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Fracture surface energy determination in $\{110\}$ planes in silicon by the double torsion method

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The fracture surface energy of $\{1\,1\,0\}$ planes of silicon were determined by the double torsion method on thin samples. Elastic anisotropy was taken into account in the calculations. The determined value of 1.81 J m^{-2} compared well with other data in the literature.

1. Introduction

The Griffith theory attributes brittle failure to pre-existing flaws in materials. It predicts that the fracture strength of a brittle material is directly proportional to the square root of Young's modulus and fracture surface energy, and the fracture strength is inversely proportional to the depth of flaws. Therefore, the strength prediction calls for a knowledge of fracture surface energy. It is known that silicon cleaves along $\{1\,1\,1\}$ planes. Gilman [1] determined the cleavage surface energy using double cantilever beam (DCB) specimens. Pre-cracking of the samples was difficult and he obtained few valid data. Jaccodine [2] carefully used his set-up with DCB specimens in the dead weight mode and was able to obtain data for $\{1\,1\,1\}$ planes for silicon. St John [3] used tapered DCB specimens and determined the fracture surface energies for $\{1\,1\,1\}$ planes. None of these experiments measured the fracture surface energies for other planes. Also, the production of precursor cracks was a major problem in all the above cases. Messmer [4] carried out fracture surface energy measurements on silicon using edge cracked specimens. He was able to produce controlled precursor cracks using the spark discharge technique. He was also able to measure the fracture surface energy on $\{1\,1\,0\}$ type planes. Chen and Leipold [5] measured the toughness values for different orientations of Knoop indented silicon. Because the cleavage plane of silicon is $\{1\,1\,1\}$, the fracture plane was different from $\{1\,1\,1\}$ the cracks branched out to $\{1\,1\,1\}$ planes. It seemed to be advisable to use some other specimen configuration, such as double torsion (DT) specimens. DT specimens can be well characterized and it makes use of compressive loading. Specimen preparation is easy. The compressive loading feature cuts down the set-up time and can easily accommodate an environmental chamber.

The DT specimen configuration was first proposed by Outwater and Jerry [6] and Evans [7, 8] detailed its useful features. So far, the DT technique has been used only once in the measurement of the fracture surface energy of boron carbide by Hollenburg and Walter [9]. Our experiments used single crystal silicon wafers, and the DT equations were modified to take into account the elastic anisotropy.

2. Theory

Lekhtinski [10] treated the case of torsion for a rectangular orthotropic bar. We modified his expressions to include elastic anisotropy.

The DT specimen configuration is shown in Fig. 1. The length l is along the z-axis, the width a is along the x-axis, and the thickness b is along the y-axis. Assuming the rectangular bar was subjected to torsion about the x–y plane, the torsion equation was written as

$$a_{44}\frac{\partial^2\psi}{\partial x^2} + a_{55}\frac{\partial^2\psi}{\partial y^2} = -2\bar{\theta} \qquad (1)$$

where $\bar{\theta}$ is the angle of twist, a_{ij}s are the elastic constants of an elastic body and ψ is the stress function. Equation 1 can be written as

$$\frac{1}{G_{23}}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{G_{13}}\frac{\partial^2\psi}{\partial y^2} = -2\bar{\theta} \qquad (2)$$

where $1/G_{23}$ is equal to a_{44}, $1/G_{13}$ is equal to a_{55} where G_{13} and G_{23} are the shear moduli in anisotropic medium. Equation 2 can be put into the following form.

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial y_1^2} = -2\bar{\theta}G \qquad (3)$$

where $x = x_1$, $y = y_1(G_{23}/G_{13})^{1/2}$ and $G = 2G_{13}G_{23}/(G_{13} + G_{23})$.

The solution to Equation 3 was given by

$$\psi = 8\bar{\theta}G_{23}\frac{l^3}{\pi^3}\sum_{k=1,3,5}^{\infty}\frac{(-1)^{k-1/2}}{k^3} \times \left[1 - \frac{\left(\cosh\dfrac{\pi k w y}{l}\right)}{\left(\cosh\dfrac{\pi k w b}{2l}\right)}\right]\cosh\frac{k\pi x}{l} \qquad (4)$$

where l is the width, b is the thickness of the bar, $w = (G_{13}/G_{23})^{1/2}$ and k is a constant. The above equation is equivalent to the equations of Timoshenko

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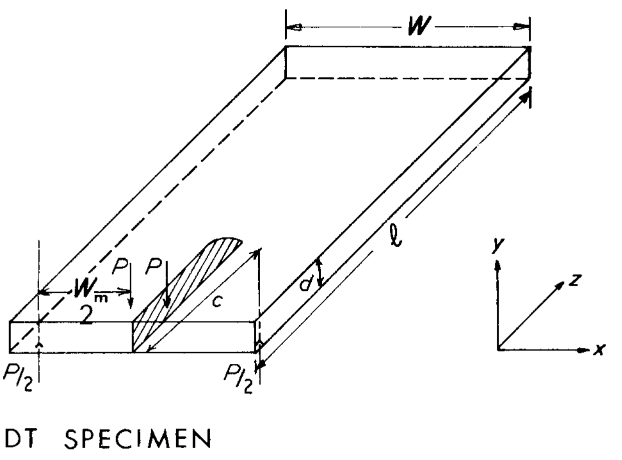

Figure 1 Testing configuration of the double torsion DT specimen. $w = 2.54 \times 10^{-2}$m, $W_m = 4.67 \times 10^{-3}$m, $d = 0.96 \times 10^{-3}$m, and $l = 7.62 \times 10^{-2}$m.

