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6 Urey, H. C., these *Proceedings*, 41, 27 (1955).

**ROTATION OF THE CRYSTAL LATTICE IN KINK BANDS, DEFORMATION BANDS, AND TWIN LAMELLAE OF STRAINED CRYSTALS**

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This paper is concerned with the geometry of rotation of the lattice of any highly strained domain in a deformed crystal with respect to the lattice of the unstrained host crystal. In particular it is a revision of the geometry of external rotation of narrow kink bands, deformation bands, and twin lamellae in experimentally deformed crystals of calcite and of dolomite. The degree and sense of external rotation are correlated with strain and with the orientation and sense of glide in the active glide system. The material studied is a series of single calcite crystals experimentally deformed by D. T. Griggs and H. C. Heard over the period 1952–1961 at the Institute of Geophysics, University of California, Los Angeles.

Correlation of External Rotation and Strain in Deformed Metal Crystals.—Metallurgists have long recognized that in experimental deformation of single crystals, strain is concentrated in local domains such as kink bands, and that the crystal lattice within such a domain becomes progressively rotated with respect to the lattice of the undeformed ends of the specimen, in which a constant orientation is maintained throughout deformation. The same effect has been observed in experimentally deformed crystals of calcite, dolomite, enstatite, and other minerals. Since rotation is measured with reference to coordinates (e.g., lattice directions in the host crystal) external to the rotated domain, it is, in Sander’s terminology, an external rotation (to be distinguished from internal rotation of passive marker planes, such as cleavage cracks, within the deformed domain).

The magnitude and sense of external rotation depend upon (1) the magnitude of strain, (2) the orientation of the active glide system in relation to the axes of principal stress \(\sigma_1\) and \(\sigma_2\) and (3) constraint of the undeformed ends of the specimen as determined by the mechanical conditions of loading. In all cases the active glide plane rotates toward the axis of minimal stress \(\sigma_3\). (In conformity with nomenclature currently in use by students of experimental deformation of rocks, compressive stresses are positive, tensile stresses negative; \(\sigma_1\) is algebraically greater than
The axis of rotation lies within the glide plane \( T \) and is normal to the glide direction \( t \). In the field of metallurgy\(^1\) external rotation has been related to linear strain \( \epsilon \) by simple equations: [1] for extension \( \sin \theta/\sin \xi = l / l_0 = (1 + \epsilon) \); [2] for compression \( \cos \theta/\cos \xi = l / l_0 = (1 - \epsilon) \); where \( \theta \) and \( \xi \) are the angles between the glide plane and the axis of the test cylinder respectively before and after the experiment, and \( l_0 \) and \( l \) are the respective lengths of the cylinder before and after the experiment. The angle of external rotation, \( \omega \), is \( (\theta - \xi) \).

**Anomalous Relations in Deformed Mineral Crystals.**—The same expressions have been applied to evaluate strain correlated with external rotation of kink bands and deformation bands in experimentally deformed mineral crystals.\(^2\)\(^3\) In these the axis of observed external rotation is invariably normal to the glide direction \( t \) in the glide plane \( T \) as deduced from other data. But there is considerable discrepancy between the magnitudes of the calculated and of the observed strain, even though the latter is always in close agreement with strain deduced from internal rotation effects.

There is good reason for such discrepancy. In experimentally and, presumably also, in naturally deformed crystals, kink bands and deformation bands develop under conditions of loading that depart markedly from those upon which equations (1) and (2) are based.

