

MECHANICAL $\langle 110 \rangle$ TWINNING IN
SHOCKED SPHENE¹I. Y. BORG, *Lawrence Radiation Laboratory,
University of California, Livermore, California 94550*

ABSTRACT

Polysynthetically twinned sphene occurs in shocked granite surrounding cavities produced by the Hardhat and Piledriver nuclear events at the Nevada Test Site. Commonly two sets of composition planes (twins) at *ca* 55 deg to each other are developed within individual grains. A few examples were observed in granites subjected to an estimated 5–8 kbar peak pressure and ~ 1 kbar stress difference, and numerous highly twinned crystals occur in the cavity walls that have experienced peak pressures greater than 40 kbar. The twin glide system is: K_1 =irrational, near $\{221\}$, $K_2 = \{\bar{1}31\}$, $N_1 = \langle 110 \rangle$, N_2 =irrational, $s = 0.60$. The twinning is of the second kind (Mügge); twin and host are related to each other by a 180 deg rotation about N_1 . The conjugate twin mode was not detected. Examination of the atomic movements involved in the twin process shows that all cations could be restored by homogeneous shear with minimal amounts of shuffling; however O atoms could not. In order to produce a twinned structure, either Si tetrahedra or Ti octahedra must rotate as well as translate during the mechanical twin glide.

INTRODUCTION

Polysynthetically twinned sphene occurs in shocked granite from the Climax Stock, Nevada, surrounding the cavities produced by the Hardhat and Piledriver Events. It is virtually absent in sphene of the unshocked granite and increases in frequency with proximity to the shot point. It was first detected in samples collected in a reopened access drift to the Piledriver cavity at 105 m from the shot point. At this point the peak pressure is estimated to be 5–8 kbar, and the stress difference is ~ 1 kbar by extrapolation from calculated as well as measured data (Cherry and Rapp, 1968). The existence of a void (the drift) at the time of the shock makes the estimate somewhat tenuous, however. Approximately 10 percent of the sphene observed contains one or more twin lamellae; accompanying biotite shows incipient kinking and secondary calcite contains a few $\{01\bar{1}2\}$ mechanical twins. Figures 1(a) and 1(b) are examples of moderate and well-developed twins in sphene from the Hardhat Event. Both are from postshot cores drilled to within 20 m of the shot point. Peak pressures in these are on the order of 30–45 kbar (Short, 1966). Numerous lamellae are developed at even greater shock pressures but are less conspicuous because of the associated high degree of fracturing and disaggregation.

ELEMENTS OF TWINNING

In 1889 Mügge considered the possibility that polysynthetic twinning

¹ This work was done under the auspices of the U. S. Atomic Energy Commission.

