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Influence of second-phase particles on plastic deformation and lattice reorientation of single crystals during uniaxial compression

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Changes in the orientation of crystal axes of Al–0.8 wt% Si single crystals in the presence of two different particle sizes and inter-particle spacings were investigated during uniaxial compression. The orientation of crystal axes before and after deformation was precisely determined by the diffractometer method in the unit triangle of the stereographic projection. The reorientation of the compression axes after deformation was found to be influenced by particle size and initial orientation of the undeformed crystals. It was found that particle size also influenced the yield strength and work-hardening characteristics which was explained on the basis of Orowan stresses and solid-solution strengthening.

1. Introduction

Knowledge of the operative slip systems during plastic deformation in single crystals is of fundamental importance because it allows mechanical as well as electrical and magnetic properties of materials to be related to the specific crystallographic orientations. The choice of slip system in the case of extension or compression depends upon the direction of the tensile or compression load in relation to the crystallographic axes [1]. It is now well understood that in an fcc metal the (1 1 1) [$\bar{1}$ 0 1] slip system has the highest value of critical resolved shear stress for all axial orientations within the unit triangle [0 0 1]–[0 1 1]–[$\bar{1}$ 1 1]. When compressive force is applied to a crystal oriented for single slip, plastic deformation commences with the activation of primary slip (1 1 1) [$\bar{1}$ 0 1] and as the deformation progresses, the compression axis moves towards the pole of the slip plane. When the compression axis reaches the symmetry boundary [0 0 1]–[0 1 1] of the unit triangle of the stereographic projection, another slip system becomes geometrically equivalent to the primary system, and duplex slip occurs. With further deformation, the compression axis seeks either [0 0 1] or [1 1 1] stable orientation depending upon the initial orientation of the undeformed crystals as predicted by Taylor [2]. Although Taylor's theory has a more rigorous basis than any other theory available so far to explain the reorientation characteristics of crystals, this theory is not always satisfied in cases when overshooting of the tensile axis near [0 0 1]–[$\bar{1}$ 1 1] or the compression axis near [0 0 1]–[0 1 1] symmetry boundaries may occur. Discrepancies exist in the literature over the overshooting of the tensile axis near the symmetry boundary during plastic deformation [3–5]. Carlsen and Honeycombe [3] reported considerable overshooting in Al–3.5% Cu single crystals. However, Silcock [4] obtained contradictory results in Al–4% Cu tested under the same conditions and concluded that overshooting of the tensile axis did not occur. Dew-Hughes and Robertson [5] studied the lattice reorientation in aluminium–copper alloys by the Laue method and registered no variation in the position of the tensile axis on the unit triangle of the standard stereographic projection. Price and Kelly [6] attributed the inconsistency in their results to the poor resolution of the Laue patterns obtained in lightly deformed single crystals. It is, therefore, possible that one of the reasons for discrepancies in the literature is due to the limitations of the experimental techniques employed in these investigations [3–6], i.e. the Laue or rotating crystal method. These techniques are sensitive to the crystal quality and in even slightly deformed crystals, the X-ray spots are no longer sharp, rendering these techniques inadequate for precise determination of crystal orientation. Moreover, when the tensile or compression axis lies near the symmetry boundary of a stereographic triangle, it is not possible to determine precisely the overshooting of the crystal axis with these methods [7].

Another method of orientation determination is the diffractometer method which is rarely used in such studies, although it allows the reorientation of the deformed crystal to be measured with great precision compared to the Laue or rotating crystal methods [8]. This method offers greater precision over conventional Laue or rotating crystal methods to identify precisely the position of the tensile or compression axes in the unit triangle of the standard stereographic projection, even though the crystal is heavily deformed.

As far as we are aware, no published work is available on the determination of the reorientation of the crystal axis during uniaxial compression in the

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presence of non-deformable second-phase particles. Thus there is a definite need for such information for the simulation of texture development during forming operations in materials containing second-phase particles such as metal-matrix composites, in which the strength of the material is reinforced by the addition of short whiskers or second-phase particles. This paper reports the reorientation characteristics during uniaxial compression of Al–0.8 wt% Si single crystals containing two different particle sizes in identical initial orientations. The differences observed in the mechanical behaviour of crystals containing different particle sizes is explained in the light of Orowan stresses and solid-solution strengthening. The orientation of the crystal axis before and after uniaxial compression was determined by the diffractometer method which has proved to be more adequate and precise compared to the conventional Laue or rotating crystal methods [7, 9].