1. Figure 1 illustrates external rotation of the lattice of a very broad kink band (between \( kk \) and \( k'k' \)) in a conventional tensile test as carried out on a single crystal of a metal.\(^4\) \( \theta_0 = 53^\circ; \theta_1 = 15^\circ; l / l_0 = 3.07; \epsilon = 2.07 (20^\circ \%) \). If the ends were free (diagram \( a \)) the axis of the strained section would be rotated counterclockwise through an angle \( \omega(38^\circ) \); the lattice, as indicated by the glide plane \( T \), would maintain a constant orientation throughout the whole specimen. Since, however, the conditions of loading constrain the ends to remain coaxial, the strained section assumes the form of a kink band within which the lattice is externally rotated clockwise through an angle \( \omega' \). Because of the difference between their respective cross sections, the kink band and the unstrained ends are not quite coaxial. They diverge by an angle \( \varphi \), which is small (in this case \( 6^\circ \)) compared with \( \omega \) provided the value of \( \epsilon \) is high and the kink band occupies most of the length of the specimen. The observed angle of external rotation \( \omega' = \omega + \varphi \), whereas the ideal angle deduced from equation (1) is \( \omega \). In tensile experiments on calcite and other mineral crystals the kink bands are usually narrow compared with the length of the cylinder. In consequence the strain calculated from \( \omega' \) is notably higher than the observed strain or the strain calculated from data of internal rotation.

2. Equation (2) applies to external rotation of \( T \) (i.e., of the lattice) in short cylinders, homo-
Fig. 2.—Sections normal to \( T \) and parallel to \( t \) to illustrate external rotation of the lattice through \( \omega = (x_t - x_0) \), during compressive test in which end surfaces of specimen remain parallel but not coaxial. (a) Before strain. (b) After strain. (c) Geometric relation \( l_t/l_0 = \cos x_0/\cos x_1 \) for zero strain in the plane \( T \).

generously strained in such a way that the end surfaces remain parallel. Figure 2 illustrates a case where \( l_t/l_0 = 0.67; \epsilon = 0.33; x_0 = 30^\circ; x_1 = 54^\circ \). The axis of the cylinder is deflected through a small angle which is the difference between the clockwise external rotation \( (x_1 - x_0) \) and the counterclockwise internal rotation \( (\theta - \alpha) \) of the cylinder surface with respect to the glide plane \( T \). Very different are the conditions familiar in compression experiments on mineral crystals, where strain is far from homogeneous but is concentrated in narrow kink and deformation bands, and the ends of the cylinder are constrained to remain coaxial. Here, too, strain calculated from observed external rotation commonly is greater than observed strain.

Clearly it is desirable to develop other relations between strain and rotation that hold good for kink and deformation bands observed in experimentally strained short cylinders cut from single crystals of minerals.

Revised Correlations of External Rotation and Strain in Kink and Deformation Bands.—The closest approach to the condition illustrated in Figure 1b is found where, in extension experiments, strain is relatively large \( (\epsilon = 0.2 \text{ to } 0.5) \) and is localized in a single kink band whose width may be as much as half the length of the cylinder. This is illustrated in Figure 3, representing the outline of a thin section of a calcite crystal deformed by extension normal to the prism \((10\overline{1}0), = m_1\), at 300°C and 5,000 bars confining pressure. The over-all strain \( \epsilon = 0.16 \); but the local strain in the kink band, calculated from reduction of one diameter from 0.49 to 0.38 inches, is 0.29. The angle \( \varphi \) between the longitudinal trace of the kink band boundary and the axis of extension (stress axis \( \sigma_3 \)) is 6°. Strain is due to gliding on \((10\overline{1}1), = r_1; \ x_0 = 45^\circ; x_1 \) has an average value of 28°, so that the mean angle of external rotation of the kink band is 17°.

To take into account the angle \( \varphi \), the equation of strain is modified to eq. (3), \( l_t/l_0 = \sin x_0/\sin (x_1 + \varphi) \). This gives a value of 1.24, and the corresponding strain, \( \epsilon = 0.24 \), corresponds reasonably well with the value 0.29 calculated from the transverse dimensions. The unmodified equation (2) on the other hand gives the impossibly high value \( \epsilon = 0.47 \).

In compression experiments on short cylinders, strain is usually localized in a single narrow oblique kink band (Fig. 4a). In some extension experiments, too, the kink band may be narrow compared with the length of the specimen, or strain may be concentrated in several narrow lamellar or lenticular deformation bands surrounded on all sides by undeformed or slightly strained material (Fig. 5a). Clearly there is no approach to the ideal conditions of Figures 1 and 2, and completely different relations between strain and external rotation must therefore be explored.
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Fig. 3.—Broad kink band (stippled) in section of calcite crystal deformed by extension normal to \( m_1 \). Translation gliding on \( r_1 \).