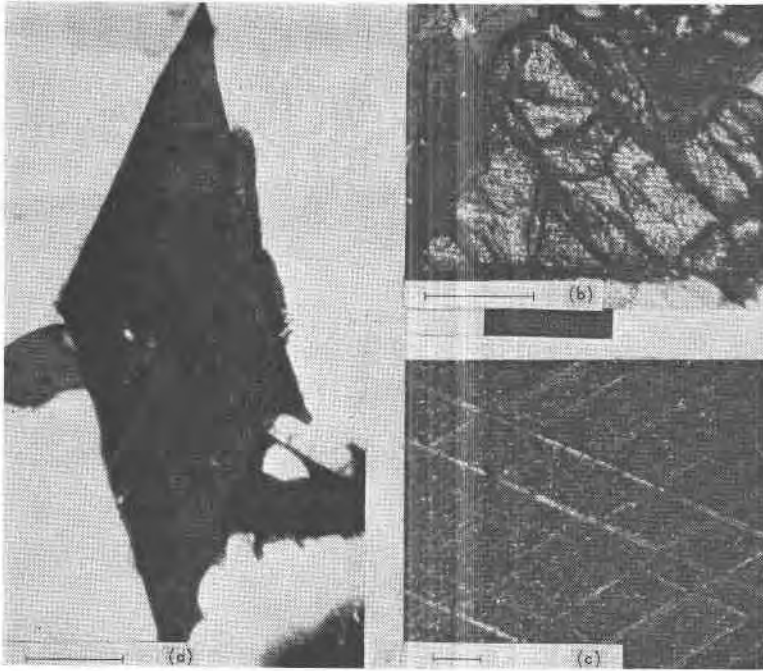


FIG. 1. $\langle 110 \rangle$ twinning in sphene: (a) Weakly developed set \approx parallel to $\{221\}$ in shocked granodiorite (Hardhat Event, B 144). (b) Well-developed set in shocked granodiorite (Hardhat Event, B 203). (c) Two sets of polysynthetic twins in sphene from Arkaroola Station, Australia. In each case bar represents 0.1 mm.

occasionally observed in monoclinic sphene, CaTiSiO_5 , was due to mechanical twin glide. Using optical goniometry he was able to prove that the composition planes (habit plane) described as (221) and $(\bar{2}\bar{2}1)$ were irrational planes near to but not coincident with $\{221\}$ and that the twinning could be described as a 180° rotation about $[1\bar{1}0]$ and $[110]$. On the assumption that the twinning was mechanical in origin he deduced the twin glide systems as follows:

$K_1 = \text{Irrational, near } \{221\}$	Slip plane or plane of no distortion
$K_2 = \{131\}$	Other plane of no distortion
$N_1 = \langle 110 \rangle$	Slip line
$N_2 = \text{Irrational}$	Axis of the principal zone (trace of K_2 on S)
$S = \text{Irrational, near } \{112\}$	Plane of deformation
$K_1 \wedge K_2 = 73^\circ 21' \quad s = 0.598$	Shear (Mügge, 1889, 1889a)
$K_1 \wedge K_2 = 73^\circ 23' \quad s = 0.597$	Shear (calculated from cell dimensions given by Zachariasen, 1930)

Mügge marshalled considerable indirect geologic evidence that some

if not all such twinning, Figure 1(c), was mechanical in origin; vis., association with other mechanically twinned minerals such as calcite and augite, and the presence in highly folded metamorphic rocks and absence in young eruptive rocks. However, he was unable to produce it in his laboratory. Mügge (1889b) subsequently designated such mechanical twinning as "twinning of the second type" as distinct from "twinning of the first type," in which the host and twin are related by a mirror operation across K_1 . Theoretically for every twin of the first or second kind there exists a conjugate or reciprocal twin of the other kind (Jawson and Dove, 1960). Examples among minerals are mechanical albite and pericline twins in plagioclase, (Borg and Heard, 1969). In the case of sphene, the conjugate twin law of the first kind is described by

$$\begin{aligned} K_1 &= \{\bar{1}31\} \text{ slip plane} \\ K_2 &= \text{Irrational, near } \{221\} \\ N_1 &= \text{Irrational slip line} \\ N_2 &= \langle 110 \rangle \end{aligned}$$

Commonly, only one of a reciprocal pair can be produced mechanically. Since the atomic movements do in fact differ, the explanations for prevalence of one type over the other have been based on energy considerations. In general mechanical twins of the second kind are most easily produced probably because the strain across the twin interface (K_1) is at minimum; it is an irrational plane containing at most a single row of atoms.

Homogeneous shear gliding rarely results in a configuration which exactly coincides with that of a perfect twin. Some indication of the ease of twinning can be gained by a close examination of the nature and size of additional adjustments or shuffles that are necessary to bring about the coincidence. To this end the atomic movements are examined in detail in the following sections.

In the present study, only $\langle 110 \rangle$ twins of the second kind were observed. It was possible to locate uniquely the composition plane to within a few degrees of $\{221\}$ by measuring well-formed faces (e.g., $\{111\}$ or $\{001\}$) and axes (XYZ , Fig. 2) of the optical indicatrix with a universal stage. In all crystals measured, the pole to the composition plane lies $34^\circ \pm 2^\circ$ to Z . Where two sets of twins are developed in a single crystal, the measured angle between them is $55^\circ \pm 2^\circ$ as compared to $54^\circ 15'$ calculated between $\{221\}$ planes and $51^\circ 40'$ between $\{131\}$ planes.

