Determination of Notch-Tip Plasticity by X-ray Diffraction and Comparison to Continuum Mechanics Analysis

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Abstract

Dislocation-free silicon crystals of (211) orientation with a hyperbolic notch, subjected to tensile deformation at 1073 K, were used as model material for the analysis of the induced plastic zone. The results obtained by X-ray topography and X-ray rocking-curve measurements were compared to theoretical calculations and predictions based on continuum mechanics. Good agreement between experiment and theory was obtained regarding the shape of the plastic zone, the contribution of the active slip systems to the size of the plastic zone and the direction of the maximum plastic strain trajectory in the zone. Discrepancies between experiment and theory regarding the symmetry relation of the plastic zone lobes and the dislocation density near the notch tip were attributed to the interactions and resulting work-hardening. These aspects were not taken into account in calculations of continuum mechanics.

Introduction

In a ductile material plastic deformation usually takes place near the crack or notch tip before the crack begins to grow. The non-linear stress–strain relationship in the plastic range makes the stress analysis a formidable task (Bilby, Cottrell & Swinden, 1963; Bilby & Eshelby, 1968; Rice, 1968; Rice & Tracy, 1973), and so far no general solution appears to exist, except for the simple case of a circular hole under tension.

In view of the importance of the shape and size of the plastic zone to fracture mechanics, a number of techniques have been employed to characterize the crack-tip yield zone. These include etching (Hahn, Hoagland & Rosenfeld, 1972; Clavel, Fournier & Pineau, 1975), image distortion interferometry (Liu & Ino, 1969; Petit & Hoeppner, 1973), X-ray microbeam (Yokobori, Sato & Yaguchi, 1973), selected-area electron channeling (Lankford, Davidson & Cook, 1977), and in situ high-voltage electron microscopy (Gardner & Wilsdorf, 1980; Kobayashi & Ohr, 1981).

Recently, a number of investigators have found that by selecting silicon as a model material X-ray topography can be used with great advantage to characterize the size and shape of the plastic zone at the crack tip in bulk specimens and to analyze the induced dislocation configuration.

The choice of silicon as a model material rests on a variety of reasons.

(1) Silicon can be obtained easily in the form of large, essentially dislocation-free, crystals which aids considerably the interpretation of the X-ray studies.

(2) Although extremely brittle at ambient temperature, silicon becomes increasingly ductile above 60% of its absolute melting temperature. At high temperatures it behaves like a metal crystal, exhibiting stress–strain curves consisting of three stages which, except for the yield points, are analogous to those of copper crystals (Alexander, 1968a, b; Alexander & Haasen, 1968).

(3) The dislocations are practically immobile at lower temperatures so that the dislocation configuration of the plastic zone developed at higher temperatures is virtually frozen-in when the specimen is cooled.

Tsunekawa & Weissmann (1974) studied notched wedge-shaped silicon crystals subjected to tensile deformation and to cantilever bending in the temperature range 773 to 1073 K. The microplastic zones were characterized by X-ray topography and by transmission electron microscopy. A quantitative evaluation was carried out experimentally by X-ray rocking-curve measurements and the residual elastic strains, constrained by the microplastic zones, were characterized by X-ray pendellösung fringe topography. The importance of microplasticity to notch-brittle sensitivity was shown. St John (1975) studied the flow and fracture associated with cracks in mode I loading of silicon under varying conditions of loading rate and temperature. The operative glide systems in crack-tip plastic regions, as revealed by X-
ray topography, were found to be those which were predicted by continuum mechanics for stress fields at sharp cracks. A detailed X-ray topographic analysis of the crack-tip dislocation arrangements was carried out by Michot, Badawi, Abdel Halim & George (1980). The shape of loops and the choice of slip systems were discussed in the light of calculations of the resolved shear stress in the silicon specimen.

Both the topographic studies of St John and those of Michot *et al.* dealt with sharp cracks. The work presented in this paper will be concerned with the analysis of the plastic zone produced by the tensile deformation of hyperbolic notched silicon crystals. It aims to correlate the quantitative X-ray measurements of the plastic zone to the predictions based on calculations of continuum mechanics. Since crack-tip blunting occurs in ductile materials the choice of a hyperbolic notch appears to represent a more realistic model than a sharp notch. Furthermore, it offers greater versatility since by a proper choice of a shape parameter the hyperbolic notch can be converted to a sharp notch.

