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Silicon Crystal Under Bending

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Abstract The mechanical behavior of a silicon crystal under bending is investigated. For a crystal of length 30 mm and thickness 3 mm, to achieve the specified bend angle of 0.64 mrad, the appropriate angle of the aluminum punches is 0.96 mrad.

1. Introduction

The beam channeling experiment (E853) requires to bend the silicon crystal to a certain degree. Fig.0 is the sketch of the situation. It is desirable to know the deformation and the stress level in the crystal under bending, and to investigate the methods of achieving such bending.

The crystal is cut in the direction shown in Fig.1, and a local coordinate system is also shown in the figure; the z -direction is along the longest edge, and the y -direction is along the shortest edge.

This work used ANSYS to study the deformation and stresses in the crystal under bending. ANSYS has the orthotropic material property capability, an essential tool for the analysis of crystals. From the crystal data provided by Thornton Murphy, the following material properties are calculated: $E_{xx} = 1.30208 \times 10^5 \text{ N/mm}^2$, $\nu_{xy} = 0.278646$, $G_{xy} = 0.39809 \times 10^5 \text{ N/mm}^2$.

Since the problem is symmetric with respect to the plane $z = 0$, only half of the crystal is modeled. The dimension of the half crystal is $15 \times 10 \times 3 \text{ mm}$.

We first use a bare crystal and specify the displacement at its surfaces, to study the basic characteristics of the crystal under bending. Then crystals with different orientations are compared with each other. After that a crystal squeezed between cylindrical aluminum punches is investigated to take into account the deformation of the punches. Finally, punches with increased curvature are used to achieve the required bend angle.

2. Crystal under Bending

The finite element mesh is shown in Fig.2 with a local coordinate system. These are 20-node solid elements, and each element is a 1mm cube. Also in the figure we marked some points which are actually some lines parallel to the z -axis. Later on we will examine the deformation along these lines.

The first analysis is for a bare crystal, with the angle $\beta = 0$ in Fig.1. Displacements are specified at its top and bottom surfaces. That is, ANSYS is told that the top and bottom surfaces are constrained to a cylindrical shape (for $x < 8\text{mm}$ and $z < 10\text{mm}$), without worrying yet about how this shape is achieved. The total bend angle at the surfaces is 0.32 mrad.

The deformed crystal is shown in Fig.3. Fig.4 shows the displacement u_y at A as a function of nodes, and Fig.5 gives the differences in u_y between A and B , and A and C . Notice that the differences are two orders of magnitude smaller than the displacement itself; that means the displacement is quite uniform. Combining the previous two figures in Fig.6 shows this result where the difference is unnoticeable. Fig.7 shows the displacement u_z at D and E , which shows a nice bending. And in Fig.8 is the displacement u_x at D and E , which shows the warping out of the bending plane.

Our main interest is in the final bend angle. Differentiating the displacement curve yields the slope, or the bend angle of the crystal. Fig.9 is the bend angle at C , D and E ; they are almost identical. Fig.10 shows the bend angle at A , F and G . Notice the big oscillation near $Z = 10\text{mm}$ in the curves for F and G . This is caused by the discontinuity in stress, since for $z < 10\text{mm}$ the displacement is specified, while for $z > 10\text{mm}$ the stress is free. Fig.11 compares the bend angle at A and C . There is a little difference near $z = 10\text{mm}$, but the bend angle at the edge $z = 15\text{mm}$ is the same.

Overall, the final bend angle, i.e. the bend angle at $z = 15\text{mm}$, is only 0.27 mrad, less than the 0.32 mrad specified at the surfaces. This is due to the flap-back tendency, a tendency of the over hanging portion of the crystal, to try to counter the bending, thus causing the bend angle to decrease after entering the stress-free region. This phenomenon is very interesting as can be noted from Fig.10. The curve for A , which is in the middle layer of the crystal, is more smooth than the curve for F and G , they are at surface, where displacement is specified for $z < 10\text{mm}$.