Fig. 4.—(a) Kink band (stippled) in section of calcite crystal deformed by compression normal to \( m_1 \). Twin gliding on \( e_1 \). The lightly stippled areas are transitional sectors of progressive strain. (b) Detail of secondary kink bands \( k_1, k_2 \), developed near \( b \) of diagram \( a \).

Fig. 5.—Glide plane \( T \) in host crystal (stippled) in and kink band (below). (a) Ideal condition for equation (4). (b) Condition for equation (5).

Fig. 6.—Longitudinal sections, parallel to the deformation plane, of calcite cylinders deformed by extension parallel to \([r_2; r_3]\). Nicols crossed. Axis of minimum stress (= axis of extension), \( e_1 \), is longitudinal. (a) Experiment 563; 500°C, 4,700 bars. Strain \( \epsilon = 10.3\% \). Strain rate \( 5 \times 10^{-4} \) sec. (b) Experiment 294; 400°C, 5,000 bars. Strain \( \epsilon = 10\% \). Strain rate \( 3.3 \times 10^{-7} \) sec.

At least one boundary surface of a kink or deformation band typically is planar through much of its length (Fig. 6b). Here extinction directions and cleavage or twin traces are sharply deflected and the trace of the boundary surface can be
located to within a degree or so. For such a band a possible relation between external rotation of the lattice and internal strain may be developed on two assumptions: (1) the boundary surface is occupied throughout progressive strain by the same mineral particles; (2) the initial angle between the active glide plane and the boundary surface approximates 90° (Fig. 6a). The first assumption can apply only to sharply defined boundaries such as A B of Figure 4a; it cannot be valid where the boundary is not a surface but rather a narrow zone of progressive strain merging into the unstrained host crystal (B C of Fig. 4a). The second assumption is consistent with a large body of evidence relating to deformed metallic and ionic crystals whose glide systems have been identified by other means.

Any passive marker surface occupied by the same set of particles becomes internally rotated with reference to the lattice of the strained band according to the equation \( \cot \alpha - \cot \beta = s \sin \gamma \) where \( \alpha \) and \( \beta \) are the angles between the glide plane \( T \) and the rotated surface after and before rotation, \( s \) is the shear (= tan \( \theta \), the angle of shear on \( T \)) and \( \gamma \) is the angle between the axis of rotation and the glide direction \( t \). Since the kink-band boundary remains fixed in space as a surface in common with the undeformed host crystal, we may consider the lattice of the kink band as being correspondingly rotated through the angle \( \beta - \alpha \) with reference to the boundary surface. Thus the angle \( \omega \) of external rotation of the kink-band lattice is \( \beta - \alpha \); and according to our second assumption \( \beta \) is 90°, and \( \alpha \) is (90° - \( \omega \)). For slip on a single glide system, \( \gamma = 90° \). Thus the relation of external rotation \( \omega \) to strain \( \epsilon \) becomes equation (4), \( \cot(90° - \omega) = s = \epsilon/S_0 \), where \( S_0 \) is the coefficient of resolved shear stress on \( T \) and the magnitude of strain is small. Equation (4) is an approximation; but for values of \( \omega \) up to 30° the error is small even where the angle \( \beta \) departs by 10° or so from 90°.

Where the kink-band boundary is sharp and the identity of the glide plane is known from other data, the relation between shear and external rotation can be defined precisely. Let \( \alpha \) and \( \beta \) be the angles between the glide plane \( T \) and the kink-band boundary in the kink band and in the host crystal, respectively. Usually the geometric relations are as pictured in Figure 5b, where the normal to the kink boundary lies in the acute angle between the two orientations of \( T \). Then (5), \( s = \cot \alpha + \cot \beta \). This relation is preferred to equation (4) because it dispenses with the assumption that the glide plane in the host lattice is normal to the kink-band boundary.