**Experimental procedure**

Wafers of 1.5 mm thickness were cut from *n*-type silicon crystals using a diamond saw. The crystals were virtually dislocation free as checked by X-ray *Pendellösung* and Lang projection topography and had a resistivity of $0.003 \pm 10\%$ $\Omega cm$. Tensile specimens with the tension axis parallel to [011] were shaped with the Servomet spark erosion machine using specially designed cutting tools. The hyperbolic notch was likewise introduced into the specimen by spark cutting. The surface damage caused by the shaping process was removed by mechanical polishing with 600-grit silicon carbide powder, followed by chemical polishing, using a solution of HF (1 part), HNO$_3$ (4 parts) and CH$_3$COOH (1 part), cooled in an ice bath. The thickness of the finished specimens ranged from 0.75 to 1.00 mm. The shape, size and orientation of the specimen is shown in Fig. 1. The geometrical relation with respect to the notch and active slip system for this crystal orientation is shown in Fig. 2.

The tensile deformation was carried out in an Instron machine at 1073 K. Since silicon is very brittle below 773 K special holders, shown in Fig. 3, were used. To maintain the exact specimen alignment throughout the course of deformation a small constant load (1.4 MPa) was applied during the heating-up period of the sample. This procedure served to compensate for the thermal expansion of the assembly. To maintain the mechanical equilibrium, the load was kept on for at least one-half hour after the desired deformation temperature was reached. Subsequently, the specimen was pulled at the constant strain rate of $\dot{\varepsilon} = 5.9 \times 10^{-3}$ s$^{-1}$ at 1073 K and the deformation was stopped when the plastic strain $\varepsilon_p$ reached 0.4%. To
avoid relaxation problems and to ensure that the deformation structure induced at 1073 K was preserved intact, the specimens were furnace-cooled to 773 K with about 60% of the applied maximum stress. All deformation processes were carried out in air since it was found experimentally that for the X-ray analysis the same results were obtained for deformation performed in argon atmosphere or in air.

The X-ray double-crystal diffractometer (DCD) method was used as the principal research tool to analyze quantitatively the lattice distortions introduced into the notched crystal by the tensile deformation. A perfect silicon crystal in (111) orientation was employed as the first, monochromating crystal in the parallel DCD arrangement shown in Fig. 4. The K\(\alpha_2\) component of the reflected radiation was removed by interposing a pinhole of 300 \(\mu\)m diameter at the far end of a 60 cm long collimator so that only a small \((350 \times 300 \mu\)m\) monochromatic and essentially parallel beam was allowed to irradiate the specimen. The test crystal was then rotated (rocked) through its reflection range and the intensity versus angular rotation - the rocking curve - was recorded on a chart recorder. For the DCD tests, Cu K\(\alpha_1\) radiation and 422 reflections were used. The rocking curve is a sensitive measure of the lattice misalignment induced by the deformation. The total width, \(\beta\), at half the intensity maximum of the rocking curve (half-width) is a sensitive indicator of the induced local lattice misorientation. It measures the induced local lattice curvature, convex or concave, which arises from the accumulation of excess dislocations of one sign. Lattice misorientations as small as 10\(^\circ\) can be analyzed by the DCD method. To investigate the distribution of excess dislocation density as a function of irradiated specimen area, the specimen was moved on a microscopic stage across the X-ray beam along the \(x\) and \(y\) axes. At each position denoted by the coordinates \((x, y)\) a rocking curve and the corresponding half-width \(\beta_{(x,y)}\) were obtained. The \(\beta_{(x,y)}\) value represents the average value of the irradiated specimen area centered at the \((x, y)\) coordinates (Fig. 7).