Figs.12 and 13 give the stresses σ_{yy} and σ_{zz} . It is seen that the maximum stress is 6.655 N/mm², much smaller than the yield stress of 100 N/mm².

We also did analysis for other cases, i.e. crystals with different orientations. The results are summarized in Table I. The results do depend on the orientation of the crystal, but the difference is not dramatic, as can be seen from Table I.

3. Crystal between Aluminum Punches

The next work is the crystal under compression by two half aluminum punches, prepared with the specified curvature. The crystal is as shown in Fig.1 with the angle $\beta = 0$. Again the stress is moderate, but the bend angle is much less than what is expected, as shown in Figs.15 and 16. In fact, the angle is only 2/3 of the required. This is due to the finite stiffness of the aluminum punches. When they are compressed against the crystal, they deform also, and thus the final curvature of the aluminum punches is less than initially specified. Furthermore, even if the final punch curvature remains unchanged, as in the previous case where displacement at the surface is prescribed, the final angle is still less than required.

To compensate for the deficiency of the bend angle, we increased the initial curvature of the aluminum punches from 0.32 mrad to 0.48 mrad. This turned out to be satisfactory. Fig.17 gives the bend angle at C , D and E , Fig.18 gives bend angle at A , F and G , and Fig.19 compares the bend angle at A , C and H .

Figs.20 and 21 give the stresses σ_{yy} and σ_{zz} . The maximum bending stress is only 9.8 N/mm² or 1420 psi. No noticeable stress concentration has been found, and the maximum compressive stress is only 2.464 N/mm² or 357 psi.

The total force required to press the punch is 23.12 newton, or 2.36 kg. Since this is a half model, the total force required to bend the crystal will be 4.72 kg.

4. Conclusions

Due to the finite stiffness of the punches and the flap-back of the bent crystal, the final bend angle is less than the initial angle specified by the curvature of the punches. For the case studied, the initial angle of the aluminum punches is set to 0.48 mrad to achieve the final bend angle of the crystal, 0.32 mrad. The maximum stress in the crystal is less than 1500 psi, and the force required to bend the crystal is less than 5 kg.

Table I. Compare results for different Orientations

Orientation of y-z plane	$\langle 111 - 7^\circ \rangle$	$\langle 111 \rangle$	$\langle 111 + 7^\circ \rangle$	$\langle 110 \rangle$
Minimum σ_z	-6.956	-6.655	-6.354	-6.419
Maximum σ_z	6.470	6.303	6.187	6.427
Maximum σ_e	6.325	6.009	5.684	5.928
Maximum displacement	2.977×10^{-3}	2.986×10^{-3}	2.991×10^{-3}	2.965×10^{-3}
Maximum difference in displacement	4.3×10^{-5}	4.4×10^{-5}	4.6×10^{-5}	6.4×10^{-5}

stress in unit of N/mm^2

displacement in unit of mm.

rotate the y-z plane about y axis

to get $\pm 7^\circ$, direction as shown.

Fig. 0 Crystal channeling experiment

Fig.1

The orientation of the crystal

$$\alpha = 90 - 35.2644^{\circ}$$

$$\beta = -7, 0, +7^{\circ}$$

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ANSYS 4.4A1
DEC 11 1992
16:20:09
PLOT NO. 1
PREP7 ELEMENTS
TYPE NUM

```