**Illustrative Examples.**—Figure 6a shows a longitudinal section, parallel to the deformation plane, of a calcite cylinder deformed by extension parallel to the cleavage edge \([r_2:r_3]\) at 500°C and 4,700 bars confining pressure (Experiment 563 of D. T. Griggs and H. C. Heard). The total strain \( \epsilon = 10.3\% \); but in the neck \( \epsilon \) is of the order of 20%, and much of this is concentrated in oblique lensoid deformation bands (dark in Fig. 6a) where the strain must be even higher. Within the deformation band adjacent to \( X \), \( e_1 \) lamellae, now \( L_{e_1} \), have been internally rotated counterclockwise along the arc \( e_1 \circ r_1 \) (the zone circle of the \( a_2 \) axis) as a result of gliding on \( r_1 \) (Fig. 7a).

For this glide system \( \alpha = 39°, \beta = 71°, \gamma = 90°, S_0 = 0.31 \). \( \epsilon = 0.31 (\cot 39 - \cot 71) = 0.275 \) (27.5%). The lattice of the kink band has been externally rotated clockwise through 40° (\( \omega \)) about the \( a_2 \) axis, the path and sense of rotation being consistent with gliding on \( r_1 \). From equation (4), \( s = \cot (90° - 40°) = \)
Fig. 7.—Projections (equal-area, lower hemisphere) of lattice directions, planes and lamellae measured in sections shown in Figure 6. Points in the undeformed sector are shown as crosses; those in the deformation or kink band are shown as circles. IR indicates internal rotation of \( e_1 \) to \( L_1 \); ER indicates external rotation of the lattice in the band. Sense of a gliding on \( r_1 \) in the band is indicated by arrows. (a) Experiment 563. Deformation band near \( X \), Figure 6a. Trend of band, \( dd \). (b) Experiment 294. Diagonal kink band, Figure 6b. Trend of band, \( kk \).

0.84. The corresponding strain, \( \epsilon = (0.31 \times 0.84) = 0.26 \) (26%), is in reasonable agreement with the values calculated from internal rotation of \( L_1 \) and from cross-sectional dimensions of the neck. On the other hand, if the standard equation (1) were used, \( \epsilon = l/l_0 - 1 = (\sin 71/\sin 31) - 1 = .83 \) (83%). This is an impossibly high value.

Figure 6b represents a longitudinal section through a similarly oriented calcite cylinder deformed by extension at a slow strain rate at 400°C and 5,000 bars confining pressure (Experiment 294, H. C. Heard). The over-all strain of 10% is localized in a single diagonal kink band inclined at 66° to \( r_1 \) of the host lattice. Gliding on \( r_1 \) within the kink band is established from clockwise internal rotation of \( e_1 \) through 28° to \( L_1 \) (Fig. 7b); and the corresponding local strain is calculated as \( \epsilon = 23\% \). Counterclockwise external rotation of the kink band through 42° about the \( a_2 \) crystal axis is consistent with gliding on \( r_1 \). Using equation (4), \( s = \cot (90 - 42) = 0.90; \epsilon = 28\% \). Since the orientation of the kink-band boundary can be measured to within a degree or two, the preferred equation (5) can be employed; and from this \( s = (\cot 66 + \cot 72) = 0.77; \epsilon = 24\% \). If, however, the standard equation (1) were employed the calculated value of \( \epsilon \) would be impossibly high: \( \epsilon = (\sin 71/\sin 29) - 1 = 95\% \).