RESULTS OF ANALYSIS

The examination subsequently described here in detail shows that mechanical twinning of the second type results in the restoration of a

Structure of Sphene. The structure was determined by Zachariassen (1930) and refined by Mongiorgi and di Sanseverino (1968).¹ The space group is $C2/c$, $Z=4$, and the cell dimensions are

$$a = 6.56 \text{ \AA} \quad b = 8.71 \text{ \AA} \quad c = 7.45 \text{ \AA} \quad \beta = 119^\circ 43' 2''$$

It consists of [101] chains of Ti octahedra linked to each other by independent SiO_4 groups and Ca polyhedra made up of seven oxygen atoms (Fig. 3).³ Edges and corners but not polyhedra faces are shared. The identity of the oxygen in the polyhedra is:

Si: 2O(B) and 2O(C)

Ti: 2O(A), 2O(B), and 2O(C)

Ca: 1O(A), 4O(B), and 2O(C)

Thus all 20 oxygen atoms in the unit cell are bound to the four Ti atoms.

Table 1 contains the atomic coordinates transposed from those given by Zachariassen so that the origin is at a center of symmetry. Appropriate symmetry operations for the new setting are:

$$\pm(xyz) : \pm(x + \frac{1}{2}, y + \frac{1}{2}, z) : \pm(x, \frac{1}{2} - y, \frac{1}{2} + z) : \pm(\frac{1}{2} - x, y, \frac{1}{2} - z)$$

Geometry of Twin Process. Left-hand portions of Figures 4 and 5 (labeled a) are projections of the unit cell onto the irrational plane of deformation, S , whose Miller indices are $(\overline{3.87} \overline{3.87} 8.18)$ or $\simeq(\overline{112})$. The two planes of no distortion, K_1 (= glide plane) and K_2 are normal to the plane of the drawing; N_1 (= glide line) is the plane of the page. Except for the Ti atom at 000, no atom lies on the plane of projection; they are distant by the amounts, D , given in Table 1. The *ideal* twin configuration is outlined in the top, right (b) and bottom, left (c) portions of Figure 4. The latter two units, b and c , are the same configuration since, in a centrosymmetric structure, a 180° rotation about the twin axis, N_1 , is equivalent to a reflection across the irrational twin plane normal to N_1 . Atoms in b are the same distance, D , from the plane of projection as those in a , whereas atoms in c have D 's of the opposite sign.

¹ Calculations reported here were carried out before the author became aware of the refinement. The improved atomic coordinates of Mongiorgi and di Sanseverino differ only slightly from Zachariassen's. For the purposes of this paper, Zachariassen's data are considered sufficiently accurate to obviate recalculation. His choice of cell has also been retained since morphological data on twinning are referred to that cell.

² The beta angle given by Zachariassen and Mügge is quoted from Des Cloizeaux's *Manual de Minéralogie* 1862, 1874.

³ This figure was drawn using the OR TEP Program (C. K. Johnson, 1965) which was used extensively throughout the study in lieu of ball- and stick-type structural models.