The shape and size of the plastic zone around the notch were qualitatively depicted by the Lang X-ray projection topography. The test specimen, mounted on the goniometer of a Lang camera at a distance of 1 m from the target of a rotating anode, was set to reflect the finely collimated beam in transmission. In this arrangement, the specimen and film were moved synchronously across the impinging X-ray beam, thereby allowing relatively large areas to be examined. While traversing the beam, the specimen was oscillated so that all the misoriented lattice regions of the plastic zone could be recorded. The resolving power of X-ray topography depends on many factors and, under optimum conditions, it is of the order of several micrometers. Because of this resolution combined with the large width of the dislocation image, the individual dislocations cannot be resolved for densities greater than about \(5 \times 10^8\) cm\(^{-2}\). For X-ray topography Mo K\(\alpha\) radiation was employed and the (022) reflecting planes were investigated.

**Continuum mechanics analysis**

Single crystals undergo plastic deformation mainly by crystallographic slip; their plastic behavior is highly anisotropic. If a crystal element is under a stress \(\sigma_{ij}\), the resolved shear stress on a slip system, \(\tau\), is given by

\[
\tau = b_i n_j \sigma_{ij},
\]

where \(b_i\) is its slip direction and \(n_j\) its slip plane normal. The usual summation convention for repeated indices from 1 to 3 is implied in this expression. When \(\tau\) reaches a critical value, say \(\tau_0\), slip will take place.

Silicon crystals have a diamond structure and their plastic flow follows the pattern of face-centered-cubic crystals. A silicon crystal, thus, has four slip planes and three slip directions on each plane. These twelve slip systems and their values of \(b_i\) and \(n_j\) under the present orientations are given in Table 1.

The value of \(\tau_0\) can be obtained from a tensile test, say with the stress applied along the \(y\) or [01\(\bar{1}\)] direction on the unnotched specimen. Then there are four potentially active slip systems: on the (11\(\bar{1}\)) plane [110] and [1\(\bar{1}\)0], and on the (1\(\bar{1}\)1) plane [101] and [110], which are equally favorably oriented. The value \(\tau_0\) is given by

\[
\tau_0 = \sigma_y / \sqrt{6},
\]

where \(\sigma_y\) is the tensile yield stress.

Because of the inherent difficulty involved in the nonlinear aspect of notch-tip plasticity we shall seek an approximate solution, based on Neuber's (1958) equations. This technique is similar to that adopted by McClintock & Irwin (1965) in their study of the size and shape of the plastic zone near a sharp crack for a plastically isotropic medium. Incorporating the shape of the notch in his formulation, Neuber elegantly introduced the curvilinear coordinates \(x\) and \(\beta\) through the following relationships, shown in Fig. 5.

![Fig. 4. Schematic drawing of X-ray double-crystal diffractometer (DCD) arrangement. (1) Monochromating crystal (Ge or Si), (2) collimator and slit system for separation of K\(\alpha_2\), (3) test specimen, (4) proportional counter.](image-url)
Table 1. Designation of slip system in a silicon crystal

<table>
<thead>
<tr>
<th>Slip plane (shown in Fig. 2)</th>
<th>(111)</th>
<th>(111)</th>
<th>(111)</th>
<th>(111)</th>
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<tbody>
<tr>
<td>(110)</td>
<td>BCD</td>
<td>ACD</td>
<td>ABC</td>
<td>ABD</td>
</tr>
<tr>
<td>[101]</td>
<td>[011]</td>
<td>[101]</td>
<td>[110]</td>
<td>[011]</td>
</tr>
<tr>
<td>h₁</td>
<td>0</td>
<td>0</td>
<td>1/2</td>
<td>1/2</td>
</tr>
<tr>
<td>h₂</td>
<td>0</td>
<td>0</td>
<td>1/3</td>
<td>1/3</td>
</tr>
<tr>
<td>n₁</td>
<td>1/2</td>
<td>1/2</td>
<td>-1/2</td>
<td>-1/2</td>
</tr>
<tr>
<td>n₂</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

where \( \varphi \) is the angle measured from the x axis to the tangent of the \( \alpha \) line at the field point. It is given by \( \varphi = \tan^{-1} (\tan \beta / \tanh \alpha) \).