2. Experimental procedure

Al–0.8 wt % Si single crystals, 5.5 mm diameter and 140 mm long, were grown by the modified Bridgeman technique. A small disc of approximately 3 mm length perpendicular to the crystal axis was cut to determine the orientation of the crystal by the diffractometer method. Three crystal orientations were selected and two different particle sizes and dispersion parameters were achieved in each of the orientations by heat treatment [10], which is given as follows. The crystals were solution treated at 580 °C followed by a cold-water quench. Fine and uniform precipitation was induced by annealing at 250 °C. The precipitates were then grown by a further anneal at high temperature either at 400 or 480 °C, and the specimens were slowly cooled to avoid any further nucleation of precipitates. This heat treatment enabled us to achieve two different particle sizes and inter-particle spacings in crystals of identical initial orientations. Furthermore, it has been shown that these particles do not deform or fracture during plastic deformation [10], which provides this system a reasonable ideal model system. Particle size and inter-particle spacing was determined by optical and electron microscopy from the linear intercept method using $\lambda = Ns^{1/2}$ [11]. The details of the dispersion parameter of silicon particles achieved in the soft matrix of aluminium single crystals are given in Table I.

Samples 11 mm long were carefully machined from the heat-treated crystals of 5.5 mm diameter, which were subjected to 50% deformation in uniaxial compression using a screw-driven Instron machine at a strain rate of $8.3 \times 10^{-4}\ s^{-1}$. Before deformation was carried out, a reference mark was inscribed along the axis of the cylindrical crystal in order to align the crystal in a fixed reference position before and after deformation with respect to the rotating goniometer axes. A special sample holder was designed to mount deformed samples which was aligned in the rotating goniometer in exactly the same position as that of an undeformed disc with the help of the reference mark. The diffractometer technique utilized in this study

TABLE I Dispersion parameters of single crystals[a]

Alloy code	d (μm)	N_s ($\mu m^{-2} \times 10^{-3}$)	λ (μm)
A, B, C,	0.66	27	6
A′, B′, C′	5	3.8	16

[a] d = mean particle diameter; N_s = number of particles per unit area; λ = inter-particle spacing.

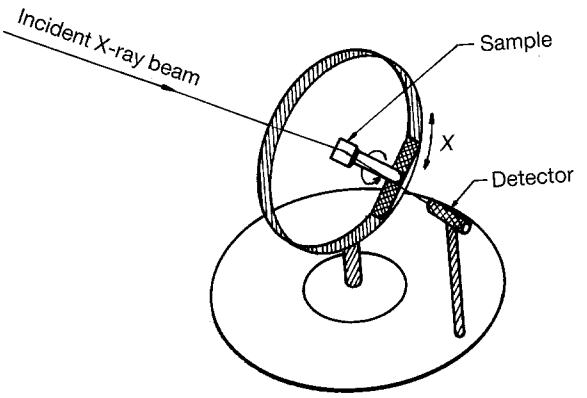

Figure 1 Basic arrangement of a texture goniometer.

involves the use of a rotating goniometer which is similar to that used in texture analysis. Fig. 1 shows the basic arrangement of the goniometer used in this work. The sample is mounted at the geometrical centre of the goniometer and the detector is preset to receive intensities from a low-index set of lattice planes of {1 1 1} type reflections. By means of two independent rotations, i.e. χ and φ, the position of these low-indexed planes on the standard stereographic projection are determined. Angle χ represents the tilt angle of the normal of the {1 1 1} crystal plane relative to the crystal axis, and angle φ represents the rotation angle of {1 1 1} plane against the crystal axis. With the help of these angles, a direct pole figure was constructed representing the crystal axis with respect to crystal planes {1 1 1} and further with the help of Wulffnet manipulation, the axis of the crystal was plotted in a unit angle triangle of a standard stereographic projection [8].

3. Results and discussion

The stress–strain curves of small particle-containing crystals (A, B, C) are plotted in Fig. 2 along with those of large particle-containing crystals (A′, B′, C′) of identical orientations. The yield stress was measured at 0.2% strain and the values thus obtained are presented in Table II.