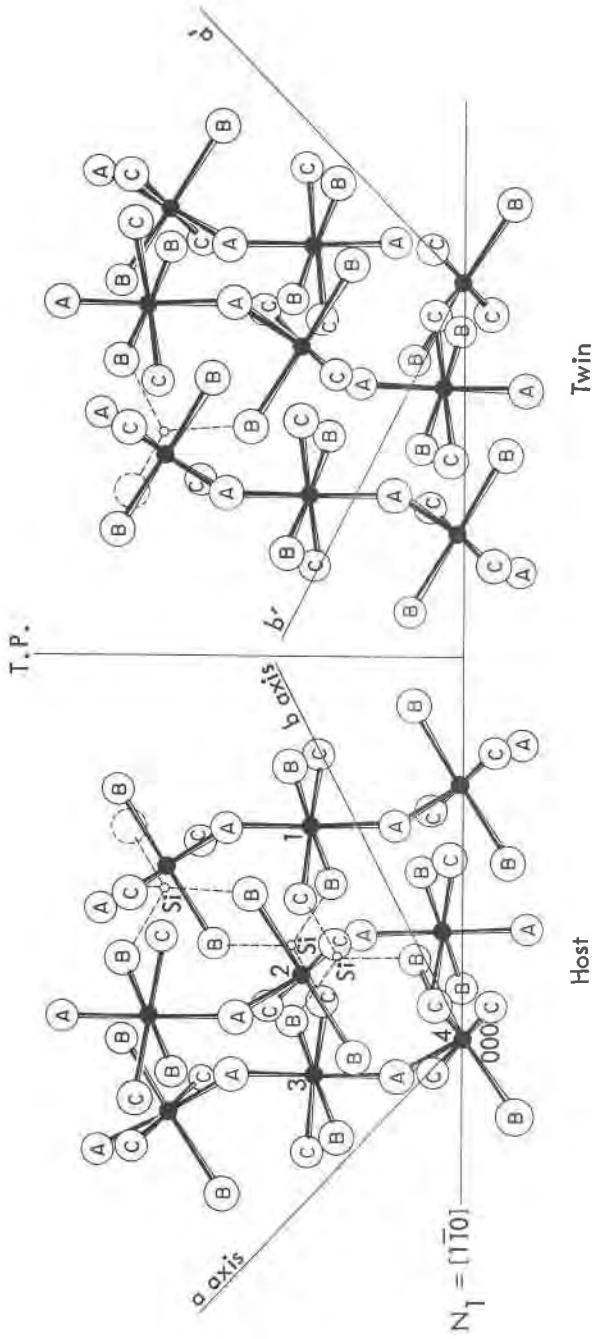


FIG. 3. Projection of chains of Ti octahedra onto the plane of deformation (*S*) in an ideal $[1\bar{1}0]$ twin configuration. Twin glide line (N_1) lies in plane of diagram. *T.P.* = twin plane. Si tetrahedra which link chains are indicated by dashed joins.