Under a prescribed nominal stress \( \sigma_n \), the yield condition at each point is determined by checking the yield condition of the twelve slip systems. Since \( \sigma_{yy} \) is the dominant term near the crack tip, only four out of these twelve are potentially active under the present plane stress state. The resolved shear stress on these four slip systems are

\[
\begin{align*}
(\bar{\text{I}}\bar{\text{I}}) & : \tau = \frac{2}{3\sqrt{6}} \sigma_{xx} + \frac{1}{\sqrt{6}} \sigma_{yy} - \frac{1}{2} \sigma_{xy}, \\
(\bar{\text{I}}\bar{\text{I}}) & : \tau = \frac{1}{\sqrt{6}} \sigma_{yy} + \frac{1}{6} \sigma_{xy}, \\
(\bar{\text{I}}\bar{\text{I}}) & : \tau = \frac{1}{\sqrt{6}} \sigma_{yy} - \frac{1}{6} \sigma_{xy}, \\
(\bar{\text{I}}\bar{\text{I}}) & : \tau = \frac{2}{3\sqrt{6}} \sigma_{xx} + \frac{1}{\sqrt{6}} \sigma_{yy} + \frac{1}{2} \sigma_{xy}.
\end{align*}
\]

The yield condition at each point then can be determined from (5)–(7), in conjunction with the critical shear stress \( \tau_0 \).

Equations (4a) and (4b), respectively, represent a family of confocal ellipses and hyperbolas. The shape of double external notches can be adequately described by choosing suitable values for \( \beta \), say \( \beta_0 \), and \( a \). Note that while \( \beta_0 \rightarrow 0 \), the double notches become sharp notches. For analytical convenience the single-notch specimen was replaced by a double-notch plate of twice the original width. The values of \( \beta_0 \) and \( a \) for the specimen tested were \( \beta_0 = 13.63° \) and \( a = 8.2 \text{ mm} \).

Under pure tension and assuming elastic isotropy, the stress field for a plate containing hyperbolic notches was obtained by Neuber:

\[
\begin{align*}
\sigma_{xx} &= A \cosh \alpha \sin \beta \left( 2 - \frac{\sin^2 \beta - \sin^2 \beta_0}{\sinh^2 \alpha + \sin^2 \beta} \right), \\
\sigma_{yy} &= A \cosh \alpha \cos \beta \left( 2 - \frac{\sin^2 \beta - \sin^2 \beta_0}{\sinh^2 \alpha + \sin^2 \beta} \right), \\
\sigma_{xy} &= -A \sinh \alpha \cos \beta \left( 2 - \frac{\sin^2 \beta - \sin^2 \beta_0}{\sinh^2 \alpha + \sin^2 \beta} \right), \\
\sigma_{ab} &= -A \sinh \alpha \cos \beta \left( 2 - \frac{\sin^2 \beta - \sin^2 \beta_0}{\sinh^2 \alpha + \sin^2 \beta} \right), \\
\end{align*}
\]

where \( A = a \cos \beta \), \( \beta_0 \), and \( \sigma_x \) is the nominal stress over the notch-root cross section.

In order to calculate the resolved shear stress on each slip system from the stress fields of \( \sigma_{xx} \), \( \sigma_{yy} \) and \( \sigma_{xy} \) of (5), we note that though the crystal orientation is fixed with respect to the \( x-y \) axes, it varies with respect to the \( \alpha-\beta \) axes. Thus, for this calculation it is more convenient to transform the stress components from the \( \alpha-\beta \) coordinate to the \( x-y \) coordinate by the stress transformation:

\[
\begin{align*}
\sigma_{xx} &= \frac{\sigma_{xx} + \sigma_{yy}}{2} + \frac{\sigma_{xx} - \sigma_{yy}}{2} \cos 2\varphi - \sigma_{xy} \sin 2\varphi, \\
\sigma_{yy} &= \frac{\sigma_{xx} + \sigma_{yy}}{2} - \frac{\sigma_{xx} - \sigma_{yy}}{2} \cos 2\varphi + \sigma_{xy} \sin 2\varphi, \\
\sigma_{xy} &= \frac{\sigma_{xx} - \sigma_{yy}}{2} \sin 2\varphi + \sigma_{xy} \cos 2\varphi,
\end{align*}
\]

