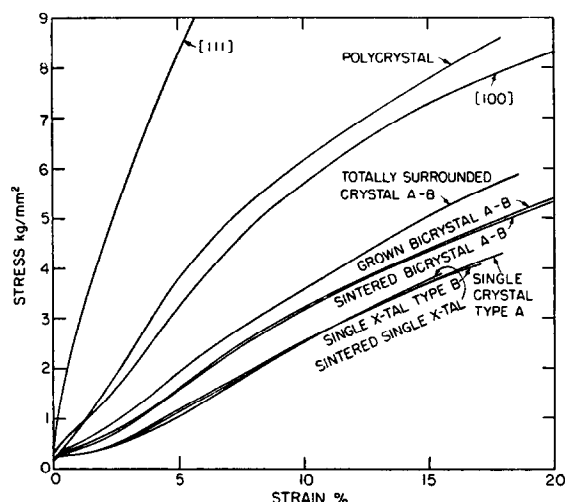


FIG. 11. Stress-strain curves up to 20 per cent elongation.

the slope of the totally surrounded bicrystal approaches that of the polycrystal. However, the totally surrounded bicrystal still exhibits a certain amount of easy glide which is nonexistent in the deformation of a polycrystal. The curves for the [100] and [111]

single crystals are shown in Figs. 10 and 11 as a means of comparison for the other stress-strain curves. It is, however, more logical to compare these various crystals on a shear stress-shear strain basis. This comparison is really only good during easy glide, when one slip system only is operative. In order to represent the polycrystal by a shear stress-shear strain curve, it is necessary to use the average Schmid factor of 3.1 used by Taylor.⁽¹³⁾ These shear stress-shear strain curves are shown in Fig. 12, and it

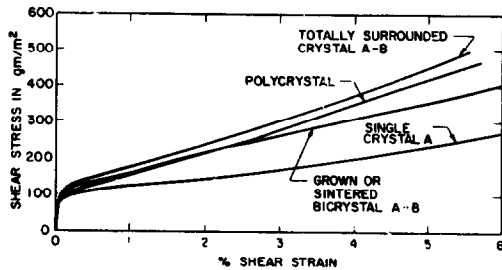


FIG. 12. Shear stress-shear strain curves.

can be seen that the totally surrounded bicrystal is a much better approximation of the polycrystal than the conventional bicrystal in the sense that the slopes of the polycrystal and the totally surrounded bicrystal curves are identical. It is also evident from Figs. 10 and 11 that the single crystal bicrystal and polycrystal curves all display the same yield point.

(b) *Single crystal surrounded by polycrystalline layer.* Single crystals were surrounded by a fine

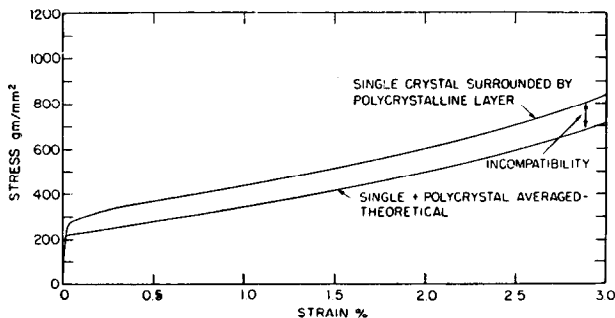


FIG. 13. Stress-strain curve for composite crystal.

polycrystalline layer approximately eight thousandths thick and with an average linear grain size of 0.1 mm. Therefore, no more than two grains on the average could be found across the layer. This polycrystalline layer represented about 10 per cent of the volume of the composite single crystal. Fig. 13

shows the stress-strain curve for such a composite single crystal up to 3 per cent elongation. On this figure, is also shown a theoretical curve calculated on the basis of 90 per cent single crystal and 10 per cent polycrystal. This latter curve is below the former one and the two curves are approximately parallel. Fig. 14 shows the stress-strain curve of the composite

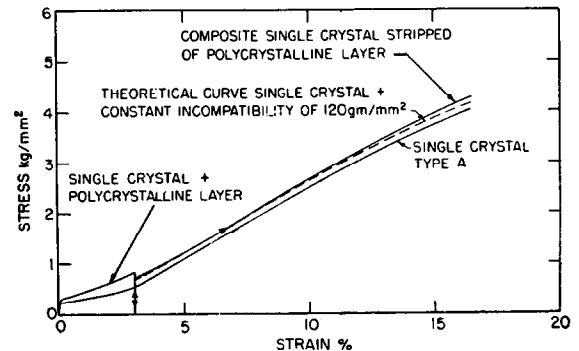


FIG. 14. Stress-strain curve of composite crystal stripped of polycrystalline layer after 3 per cent elongation.