It is instructive to recompute strain on the basis of equations (4) and (5) using published data on experimentally deformed crystals of calcite for which the value of \( \epsilon \) has been determined independently from data of internal rotation or from the geometry of \( \epsilon \) twinning. Figure 4a shows a longitudinal section through a calcite cylinder deformed by compression normal to the prism (1010), \( = m_1 \), at 20°C and 10,000 bars. The over-all strain is a shortening of 15%. But this is concentrated in a diagonal kink band within which twinning on \( e_1 \) is complete, so that the local strain is accurately known: \( s = 0.694; \epsilon = 26\% \). The angle of external rotation of the kink-band lattice, \( \omega \)—shown by counterclockwise deflection of \( r_1 \) in Figure 4a—is 37°. From equation (4), \( s = \cot 53 = 0.75; \epsilon \) the error is +8%. Contrast this
with the value of $\epsilon$ calculated from equation (2). $\epsilon = 1 - (\cos 63/\cos 26) = 0.50$; the error is +90%. At the edges of the main kink band of Figure 4a (e.g., near point $D$) there are local microscopic, sharply defined kink bands showing different degrees of strain ($e_1$ twinning) and of external rotation. Data for one of these bands ($k_1$ in Fig. 4b) are as follows: Angle of internal rotation of $e_2$ to $L_{e_2}$ = 18° (clockwise). Angle of external rotation of lattice in $k_1$ = 28° (counterclockwise). Twinning on $e_1$ in $k_1$ is about 80% complete ($s = 0.56$). From internal rotation $s = (\cot 45 - \cot 63)/\sin 57 = 0.58$. From external rotation, using equation (4), $s = \cot 62 = 0.53$. All three values of $s$ are mutually consistent.

Finally, Higgs and Handin7 have recorded rotational data for experimentally deformed crystals of dolomite. In most of these experiments $T = \{0001\}$ and $t$ is an a axis of the lattice. Values of the angle of external rotation are not large and are correct only to within one or two degrees. Nevertheless, as shown in Table 1,

### Table 1

<table>
<thead>
<tr>
<th>Specimen number</th>
<th>Orientation</th>
<th>Over-all, from dimensions</th>
<th>Computed Values of $\epsilon$ (%)</th>
<th>Local, from internal rotation</th>
<th>Local, from external rotation</th>
</tr>
</thead>
<tbody>
<tr>
<td>160 (p. 268)</td>
<td>Extension</td>
<td>$\omega$</td>
<td>$\epsilon$</td>
<td>Eq 1</td>
<td>Eq 4</td>
</tr>
<tr>
<td>170 (p. 269)</td>
<td>normal to $r$</td>
<td>$12^\circ$</td>
<td>11.9</td>
<td>9.2-14.9</td>
<td>30.0</td>
</tr>
<tr>
<td>529 (p. 270-271)</td>
<td>Compression</td>
<td>$14^\circ$</td>
<td>10.4</td>
<td>12.3</td>
<td>11.4</td>
</tr>
<tr>
<td>156 (p. 269-270)</td>
<td>normal to $r$</td>
<td>$10^\circ$</td>
<td>7.8</td>
<td>12.0</td>
<td>29.0</td>
</tr>
<tr>
<td>161 (p. 271)</td>
<td>Extension parallel to $[f_1,f_3]$</td>
<td>$10^\circ$</td>
<td>7.5</td>
<td>7.9 or 9</td>
<td>26</td>
</tr>
<tr>
<td>622 (p. 266)</td>
<td>gliding on f $= {02\overline{2}1}$</td>
<td>$22^\circ$</td>
<td>20</td>
<td>37</td>
<td>12.7</td>
</tr>
</tbody>
</table>

the strain calculated from equation (4) commonly agrees satisfactorily with that computed from internal rotation and from dimensional data, especially where (as in specimen 161) strain is concentrated in a sharply defined kink band. In one specimen (170) the value of $\epsilon$ computed from the standard equation (1) is more satisfactory than that obtained from equation (4); but here the kink band is ill defined. Experiment 622 was complicated by failure by shear fracture following twin gliding on $\{02\overline{2}1\} = f$.

Collectively the experimental data relating to calcite and dolomite confirm the general validity of equations (4) and (5) as applied to narrow kink bands and deformation bands.