Fig. 5. Curvilinear coordinates.
Experimental results

The shape and extent of the plastic zone which developed at the notch is pictorially shown by the Lang X-ray projection topograph of Fig. 6. A quantitative determination of the plastic zone in terms of local lattice misalignment (or excess dislocation density) was carried out by DCD measurements. The half-width values of the rocking curves $\beta_{(x,y)}$ – not to be confused with Neuber's curvilinear $\beta$ coordinates – corresponding to the coordinates $x_i$, $y_j$ on the specimen's surface are shown in Fig. 7. Although these values were determined with a precision of seconds of arc they are given in Fig. 7, for the sake of clarity, rounded up to the nearest value of minutes of arc. It will be seen that Fig. 7 represents thus a contour map of the plastic zone expressed in terms of excess dislocation densities. It resembles quite closely the X-ray topograph of Fig. 6. Inspection of Figs. 6 and 7 reveals that the plastic zone consists of two lobes of unequal size which are distributed on both sides of the central plane passing through the notch ($y = 0$). The following observations appear to be instructive.

(1) If in Fig. 7 the distribution of the $\beta$ values relative to the central plane is closely studied, it may be seen that near the notch tip this distribution was nearly symmetrical around the $x$ axis ($y = 0$).

(2) The maximum of the $\beta$ value for each lobe, namely 18' for the upper and 15' for the lower lobe, did not occur at the notch surface but at a distance of about 0.15 mm from the surface.

(3) There was a preponderance of slip activity in the upper lobe and consequently the distribution of the $\beta$ values relative to the central plane became increasingly asymmetrical with increased distance from the notched surface.

(4) Connecting the $\beta$ maxima of each lobe in Fig. 7 and supported by the visualization of slip interaction shown in the topograph of Fig. 6, one obtains the direction of the maximum plastic strain trajectories. They are indicated by the solid lines in Fig. 7. It will be seen that they subtended an angle of approximately 24° with the direction of the $x$ axis.

(5) Of considerable interest is the distribution of lattice misorientation in the regions adjacent to the flanks of the notches. It will be seen that the $\beta$ values near the edge of the specimen were very small and that there was only a slight monotonic increase as the flanks of the notches were approached.

Discussion of numerical results

The elastic–plastic boundaries near the notch root corresponding to various nominal stresses were plotted in Fig. 8. The shape of the plastic zone in single crystals is usually not symmetric, but because of the particular orientation of this specimen, it is always symmetric with respect to the central plane ($y = 0$). Indeed, this can be anticipated from (7) and from the nature of the stress distribution in this geometrically symmetric specimen. With respect to the central plane $\sigma_{xx}$ and $\sigma_{yy}$ are both symmetric, and $\sigma_{xy}$ anti-

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Fig. 6. X-ray oscillation-projection topographs of silicon crystal tensile deformed at 1073 K; $N$ refers to the notch, Mo Kα (022) reflection.

Fig. 7. Quantitative mapping of plastic zone in regions of equal lattice misalignment, $\beta$. 
symmetric. Thus, the resolved shear stresses of \(\{11\} [10T]\) and \(\{11\} [110]\) on the upper half of the specimen are, respectively, equal to those of \(\{11\} [101]\) and \(\{11\} [110]\) on the lower half, and vice versa.

The elastic-plastic boundary under a given nominal stress was obtained by considering the contour of the isoforce line of each slip system, for the special case when this force was equal to \(\tau_0\). For instance, at \(\sigma_n=0.68\ \tau_0\), which corresponds to the outermost boundary in Fig. 8, the contours for these four most favorably oriented slip systems were plotted in Figs. 9(a) and (b). The envelope of these contours leads to the elastic–plastic boundary in Fig. 8. Besides being useful for the determination of elastic–plastic boundary, these isoforce lines are very revealing to the relative extent of plastic deformation of slip systems. It is evident that on the upper half of the specimen, system \(\{11\} [101]\) is dominant while on the lower half system \(\{11\} [101]\) is most active. This also suggests that these two systems possess the highest dislocation density in these two respective regions. Moreover, the single slip, double slip and even quadruple slip zones can also be identified from this figure. The extended plastic region which flanks the notch surface, as shown in Fig. 8, is seen to be contributed by the second, relatively weak, plastic zone of \(\{11\} [10T]\) and \(\{11\} [110]\).