single crystal after 3 per cent elongation and the stripping of the polycrystalline shell by electro-polishing. Its curve coincides approximately with a theoretical curve which is derived from the single crystal curve by a translation of 120 g/mm² parallel to the stress axis. After 3 per cent elongation, the composite single crystal was stripped of approxi-

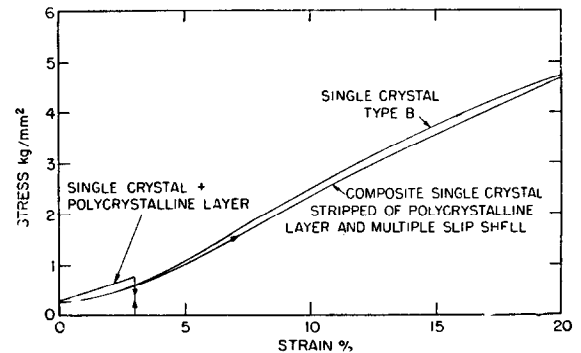


FIG. 15. Stress-strain curve of composite crystal stripped of polycrystalline layer and multiple slip shell after 3 per cent elongation.

mately fifteen thousandths, which is twice the thickness of the polycrystalline layer. The resulting stress-strain curve is shown in Fig. 15, and it can be seen that the stripped composite single crystal now behaves similarly to a normal single crystal. The final experiment consisted in extending the composite single crystal up to 6 per cent elongation. After removal

of the polycrystalline layer only, the resulting crystal is found to have the same stress-strain curve as a single crystal of the same type as evidenced by Fig. 16.

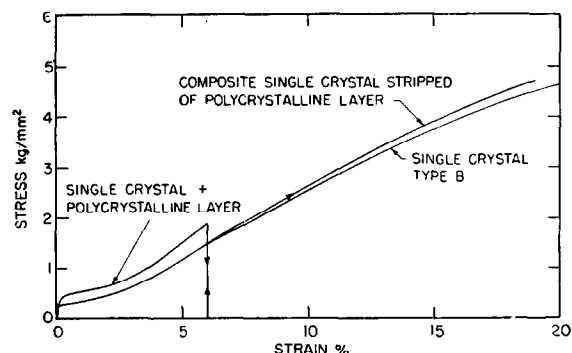


FIG. 16. Stress-strain curve of composite crystal stripped of polycrystalline layer after 6 per cent elongation.

3.3. Discussion

(a) *Bicrystals*. The new technique used in this investigation has made possible the formation of grain boundaries by sintering rather than from the melt as was customary so far. The first question which arises is whether a grain boundary produced by sintering behaves in the same way as one produced from the melt. The formation of a grain boundary by sintering takes place by a diffusion process. Consequently, as the processes of formation are different, one could expect differences in the properties of the two types of boundaries. However, Chalmers and Davis⁽²²⁾ obtained small tricrystals, where a single crystal of silver was sintered onto a grown bicrystal of silver. The two boundaries, which were originally at 90°, moved during annealing and reached the equilibrium dihedral angles of 120°.

Thus it is demonstrated that the sintered boundary can move in the same way as a grown boundary and that it has the same specific free energy when it has reached its equilibrium configuration. The sintering operation leaves some spherical cavities along the grain boundary. It is possible by prolonged sintering to remove most, if not all, of these cavities. This was nevertheless not done, because if all the cavities were removed in the case of the totally surrounded bicrystal, the center crystal would then shrink by inward migration of the boundaries.

A comparison was made between the tensile properties of a grown bicrystal and a sintered bicrystal. It is expected, if one ignores the microscopic com-

patibility argument, that these microcavities should not affect the plastic properties as long as there is enough sintered boundary for the macroscopic compatibility equations (5) to be felt. Figs. 10 and 11 show that the grown bicrystal and the sintered bicrystal have the same stress-strain curve. Therefore, even though a sintered boundary contains cavities, it is still identical in its plastic behaviour to a grown boundary.

For the bicrystal used here the N_{ij} factors predict slip in B only, which was observed experimentally. The solution of the equations (4) yields $s_u^A = 1.3 s_u^B$ (s_u meaning slip on the secondary system) which represents a fair amount of incompatibility. For such a bicrystal $\Delta\omega_y = 0.58$.