It is observed that small particle-containing crystals have higher values of yield strength compared to large particle-containing crystals in all the orientations studied. The yield stress of crystals containing particles is a combination of the contribution from the particle–dislocation interactions, and the flow stress of the matrix crystal. As these particles are non-deformable [10], the observed yield stress is partly due to the force needed for dislocations to bypass the

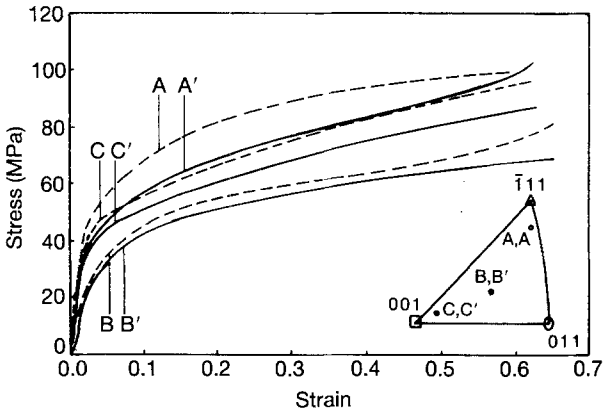

Figure 2 Stress–Strain curves of crystals containing small particles (A, B, C) compared with crystals containing large particles (A′, B′, C′). The orientation of the undeformed crystals is also shown in the unit triangle.

TABLE II Yield stress and Orowan stress of small particle-containing crystals and large particle-containing crystals

Crystal code	Yield stress (MPa)	Orowan stress (MPa)
A	33.4	0.62
B	15.9	0.62
C	30.3	0.62
A′	28.8	0.23
B′	15.2	0.23
C′	27.3	0.23

particles. The spacing and distribution of the particles play a significant role in determining the yield strength of materials as proposed by Orowan [12]. A simplified form of the relationship for the yield stress of the alloy may be given as follows.

$$\sigma_y = \sigma_m + 2T/b\lambda \quad (1)$$

where σ_y is the yield stress of the alloy, σ_m the yield stress of the matrix, T the line tension of the dislocation which is $Gb^2/2$ (where G is the shear modulus), b Burger's vector, and λ the effective inter-particle spacing.

Although there has been some modification to the above equation [13], it is adequate for rough-order-of-magnitude calculations of the yield stress [14]. Orowan stresses calculated for crystals containing large and small particles with the help of the above equation by taking G (shear modulus) $= 2.6 \times 10^4$ MPa [1], the values thus obtained are presented in Table II. The calculated Orowan stresses in small-particle-containing crystals are higher than for those containing large particles. However, the Orowan stresses alone cannot account for the difference in the yield stress of the two different particle-containing crystals. This is probably due to the solution-hardening effect, because the heat treatment used to obtain different particle sizes may have caused different amounts of solute (silicon) to remain in the solvent (aluminium).

The influence of initial orientations of the crystals on the stress–strain curves can be seen in Fig. 2. It is observed that crystals (B, B′) whose initial orientations lie in the centre of the unit angle triangle (soft orientation) exhibits least yield stress and low work-hardening characteristics compared to other crystals (A, A′, and C, C′) whose initial orientations lie near the corners of the triangle (hard orientations). Low work-hardening of B, B′ crystals is due to their initial orientations which lie in the middle of the triangle, i.e. in the region representing "soft orientations". It is, therefore, expected that the deformation process commences with the activation of only primary slip, because these crystals are least likely to experience slip on the conjugate system because the resolved shear stress on this system in the soft region of the triangle is low. Secondary slip in these crystals is activated when the crystal axis reaches the symmetry boundary [0 0 1]–[1 1 0] to explain further deformation. On the other hand, multiple slip at the beginning of the deformation in crystals (A, A′, and C, C′) is expected, owing to their initial orientations which lie near the edges of the unit angle triangle. Although these crystals are not precisely oriented for multiple slip to occur, however, near [1 1 1] and [0 0 1] three and four slip systems tend to operate, respectively, because they have nearly the same values of critical resolved shear stress. Therefore, the interaction between dislocations from different slip systems results in an increase in the dislocation density leading to high work hardening. Such an orientation dependence has been reported earlier in copper [15], silver [16] and recently in Al–4%Cu–0.1%Fe [17] single crystals.