An interesting property which can be extracted from Fig. 8 is that, along the \(y\) axis, or \([01T]\) direction at a constant \(x\), the maximum resolved shear stress (with all twelve systems considered) exists at an angle of about \(13^\circ\) emanating from the notch root with respect to the \(x\)-axis. This line indicates the possible site where the maximum absolute dislocation density could be developed. Indeed, the profiles of highest resolved shear stress along the \(y\) direction, as shown in Fig. 10 for various distances \(d\) from the notch root, suggest both the extent of plastic deformation and distribution of dislocation density at notch proximity. These profiles are symmetric; the nonsymmetric behavior observed experimentally appear to be attributed to the possible nonaxial loading and dislocation kinetics and interactions.

The furthest extension distance of the lobes to the elastic–plastic boundary denoted by \(\gamma_{\max}\) in Fig. 8, is seen to occur at an angle of about \(23^\circ\). This value is known to be about \(70^\circ\) for a plastically isotropic material [such as a polycrystalline metal (Rice & Tracy, 1973)]. Since calculations for the isotropic materials were based on a sharp notch and not on a round one, as was considered here, it was suspected that this difference might be attributed to the notch shape. To clarify this shape effect, another calculation was performed for the single crystal, reducing the round notch into a sharp one by setting \(\beta_0=0^\circ\). The obtained plastic zone again showed the same charac-

![Fig. 8. Theoretical elastic–plastic boundaries in front of the notch at different nominal stress levels. \(N_{\max}\): direction of maximum dislocation density; \(\gamma_{\max}\): furthest extension distance of the lobe.](image)

![Fig. 9. Isoforce lines of the active slip systems on corresponding slip planes.](image)

![Fig. 10. Variation of normalized maximum shear stress along tensile direction at different distances from notch tip. [See equation (5) for the value of \(A\).](image)
teristics as plotted in Fig. 8: $\theta = 23^\circ$ for the furthest extension distance to the elastic-plastic boundary and $13^\circ$ for the maximum resolved shear stress along the y direction at a constant x.

Directly ahead of the notch root along the symmetry line, the maximum $\tau$, as shown by the midpoints of the stress profiles in Fig. 10, is seen to decrease drastically from the notch tip. This suggests a drastically decreasing profile for the dislocation density, which vanishes at the elastic-plastic boundary. According to this analysis, the maximum dislocation density should be at the crack tip. The experimental observations of this study and the results of a previous investigation (Tsunekawa & Weissmann, 1974), as well as the in situ electron microscope studies of Kobayashi & Ohr (1981), are in conflict with this concept and the possible causes of this disagreement will be discussed in the next section.

**Correlation of microstructural X-ray analysis to analysis of continuum mechanics**

Comparing the experimental results to the predictions based on continuum mechanics, one finds a number of agreements but also certain discrepancies which require clarification. The theoretical calculations have shown that for the given crystal orientation and notch geometry the direction of greatest shear strain in the plastic zone, produced by tensile deformation, should not be located in the central plane ($y=0$) but at an angle of $23^\circ$ with respect to the x axis. The quantitative X-ray measurements give corroborative evidence to this prediction when it was shown that the maxima of the excess dislocation densities, measured in terms of the $\beta(x, y)$ values of the rocking curves, did not lie in the central plane passing through the notch, but were located at an angle of about $24^\circ$ relative to the central plane.

The continuum-mechanics calculations predicted a shape for the plastic zone which should be symmetrical with respect to the central plane (Fig. 8). The X-ray measurements have confirmed this prediction only to a certain degree. Inspection of Fig. 7 will show that there exists a reasonably symmetrical relationship of the $\beta$ values relative to the x axis up to about 0.5 mm from the notch surface. On a microscopic level, however, one cannot realistically expect that in the upper and lower lobe of the plastic zone the two operative slip systems will be activated with equal strength. Indeed, it may be seen from the topograph of Fig. 6 and from the $\beta$ measurements that the slip activity in the upper lobe was much stronger and more extended, resulting in larger values for the upper lobe and accounting for the asymmetry of the zone shape at larger distance from the notch surface.

There was a remarkable agreement between the theoretical prediction of a weak plastic zone flanking the notch surface (Fig. 8), being produced by the activities of the weaker (111) [101] and (111) [110] slip systems (Fig. 9), and the experimental result of the topograph (Fig. 6) and $\beta$ measurements (Fig. 7) which offered corroborative evidence.