TABLE 1. ATOMIC COORDINATES

Atom	Original				Transformed by homogeneous shear (“twinned”)				Corre- sponding atom in original	Translated 1/2 1/2 0			Corre- sponding atom in original	Components of shuffle ^a	
	x	y	z	D(Å)	x'	y'	z'	D(Å)		x''	y''	z''		Δx	Δy
Ca 1	0.75	0.167	0.25	-1.27	0.75	0.17	0.25	-1.27	Ca-1	0.25	0.67	0.25	Ca-2	0.00	0.00
2	.25	.667	.25	-1.27	1.25	-.33	.25	-1.27	Ca-2	.75	.17	.25	Ca-1	.00	.00
3	.75	.333	.75	1.64	1.25	-.17	.75	1.64	Ca-4	.75	.33	.75	Ca-3	.00	.00
4	.25	.833	.75	1.64	1.75	-.67	.75	1.64	Ca-3	.25	.83	.75	Ca-4	.00	.00
Ti 1	.0	.5	.5	1.82	1.0	-.5	.5	1.82	Ti-1	.5	.0	.5	Ti-3	.00	.00
2	.5	.5	.0	-3.26	1.0	.0	.0	-3.26	Ti-4	.5	.5	.0	Ti-2	.00	.00
3	.5	.0	.5	1.82	0.5	.0	.5	1.82	Ti-3	.0	.5	.5	Ti-1	.00	.00
4	.0	.0	.0	0.0	0.0	.0	.0	0.00	Ti-4	.5	.5	.0	Ti-2	.00	.00
4'	.0	1.0	.0	-3.26	1.5	-.5	.0	-3.26	Ti-2	.0	.0	.0	Ti-4	.00	.00
Si 1	.75	.02	.25	-3.40	1.73	-.16	.25	-3.39	Si-1	.23	.34	.25	Si-2	-.02	+.02
2	.25	.32	.25	-0.14	0.73	-.16	.25	-0.14	Si-1	.23	.34	.25	Si-2	-.02	+.02
3	.75	.68	.75	0.51	1.77	-.34	.75	0.51	Si-3	.27	.16	.75	Si-4	+.02	-.02
4	.25	.18	.75	3.77	0.77	-.34	.75	3.77	Si-3	.27	.16	.75	Si-4	+.02	-.02
2'	.25	.32	1.25	6.76	1.23	-.66	1.25	6.76	Si-2	.73	.84	.25	Si-1	-.02	+.02
4'	.25	1.18	.75	0.51	2.27	-.84	.75	0.51	Si-4	.77	.66	.75	Si-3	+.02	-.02
O(A) 1	.75	.438	.25	-2.15	1.16	.03	.25	-2.15	O(A)-3	.66	.53	.25	O(A)-1	-.09	+.09
2	.25	.562	.75	2.52	1.34	-.53	.75	2.52	O(A)-2	.04	.97	.75	O(A)-4	+.09	-.09
3	.25	.938	.25	-2.15	1.66	+.47	.25	-2.15	O(A)-1	.16	.03	.25	O(A)-3	-.09	+.09
4	.75	.062	.75	2.52	0.84	-.03	.75	2.52	O(A)-4	.34	.47	.75	O(A)-2	+.09	-.09
O(B) 1	.5	.711	.1	-3.26	1.37	.84	.1	-6.52	O(B)-1	.87	.34	.1	O(B)-5	-.13	+.13
2	.0	.289	.6	3.20	0.73	-.45	.6	3.22	O(C)-1	.23	.05	.6	O(C)-3'	-.05	+.02
3	.5	.789	.6	-0.07	0.73	-.45	.6	3.21	O(C)-1	.23	.05	.6	O(C)-3'	-.05	+.02
4	.0	.789	.9	3.63	1.63	-.84	.9	3.64	O(B)-6	-.13	.66	.9	O(B)-4	+.13	-.13
5	.0	.211	.1	0.00	0.37	-.16	.1	0.00	O(B)-1	.87	.34	.1	O(B)-5	-.13	+.13
6	.5	.289	.9	3.63	1.13	-.35	.9	3.65	O(B)-4	.63	.15	.9	O(B)-6	+.13	-.13
7	.0	.711	.4	0.44	1.27	-.56	.4	0.42	O(C)-6	.77	.94	.4	O(C)-5	+.05	+.01
8	.5	.211	.4	0.44	0.77	-.06	.4	0.42	O(C)-5	.27	.44	.4	O(C)-6	+.05	+.01
3'	.5	.789	1.6	6.83	2.23	-.94	1.6	6.83	O(C)-3	.73	.56	1.6	O(C)-1	-.05	-.01
5'	.0	.211	1.1	6.90	0.87	-.66	1.1	6.89	O(B)-5	.37	.83	1.1	O(B)-1	+.13	+.13
O(C) 1	.778	.572	.6	-0.27	1.55	-.20	.6	-0.28	O(B)-3	.05	.30	.6	O(B)-2	+.05	+.01
2	.278	.428	.1	-1.61	0.83	-.13	.1	-1.61	O(C)-8	.33	.37	.1	O(C)-2	+.05	-.06
3	.278	.072	.6	3.00	0.55	-.20	.6	3.00	O(B)-3	.05	.30	.6	O(B)-2	+.05	+.01
4	.222	.072	.9	5.25	0.67	-.38	.9	5.24	O(C)-7	.17	.12	.9	O(C)-4	-.05	+.05
5	.722	.928	.4	-2.63	1.95	-.30	.4	-2.61	O(B)-7	.45	.20	.4	O(B)-8	-.05	-.01
6	.222	.428	.4	0.64	1.95	-.30	.4	-2.63	O(B)-7	.45	.20	.4	O(B)-8	-.05	-.01
7	.722	.572	.9	1.99	1.67	-.38	.9	2.00	O(C)-7	.17	.12	.9	O(C)-4	-.05	+.05
8	.778	.928	.1	-4.88	1.83	-.13	.1	-4.86	O(C)-8	.33	.37	.1	O(C)-2	+.05	-.06
3'	.278	.072	1.6	9.00	1.05	-.70	1.6	9.09	O(B)-2	.55	.80	1.6	O(B)-3'	+.05	+.01
4'	.222	.072	1.9	12.1	1.17	-.87	1.9	12.13	O(B)-8	.67	.63	1.9	O(C)-7	-.05	+.06
6'	.222	.428	1.4	7.54	1.45	-.80	1.4	7.55	O(C)-2	.95	.70	1.4	O(B)-7	-.05	-.01
8'	.778	.928	1.1	2.02	2.33	-.63	1.1	2.02	O(C)-4	.83	.87	1.1	O(C)-8	+.05	-.06
a axis	1	0	0	-3.26	.5	.5	0	-3.26							
b axis	0	1	0	-3.26	1.5	-.5	0	-3.26							
c axis	0	0	1	6.90	.5	-.5	1	6.90							
N ₁	1	-1	0	0.0	-1	1	0	0.00							
K ₂	-1	3	1		1	-3	-1								