It has been shown by von Mises⁽²³⁾ that the unrestricted change of shape without change in volume of a grain in a polycrystal would require slip to take place on at least five different slip systems. From another point of view, the bicrystal only requires four slip systems even in the worst case of incompatibility. This difference between the number of slip systems required in these two cases reflects the difference in the constraint imposed. It was the need for a better physical approximation of the polycrystal which prompted the development of the totally surrounded bicrystal.

Physically, it is obvious that the totally surrounded bicrystal is a better approximation to the polycrystal, since most of the grains in a polycrystal are fully surrounded by other grains. Furthermore, the totally surrounded bicrystal shown in Fig. 5 has two parallel $A-B$ boundaries which are similar to the zx boundary shown for a regular bicrystal in Fig. 1. The totally surrounded bicrystal has, in addition, two other $A-B$ boundaries which are in the zy plane. The relations (4) still hold for the zx boundaries and the following relations hold for the other two boundaries:

$$\epsilon_{zz}^A = \epsilon_{zz}^B \quad \epsilon_{yy}^A = \epsilon_{yy}^B \quad \epsilon_{zy}^A = \epsilon_{zy}^B. \quad (25)$$

If one combines equations (4) and (25) one does not obtain six equations, first of all because $\epsilon_{zz}^A = \epsilon_{zz}^B$ is common to both and then because ϵ_{zz}^A , ϵ_{xx}^A and ϵ_{yy}^A are not independent as the volume may be treated as constant. Therefore the relations (4) and (25) combine to give four independent relations:

$$\epsilon_{zz}^A = \epsilon_{zz}^B; \quad \epsilon_{xx}^A = \epsilon_{xx}^B; \quad \epsilon_{zx}^A = \epsilon_{zx}^B; \quad \epsilon_{zy}^A = \epsilon_{zy}^B. \quad (26)$$

However, at the intersection of the two types of boundaries the following relation must be satisfied if no gap is to be opened at the corners of the inner crystal:

$$\epsilon_{xy}^A = \epsilon_{xy}^B.$$

As in addition to these five independent relations, the amount of ϵ_{zz} is fixed in a tension test, this makes six independent relations which in the worst case of incompatibility will require deformation on six different slip systems.

Although mathematically a certain orientation relationship requires six slip systems, this might not be true physically. In the center of a grain boundary far enough from the other two orthogonal boundaries, the effect of the other boundaries might not be felt. In this region therefore, compatibility will be satisfied by either relations (4) or (25) but not both at the same time, and consequently, in this region four slip systems only will be sufficient. In a region close to a corner of the inner single crystal the two sets of relations (26) and (27) must be satisfied and in this region deformation must take place on six slip systems. There might also exist a transition region with five slip systems. The relative extent and the existence of these various regions depend on the relative size of the center single crystal.

As was pointed out, the totally surrounded bicrystal possesses a boundary in the yz plane which is different from the other boundary in the xz plane; this latter boundary is the same as the one found in the planar bicrystal. For this new boundary as $\Delta\theta$ is still 45° the N factors are unchanged and secondary slip is still only predicted in crystal B . The solution of the relations (4) for this case is $s_z^A = 0$ if one rounds off the geometrical factors to the nearest tenth. Consequently, the solution required for compatibility is in agreement with the result predicted by N factors. As the $\Delta\omega$, for this boundary is 0.50, it is safe to conclude that this boundary will produce much less hardening than the other boundary and therefore, any difference between the bicrystal and the totally surrounded bicrystal is caused by the different geometries of the two bicrystals.

From another point of view, as the orientations of the individual single crystals were determined at best with an accuracy of $\pm 2^\circ$, it might be suggested

that if the totally surrounded bicrystal is found to be harder than the planar bicrystal, it is due to the fact that the outside A crystal is not a continuous single crystal, but really four single crystals separated by low angle boundaries. For that reason, a single crystal was made by sintering two identical single crystals with a slight misorientation of 3° . The stress-strain curve for such a sintered single crystal is the same as the stress-strain curve for the normal single crystal. As expected from the previous discussion the totally surrounded bicrystal is indeed harder than the bicrystal. But the totally surrounded bicrystal still exhibits some easy glide which is absent in a polycrystal. The presence of this easy glide could be attributed to the absence of transverse boundaries which are present in a polycrystal. It is of course possible to vary the geometry so that the totally enclosed bicrystal be a still better approximation of the polycrystal.