Of particular interest and controversial impact was the experimental observation that the largest amount of lattice misalignment, i.e. greatest degree of excess dislocation density, was not located at the notch tip but about 0.15 mm ahead of the tip. Previous deformation studies of silicon (Tsunekawa & Weissmann, 1973) carried out at different temperatures and different applied stress levels showed similar results. Thus, an increase of applied stress at 1073 K to $\sigma/\sigma_{nc} = 0.95$, where $\sigma_{nc}$ is the nominal fracture stress, resulted in large $\beta$ increases at sites 1 and 2 mm ahead of the crack tip but only in small increases at the tip.

A very recent X-ray study of the plastic zone ahead of a hyperbolic notch of 304 austenitic stainless steel deformed in tension gave corroborative results (Mayo, Yazici, Takemoto & Weissmann, 1981). X-ray rocking curves of the reflecting grain population were rapidly recorded and analyzed using a position-sensitive detector with interactive computer controls. It was found that the excess dislocation densities a few grain diameters ahead of the crack surface were considerably larger than in the grains immediately surrounding the crack tip. Kobayashi & Ohr (1981), carrying out in situ electron microscopy studies of the plastic zone ahead of the crack in tensile deformed polycrystalline copper, found part of the plastic zone immediately ahead of the crack tip free of dislocations. Beyond this dislocation-free zone, dislocations in the plastic zone formed an inverse pile-up of dislocations. Because of the thinness of the sample the results of the electron microscopy studies should be viewed, however, with caution and the difficulties encountered in interpreting the results have been recognized by one of these authors in a previous publication (Ohr & Narayan, 1980).

The experimentally observed dislocation-poor zone, immediately surrounding the crack tip, is in gross variance with the dislocation-rich zone predicted by continuum mechanics. The calculations of continuum mechanics, however, did not include considerations of dislocation kinetics in the work-hardening process of the plastic zone. The results of the X-ray studies suggest strongly that the dislocations emitted from the crack surface pertaining to different slip systems interacted ahead of the crack and gave rise to work-hardened sites in the plastic zone ($\beta$ maxima in the X-ray analysis) with concomitant increased lattice misalignment as soon as excess dislocations of one sign began to accumulate. It is because of these dislocation interactions that such a discrepancy arises between the X-ray measurement and continuum theory. It is tentatively suggested that
these work-hardened sites may form barriers to the dislocations subsequently emitted from the crack surface. The interaction of the emitted dislocations with these work-hardened sites in the plastic zone may generate microcracks which, with increased applied stress, become linked up with the main propagating crack (Gardner & Wilsdorf, 1980).

Summary and conclusions

Dislocation-free silicon crystals of (211) orientation with a hyperbolic notch were used as model material and subjected to tensile deformation at 1073 K. The plastic zone formed ahead of the notch was analyzed by X-ray topography and X-ray rocking-curve measurements. The results were compared to calculations and predictions based on continuum mechanics. The following conclusions were drawn.

Good agreement was obtained between the X-ray measurements and theoretical calculations regarding

1. the general shape characteristics of the plastic zone,
2. the contribution of the active slip systems to form the two-lobe characteristic of the plastic zone,
3. the contribution of the weakly active slip systems in shaping the plastic zone at the flanks of the notch,
4. absence of the greatest dislocation density in the direction of the central plane passing through the notch tip, and
5. the angle of ∼23° which the maximum plastic strain trajectory and furthest extension distance of the lobe to the elastic–plastic boundary subtended relative to the central plane.

Discrepancies between experiment and theory arose on

1. the deviation from the strict symmetry relation of the two lobes relative to the central plane of the plastic zone and greater extension of the upper lobe, and
2. development of an experimentally observed zone at the notch surface with a smaller excess dislocation density than the region about 150 μm ahead of this zone.

The discrepancies arising between micromechanic observations, based on X-ray measurements, and calculations, based on continuum mechanics, were rationalized in terms of dislocation kinetics, dislocation interactions with concomitant work-hardening and the possible specimen nonaxial alignment which were not taken into account in calculations of continuum mechanics.

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