^aΔz = 0 for all atoms.

Two of the four Ti-octahedra are shown in Figure 4. For clarity most of the oxygen atoms are omitted from the sketch. (See Fig. 5 for all O positions.)

Shearing of the original network results in a new network part of which is shown in the right-hand portion (b) of Figure 5. The “path” is shown for Ca-4 and Ti-4' of the original cell. The “paths” and positions of the

remainder of the sheared atoms of the original cell are not shown in order to avoid confusion resulting from the overlap. The bulk of the atoms constituting 5(b) are from cells adjacent to the original. D 's are given for sheared ("twinned") atoms in Table 1. The repeat distance normal to the S plane of projection is 3.26 Å. Small differences in D 's of original and sheared atoms are due to rounding of the coordinates of the sheared atoms.

A comparison of Figure 5 with Figure 4, the ideal twin configuration, demonstrates that the cations assume nearly perfect twin positions but that the oxygens do not. Si-tetrahedra or Ti-octahedra, particularly Ti-2, must rotate in order to be in true twin positions. By necessity this involves severance of the Ti-O(B)-Si, Ti-O(C)-Si, Ti-(B)-Ca, and Ti-O(C)-Ca links between the chains.

Alternatively, if bonds can be broken, a reorganization of the sheared oxygen, Ti and Si can be carried out which results in a largely restored cation network coordinated to oxygen in distorted polyhedra which are more nearly in the ideal twin position. The extent of the hypothetical distortions is best illustrated by an examination of the coordinates of the individual sheared atoms.

Transformation of Coordinates during $[\bar{1}10]$ Twin Gliding. Equations describing the transformation of indices in twin gliding (Mügge, 1889a), e.g., $\rho h' = 2H(Uh + Vk + Wl) - h(UH + VK + WL)$, etc. where $(HKL) = K_1$ or K_2 and $[UVW] = N_1$ or N_2 , can be put into matrix form (Pabst, 1955; Andrews and Johnson, 1955). For $K_2 = (\bar{1}31)$ and $N_1 = [\bar{1}10]$, the matrix is

$$\rho \begin{vmatrix} 110 \\ 3\bar{1}0 \\ \bar{1}12 \end{vmatrix} \quad \text{where } \rho = 2$$

The inverse transpose of the matrix is applicable for the transformation of points, *i.e.*, atomic coordinates or axes:

$$\rho \begin{vmatrix} 131 \\ \bar{1}\bar{1}\bar{1} \\ 002 \end{vmatrix} \quad \text{where } \rho = 2$$

The x , y , z coordinates of all atoms in the unit cell including those shared with adjacent cells are transformed to x' , y' , z' by twin gliding (Table 1).

Ca and Ti atoms transform into themselves or equivalent positions.

Si are slightly displaced. On the other hand larger disparities in coordinates (± 0.09) exist between original and twin in the case of O(A) and even larger up to (0.25) in the case of some O(B) and O(C) atoms. Atoms in general symmetry positions (*i.e.*, O(B) and O(C)) are no longer related to each other by the symmetry operations appropriate to the setting within the space group. All of the polyhedra are thus distorted and misoriented by homogeneous shear.