From the study of the cases of compatibility made previously for bicrystals, it is obvious that the only compatible totally surrounded bicrystal is pseudo-identical. All other totally surrounded bicrystals represent various degrees of incompatibility. Consequently, it is proposed that a polycrystal is the average of such totally surrounded bicrystals, averaged over all orientations and all degrees of incompatibility.

In all the experiments performed by Livingston with aluminium, and in this investigation with silver, the yield stress was always the same. This shows that the f.c.c. case is quite different from the b.c.c. case with interstitials, where the yield points are changed by grain size to a very definite extent. The difference is that in f.c.c. the flow stress is the "friction stress" while in b.c.c. the "starting stress" can be much higher than the friction stress. Thus the explanation of the effect of grain size on the yield point in iron (or silicon-iron) does not apply here.

(b) *Single crystals surrounded by polycrystalline layer.* So far, the cases of compatibility have been established, and when a bicrystal is incompatible, certain mathematical factors can be used to evaluate the degree of incompatibility. However, this still does not provide a physical evaluation of incompatibility. From the stress-strain curves shown in Figs. 10 and 11, it is seen that incompatibility is observed mainly during easy glide. This is the expected result as incompatibility causes multiple slip to

occur in the vicinity of the grain boundary, when otherwise the individual single crystals could still deform on a single slip system. Later on, during deformation, the self-incompatibility of the single crystals themselves becomes more important. In other words, after easy glide a single crystal deforms on more than one slip system, and the multiple slip of the individual single crystals overshadows the multiple slip caused by the grain boundary interactions. This is especially true in the case studied here, where the secondary slip system introduced by the boundary forms sessile jogs with the primary, while the secondary slip system ending easy glide in a single crystal forms Cottrell-Lomer locks with the primary. The single crystals surrounded by a polycrystalline layer were examined in order to study experimentally the nature of incompatibility.

The stress-strain curve for a single crystal surrounded by a polycrystalline layer is shown in Fig. 13. This crystal is composed of 90 per cent single crystal and 10 per cent polycrystal by volume. Therefore, one could assume that the stress-strain curve of such a crystal is the result of the superimposition of the single crystal and the polycrystal stress-strain curves in the above mentioned proportions. The theoretical curve based on this averaging of polycrystal and single crystal is shown in Fig. 13 and is found to fall below that of the composite crystal.

However, the composite crystal is not equivalent to a polycrystal plus a single crystal, but because of the incompatibility at the boundary of the single crystal there is a layer of multiple slip which was ignored in the theoretical curve. Consequently, the difference in stress between the theoretical and the experimental curves is a measure of the incompatibility. This difference is equal to 120 g/mm^2 at 3 per cent strain.

This composite single crystal was stripped of its polycrystalline layer after the 3 per cent strain i.e. at the end of easy glide. The composite single crystal, stripped of its polycrystalline shell, was then reloaded and the resulting stress-strain curve is shown in Fig. 16. This stripped composite crystal should be harder than a single crystal, as it still contains the multiple slip layer left by the presence of the polycrystalline layer. This is evidenced in Fig. 14. The difference between these two curves is again a measure of the incompatibility. If one adds to the stress-strain curve of the single crystal

the amount of incompatibility found in Fig. 13, i.e. if one translates the single crystal stress-strain curve by 120 g/mm^2 parallel to the stress axis, one obtains the dashed curve of Fig. 14. This dashed curve coincides as was expected with the experimental curve at 3 per cent strain. However, the experimental curve and the dashed curve diverge with increasing strain. As this divergence is very small and falls very close to the experimental accuracy of these curves, it could be meaningless. If this divergence were a real effect, it would mean that the incompatibility caused by the grain boundary interaction is still effective in the second stage. This would be consistent with Seeger's⁽²⁴⁾ theory of stage II, which proposes that the linear slope of stage II is caused by the progressive creation of Cottrell-Lomer locks. Therefore, it is reasonable to assume that enough Cottrell-Lomer locks will be needed to completely mask the effect of the grain boundary, and during the early parts of stage II the effect of the grain boundary should still be apparent.

Another composite single crystal was stripped of a layer twice as thick as the polycrystalline layer after 3 per cent elongation. This experiment was performed in an attempt to remove the multiple slip layer, as it was felt that a polycrystalline layer could not affect a layer greater than its own thickness inside the single crystal. That this is true is demonstrated in Fig. 15 where the composite single crystal stripped of a fifteen thousandths thick layer has more or less the same stress-strain curve as the single crystal. Actually, the stress-strain curve for the stripped crystal falls slightly below that of the single crystal, but this effect is most probably due to grip slippage.