```

XP =1
YV -2
ZV t-3
DIST=12.225
XF -8.392364
YF -7.483
ZF =5.258
ANGZ=90
PRECISE HIDDEN

```

Crystal

Fig.2 Finite element model

ANSYS 4
DEC 14 1992
8:38:50
PLOT NO. 1
POST1 DISPL.
STEP=1
ITER=1
DMX =0.002988
ERPC=41.267

DSCA=489.431
XV =1
YV =2
ZV =-3
DIST=12.225
XF =-0.392354
YF =7.483
ZF =5.258
ANGZ=90
PRECISE HIDDEN

Fig.3 Deformed model

Crystal

Since the element mesh is 1 mm³ cubes, the distance along the Z direction can be obtained in unit of mm by subtracting 1 from the node number. All the displacements are in mm.

Fig.4 Displacement u_z at point A

Fig.5 Differences in u_y

Fig.6 Difference in u_y compared with u_y

Fig.7 Displacements u_z

Fig.8 Displacements u_x

Fig.9 Bend angles at C, D, E (Bare crystal)

Fig.10 Bend angles at *A, F, G* (Bare crystal)

Fig.11 Bend angles at A, C (Bare crystal)

ANSYS 4.4A
DEC 14 1992
9:40:04
PLOT NO. 2
POST1 STRESS
STEP=1
ITER=1
SY (AVG)
CSYS=11
DMX =0.002986
SMN =-3.574
SMNB=-5.459
SMX =3.625
SMXB=5.483

XV =1
YV =2
ZV =-3
DIST=12.225
XF =-0.392354
YF =7.463
ZF =5.258
ANGZ=90
CENTROID HIDDEN
-3.574
-2.775
-1.975
-1.175
-0.374829
1.225
2.025
2.825
3.625

ANSYS 4.4
 DEC 14 1992
 9:40:18
 PLOT NO. 3
 POST1 STRESS
 STEP=1
 ITER=1
 SZ (AVG)
 CSYS=11
 DMX =0.002986
 SMN =-6.655
 SMNB=-7.813
 SMX =6.303
 SMXB=7.368

 XV =1
 YV =2
 ZV =-3
 DIST=12.225
 XF =-0.392354
 YF =7.463
 ZF =5.258
 ANGZ=90
 CENTROID HI^o DEN
 -6.655
 -5.215
 -3.776
 -2.336
 -0.896^o92
 1.983
 3.423
 4.863
 6.303

Fig.13 Stress σ_z (Bare crystal)

ANSYS 4.4,
JAN 11 1993
11:15:39
PLOT NO. 3
POST1 ELEMENTS
TYPE NUM

XV =1
YV =2
ZV =-3
DIST=17.183
XF =-0.07884
YF =5.736
ZF =3.216
ANGZ=70
CENTROID HIDDEN

Fig.14 Crystal between aluminum punches

Crystal Under Bending (exaggerated punch)

Fig.15 Displacements for bare crystal and crystal between punches

Fig.16 bend angles for bare crystal and crystal between punches

Fig.17 Bend angles at *C, D, E* (exaggerated punches)

Fig.18 Bend angles at *A, F, G* (exaggerated punches)

Fig.19 Bend angles at A, C, H (exaggerated punches)

ANSYS 4.4
 JAN 8 1993
 10:03:07
 PLOT NO. 1
 POST1 STRESS
 STEP=1
 ITER=10
 SY (AVG)
 CSYS=11
 DMX =0.003842
 SMN =-2.464
 SMNB=-3.584
 SMX =1.511
 SMXB=3.002

XV =-1
 YV =-2
 ZV =3
 DIST=12.225
 XF =-0.392354
 YF =7.463
 ZF =5.258
 ANGZ=90
 CENTROID HIDDEN

Blue	-2.464
Dark Blue	-2.022
Light Blue	-1.581
Teal	-1.139
Green	-0.697338
Yellow	0.185958
Orange	0.627605
Red	1.069
Dark Red	1.511

Fig.20 Stress σ_y (Shown is the bottom surface)

```

ANSYS  4.4
JAN  5 1993
10:09:09
PLOT NO.  1
POST1 STRESS
STEP=1
ITER=10
SZ  (AVG)
CSYS=11
DMX =0.003842
SMN =-9.797
SMNB=-11.276
SMX =8.878
SMXB=10.246

XV  =1
YV  =2
ZV  =-3
DIST=12.225
XF  =-0.392354
YF  =7.463
ZF  =5.258
ANGZ=90
CENTROID HIDDEN
      -9.797
      -7.722
      -5.647
      -3.572
      -1.497
      2.653
      4.728
      6.803
      8.878

```

Fig.21 Stress σ_z

Crystal Under Bending (exaggerated punch)