Since all O in the cell are bound to one of the four Ti atoms, restoration of the Ti octahedra is equivalent to restoring the structure. It is therefore convenient to focus on these groups. From Table 1 it can be seen that a closer approximation of the Ti-octahedra is possible by reconstruction; *i.e.*, by coordinating Ti to an entirely different set of sheared oxygen atoms. The tenth column in Table 1 gives the new identification which involves interchanging O(B) and O(C) atoms.¹ Reidentified O(B) and O(C) atoms are almost restored to positions appropriate to the space group and setting. Their departure from the ideal O(B) and O(C) given in the last columns of Table 1 is a measure of the additional shuffles necessary. Components of the shuffles in the three principal directions are of the form $\pm(\Delta x, -\Delta x, 0)$ for Si and O(A) atoms and for half of the O(B) and O(C) atoms. In these instances the required adjustments are parallel to the slip line, $[1\bar{1}0]$. These atoms thus fulfill a geometric criterion governing twinning modes; namely, that the shuffles be parallel to the twinning direction rather than normal thereto (Bilby and Crocker, 1965). As a group the requisite movements necessary to exactly restore the structure are smaller than those involved in rotation of Ti-octahedra or Si-tetrahedra; however, they are probably too large to be considered likely. In the reconstructed Ti groups, before shuffling Ti-O distances become 1.86–2.30 Å (Ti-1, 3) and 1.64–2.35 Å (Ti-2, 4) as compared to 1.85–2.04 Å in the host (Zachariasen).²

In both models discussed, the nature and number of bonds broken is the same. By analogy with the behavior (rotation) of the CO_3^{2-} groups during $\{01\bar{1}2\}$ twin glide in calcite, the rotation model is the more acceptable of the two, for it is difficult to envisage oxygen of the presumably stable Si-O and Ti-O groups shearing independently. Rupture of Si-O-Ti bonds is the chief obstacle to rotation of the polyhedra during the shearing process. It seems likely that the SiO_4 groups remain intact

¹ In order to conform to the graphical description of the shear shown in Figure 4 (b), coordinates (x'' , y'' , z'') are given for atoms referred to another origin at $\frac{1}{2} \frac{1}{2} 0$. Symmetry operations in this new setting remain the same. Correspondence between the original atoms and the sheared set described by x'' , y'' , z'' (columns 11–13 of Table 1) does not differ in any way from that between the x , y , z and x' , y' , z' sets.

² Improved values by Mongiorgi and di Sansverino (1968) are 1.874–2.024 Å.

during the rotation and that Ti-O bonds are broken and reformed.

The Ca-O-Ti and Ca-O-Si links are probably relatively weak in view of the seven-fold coordination about Ca. As the structure is restored during the twin process, the linkage between Ti-O chains must be re-established.

Partings repeatedly reported parallel to the habit plane (≈ 221) in twinned sphene (Mügge, 1889a; Dana, 1892; Tröger, 1959) indicate that the links between the Ti octahedra within the chains (O(A) of Fig. 2) can also be broken. The oxygen position common to two Ti octahedra is reported to contain the OH consistently found in sphene chemical analyses.¹ Thus during strain of the structure, breaks at these points are not improbable.

SUMMARY

Mechanical twinned sphene occurs in weakly-to-strongly shocked rocks. The elements of the twin glide, $K_2 = \{\bar{1}31\}$, $N_1 = \langle 110 \rangle$, are as predicted by Mügge (1889a). The reciprocal twin mode was not observed. The cation network can be almost perfectly restored by homogeneous shear, but additional movements or shuffles are necessary in order to restore the oxygen atoms to their proper positions about the cations. Either Ti or Si polyhedra apparently rotate as discreet units during the twin process. Despite the magnitude of the shear ($s = 0.60$) and the fact that the cross linkage between chains of Ti-octahedra must be broken in order that the rotation occur, the twin process apparently proceeds with little difficulty.

ACKNOWLEDGMENTS

I am particularly grateful to R. Braun for aid in solving many of the crystallographic and geometric problems encountered. In addition to R. Braun, Gordon Smith and S. Weissman acted as sounding boards during the course of the analysis and by doing so were very helpful.

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¹ 0.5-1.0 formula units/20 O.

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Manuscript received, April 28, 1970; accepted for publication, June 8, 1970.