A single crystal with a polycrystalline layer was extended up to 6 per cent strain and then unloaded. After removing the polycrystalline shell, the resulting single crystal with the shell of multiple slip caused by the polycrystalline layer was reloaded. The resulting stress-strain curves are shown in Fig. 16, and it can be seen that the stress-strain curve of the composite single crystal without its polycrystalline shell coincides with that of the single crystal at 6 per cent strain. The slopes of the composite single crystal and of the single crystal are approximately equal at 6 per cent strain. This fact shows that the grain boundary interaction is masked by the Cottrell-Lomer locks. It is nevertheless necessary in second

stage, to remove the polycrystalline shell to return to the single crystal state. This is due to the fact that even in second stage, where grain boundary interaction is negligible, the stress-strain curve of the composite single crystal still remains the average of the stress-strain curves of the single crystal and the polycrystal.

CONCLUSIONS

Assuming that the continuity of strain across the boundary of a bicrystal is the important criterion and ignoring the state of stress, it has been established that there exist only four different cases of compatibility, namely: symmetry, pseudosymmetry, pseudo-identity and the case $n = p = 0$. All other cases can be at best transiently compatible, i.e. compatible at the onset of deformation, and more incompatible as deformation proceeds. The importance of $\Delta\omega$, is questionable from the fact that Δp is proportional to $\Delta\omega$, which in turn means the greater the degree of incompatibility for a certain percentage of strain.

At the very onset of deformation, dislocation pile-ups can be responsible for the formation of fairly long slip bands of secondary slip system in the neighboring crystal. However, the main effect of dislocation pile-ups results in the formation of a multiple slip layer in the vicinity of the grain boundary, of which the thickness is comparable to the separation of the slip bands, i.e. a few microns. These microscopic effects can cause a macroscopically compatible bicrystal to be harder than its component single crystals. The macroscopic layer of multiple slip found in an incompatible bicrystal is believed to be caused by the superimposition of the shear taking place in one crystal on the deformation of the adjoining crystal.

As the microscopic layer has a constant thickness independent of grain size, it could explain the grain size effect that is believed to exist in polycrystals. The secondary slip systems activated by either mechanism can be predicted with the use of the N_{ij} factors.

Although no rigorous theory has been established to predict the stress-strain curve of a bicrystal some factors of importance are pointed out, which could explain the relative level of the stress-strain curves of some bicrystals. The Schmid factor and hence the resolved shear stress on all slip systems are of primary importance. Size effects which are

present in both single crystals and bicrystals should be taken into account especially when comparing a bicrystal with its component single crystals. The most important factor controlling the stress-strain curve of a bicrystal is its degree of compatibility as determined by the strain relations at the grain boundary. When the bicrystal is incompatible the degree of agreement between the predictions of the N_{ij} factors and the requirements to maintain compatibility will determine the relative strength of the bicrystal. The type of secondary slip system activated and its amount relative to primary slip are also very important as they determine the magnitude of the interaction. Finally, the stress-strain curve will depend on the extent of the multiple slip layer produced at the grain boundary. All these factors can successfully be used to rationalize the relative levels of the stress-strain curves of various bicrystals.

Bicrystals were obtained by sintering two single crystals. The sintered boundary behaved plastically in an identical manner to the grown boundary. A sintered single crystal with a slight misorientation at the sintered boundary has the same stress-strain curve as a normal single crystal. This sintering technique has made possible the achievement of a totally surrounded bicrystal, in which one crystal is fully surrounded by another.

This totally surrounded bicrystal can deform on as many as six slip systems in the worst case of incompatibility, while in a similar situation a bicrystal would deform on only four slip systems. The totally surrounded bicrystal is harder than the bicrystal and is a better approximation of the polycrystal. The slope of the shear stress-shear strain curve of the totally surrounded bicrystal is the same as that of the polycrystal. The polycrystal could therefore be considered to be the average of such totally surrounded bicrystals over all orientations and all degrees of incompatibility.

Single crystals surrounded by a polycrystalline layer were pulled in tension to study the nature of incompatibility. It was indirectly shown that incompatibility produces a multiple slip layer in the vicinity of the grain boundary. The major effect of incompatibility is felt during easy glide, although some effect still exists during the early part of stage II, when only a few Cottrell-Lomer locks have been produced. This corroborates the fact that most

of the difference between the stress-strain curves of a single crystal and a bicrystal occurs during easy glide and only a small divergence occurs thereafter.

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