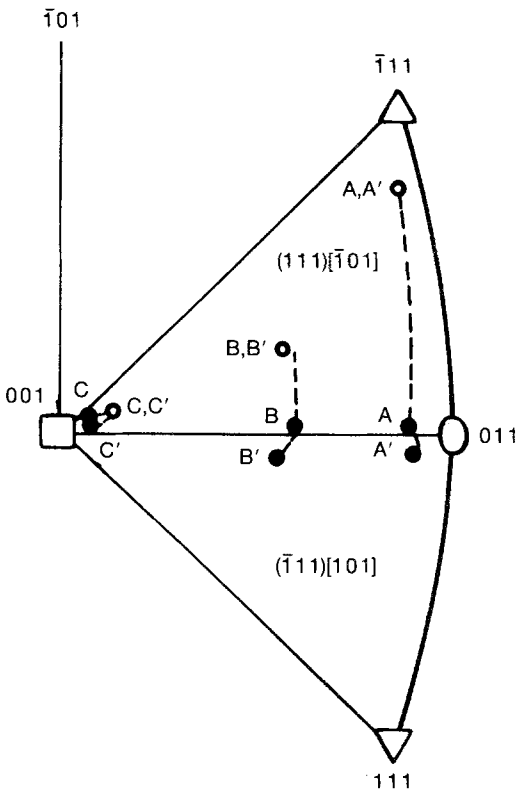

Figure 3 Reorientation of crystal axis (○) before and (●) after deformation.

The reorientation of crystal axes after 50% compression is shown in Fig. 3. It is interesting to note that small-particle-containing crystals in all the orientations studied never overshot the [0 0 1–0 1 1] symmetry boundary. On the other hand, in large-particle-containing crystals A′, and B′ overshooting of the

symmetry boundary to the extent of 3° and 4°, respectively, occurred. Another significant observation is the reorientation of crystal C′ which, although it contained large particles, moved very little from its initial orientation which lies near the [0 0 1] pole.

Although no comprehensive theory is available on the plasticity of particle-containing materials to explain the reorientation characteristics of crystals after plastic deformation, the subject can be discussed in the light of the effect of particle sizes on the microstructural development during plastic deformation. It has been observed that second-phase particles act as dislocation sources on a large number of slip systems [18] and therefore considerably modify the dislocation structure depending on the particle size and amount of strain. The deformation process in the presence of second-phase particles is inevitably inhomogeneous [19, 20] which leads to the formation of deformation bands from the early stages of the deformation process. Deformation bands are regions of different orientations within a deformed grain and can be readily recognized as differentiated bands of contrasting shading [21]. These microstructural inhomogeneities form a very significant part of the deformed structure [21]. Price and Kelly [6] found that single crystals of Al–3.7%Cu in hard orientations were deformed by the propagation of deformation bands. A similar observation was also made by Gonzalez *et al.* [17] in the presence of second-phase particles. These microstructural inhomogeneities are formed due to the strong interaction between dislocations of the primary slip system and second-phase particles resulting in strong latent hardening of the secondary slip system. It has also been reported that particle size also influences the scale of the deformation bands formed, because there is evidence that particles may effect the nucleation of these bands [22]. It is therefore expected that reorientation characteristics of crystals will be influenced in the presence of microstructural inhomogeneities, the scale and nature of which are dependent on particle sizes. Although there have been numerous experimental investigations of deformation band formation, understanding of their origin and their formation remains inadequate. The understanding of the origin and nature of microstructural inhomogeneities is extremely valuable in the formation of a theory to predict the reorientation characteristics of crystal axes and hence texture development in particle-containing materials.

The crystal axes near the [0 0 1] direction moved very little from their initial orientations in both the small-particle-containing crystal (C) and the large-particle-containing crystal (C′). This small movement of crystal axes may be attributed to the fact that in this orientation four slip systems are equally stressed, preventing the axes from considerable movement. Homogenized microstructure has been observed in crystals near [0 0 1] orientation, compared to other orientations in which considerable movement of the crystal axes occurred, the microstructure of which is predominated by deformation bands of various scales [21].

4. Conclusions

1. Small-particle-containing crystals show higher yield strength and work hardening compared to large-particle-containing crystals, which is explained on the basis of Orowan stresses and solid-solution strengthening of the crystals.

2. The reorientation of the crystal axes after plastic deformation was found to be influenced by the particle size as well as the initial orientation of the crystal axis.

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