**Lattice Rotation in Complementary Twinning.**—When twin gliding on $e_1$ proceeds to completion in a calcite crystal, any pre-existing $e_2$ twin lamella retains its identity and becomes internally rotated through $22^\circ$ (Fig. 8a). As an $L_{e_1}$ lamella it becomes reoriented so as to coincide with $\{1120\} = a$ of the twinned host crystal.5,6 Dr. Iris Borg has drawn the author’s attention to an accompanying effect which she observed in completely rotated $L_{e_2}$ lamellae: these themselves become strained in sympathy with the enclosing host crystal, by internal twinning on $e_2^\parallel$ (the twinned equivalent of $e_2$ in the $e_2$ lamella); and the orientation of the lattice so formed is identical with that of the completely twinned host. The boundary surfaces of the lamella are still recognizable in arrays of microscopically visible discontinuities.

The geometry of the reorienting process may be followed on a projection upon the only recognizable plane that survives the process of complementary twinning, namely $L_{e_2}^\parallel$ (Fig. 8b). This
is held in a fixed position, and the two lattices—that of the host and that of the lamella—are shown as rotating in opposite senses as required by the geometry of twinning. The axis of rotation is the same for both lattices, the common edge R between e, e% and e,'. In Fig. 8b what is conventionally described as internal rotation of the lamella within the host lattice is shown as external rotation of the twinned lattice in the opposite sense with reference to a fixed level.

To illustrate the general case, let a crystal lattice become completely twinned by gliding on a plane h. And let a pre-existing twin lamella k (twinned on a plane k of the host lattice) thereby become rotated to a new orientation Lkh. Lkh must be rationally oriented as a simple plane of the twinned host lattice. If the lamella simultaneously twins on its own h plane, f2, the twinned lamella and the twinned host are finally related by twinning with f2 as twin plane. This may be demonstrated by geometric construction along the same lines as Figure 8b.

Summary.—New equations are offered for correlating longitudinal strain ε or shear s (the tangent of the angle of shear on the glide plane) with external rotation of the crystal lattice in narrow kink bands and in deformation bands in experimentally deformed crystals. Where χ0 and χ1 are the respective angles between the single active glide plane and the longitudinal axis of the specimen (σ1 or σ2 of an axial stress system), (1) for extension experiments in which the kink band is
wide compared with the length of the specimen, and \( \phi \) is the angle between the lateral edge of the kink band and the axis of extension, \( e = \frac{\sin \chi_0}{\sin (\chi_1 + \phi)} - 1 \). (2) For narrow kink bands and deformation bands, (a) an approximate relation is 
\[ s = \cot (90^\circ - \omega) \]; (b) a more precise relation where \( \alpha \) and \( \beta \) are the respective angles between the kink-band boundary and the active glide plane in the band and in the unstrained ends, \( s = \cot \alpha + \cot \beta \). The validity of these equations has been tested against rotational and strain data for experimentally deformed crystals of calcite and dolomite.

The above relations are based on the assumption that throughout progressive strain the boundary surface of a kink or deformation band is occupied by the same material particles and serves as a datum with reference to which the crystal lattice of the band may be considered to rotate about the intersection of the kink-band boundary surface and the glide plane \( T \). By making a similar assumption with regard to a twin-lamella boundary in calcite, it is possible to explain complex rotational effects leading to simple geometric relations previously observed between a completely twinned crystal lattice and the completely twinned lattice of an enclosed rotated lamella.

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6 Ibid., 907, experiment 190.

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**ON THE MARTIN BOUNDARY FOR MARKOV CHAINS**

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The Martin boundary for a discrete parameter Markov chain was first considered by Doob, using the theory of R. S. Martin after whom the boundary is named. A direct and ingenious method was later found by Hunt, who also strengthened Doob's results in several points. In this note, I shall sketch a natural approach to the theory in the continuous parameter case. There, upon the introduction of certain intrinsic quantities (probabilities) which have no obvious discrete analogues, it is possible to derive the main results by familiar methods developed in reference 1. They cover the discrete case through a simple transformation. Thus, in a sense, what has been artificial becomes now the inevitable. It appears at the same