and Goodier [11] for the torsion of the isotropic rectangular beam. Torque, M, is given by

$$M = 2\int_{-\frac{a}{2}}^{\frac{a}{2}}\int_{-\frac{b}{2}}^{\frac{b}{2}} \psi \, \mathrm{d}x \, \mathrm{d}y \tag{5}$$

$$= \bar{\theta} G_{13} l b^3 \beta(\phi) \tag{6}$$

where

$$\phi = \frac{l}{bw} = \frac{l}{b}\left(\frac{G_{23}}{G_{13}}\right)^{1/2} \tag{7}$$

and

$$\beta(\phi) = \frac{32\phi^2}{\pi^4} \sum_{k=1,3,5}^{\infty} \frac{1}{k^4}\left(1 - \frac{2\phi}{\pi}\tanh\frac{k\pi}{2\phi}\right) \tag{8}$$

From the above we have

$$M = \bar{\theta} G_{23} \frac{l^3 b}{\pi^4} \left\{ \sum_{k=1,3,5}^{\infty} \frac{1}{k^4} \left[1 - \frac{2l}{k\pi b}\left(\frac{G_{23}}{G_{13}}\right)^{1/2} \times \left(\tanh \frac{k\pi}{2\frac{l}{b}\left(\frac{G_{23}}{G_{13}}\right)^{1/2}} \right) \right] \right\} \tag{9}$$

We note that

$$\frac{1}{1^4} + \frac{1}{3^4} + \frac{1}{5^4} + \cdots = \frac{\pi^4}{96} \tag{10}$$

Also, we assumed that, for a very narrow rectangle (a condition that fitted our case)

$$\tanh \frac{k\pi}{2}\frac{b}{l}\left(\frac{G_{23}}{G_{13}}\right)^{1/2} = 1 \tag{11}$$

From Equations 9, 10 and 11

$$M = \tfrac{1}{3}\bar{\theta} G_{23} l^3 b \left[1 - 0.64 \frac{l}{b}\left(\frac{G_{23}}{G_{13}}\right)^{1/2} \right] \tag{12}$$

$$M = \tfrac{1}{3}\bar{\theta} G_{23} l^3 b \quad \text{[For a narrow rectangle]} \tag{13}$$

In the case of a DT sample having crack length c, and for $b = d$, $l = w/2$

$$Mc = \tfrac{1}{6}\bar{\theta} G_{23} d^3 w \tag{14}$$

For a DT specimen, $M = PW_m/4$ and $\bar{\theta} \approx 2y/W_m$, and the angle of torsion is very small, where P is the applied load, W_m is half the moment arm and y is the displacement of loading points. Thus, from Equation 14

$$y = \frac{3}{4}\left(\frac{PW_m^2 c}{G_{23} d^2 w}\right) \tag{15}$$

or

$$C = \frac{y}{P} = \frac{3}{4}\left(\frac{PW_m^2 c}{G_{23} d^3 w}\right) \tag{16}$$

where C is the compliance.

Here, the axis 2 is $[0\,0\,\bar{1}]$ and the axis 3 is $[\bar{1}\,1\,0]$. The transformation [13] of G is the following

$$\tfrac{1}{4}G' = \tfrac{1}{4}S_{44} + [S_{44} - 2(S_{11} - S_{12})] \times (\alpha_{11}\alpha_{21}\alpha_{22}\alpha_{21} + \alpha_{11}\alpha_{21}\alpha_{13}\alpha_{23} + \alpha_{12}\alpha_{22}\alpha_{13}\alpha_{23}) \tag{17}$$

where S_{44}, S_{12}, S_{11} are the compliances for a crystalline material, α_{ij}s are direction cosines, $i, j = 1, 2, 3$. In the present case, $\alpha_{11} = -1$, $\alpha_{12} = 0$, $\alpha_{13} = 0$

$$\alpha_{21} = 1/2^{1/2}, \quad \alpha_{22} = 1/2^{1/2}, \quad \alpha_{23} = 0 \tag{18}$$

From Equations 16 and 17

$$G_{23} = \frac{1}{S_{44}} \tag{19}$$

and hence

$$y = \frac{3}{4}\frac{PW_m^2 c S_{44}}{d^3 w}$$

and

$$C = \frac{3}{4}\frac{cW_m^2 S_{44}}{d^3 w} \tag{20}$$

Now, $\mathscr{G}_\mathrm{I} = (P_\mathrm{I}^2/2d)(\mathrm{d}C/\mathrm{d}c)$ where $\mathscr{G}_\mathrm{I}$ is the strain energy release rate, d is the thickness of the sample and c is the crack length. To obtain a relation between $\mathscr{G}_\mathrm{I}$ and K_I in the elastic anisotropic case, the Sih–Paris–Irwin relations [13] was used. Wachtman [14] made detailed calculations using different combinations of fracture planes and directions. In the present case, the fracture was $(1\,1\,0)[\bar{1}\,1\,0]$ type and of mode I in nature. The Sih–Paris–Irwin relation was cast into the form

$$\mathscr{G}_\mathrm{I} = \frac{\pi K_\mathrm{I}^2}{2}\left[S_{11}\left(1 + \frac{2S_{11} + S_{44}}{2}\right)\right]^{1/2} \times \left[\frac{1}{2^{1/2}}\left(1 + \frac{2S_{11} + S_{44}}{2S_{11}}\right)^{1/2} + \frac{2S_{11} + S_{44}}{2S_{11}}\right]^{1/2} \tag{21}$$

where $\mathscr{G}_\mathrm{I}$ is the strain energy release rate, K_I is the stress intensity factor and S_{11}, S_{12} and S_{44} are compliances of silicon. Metzger and Kessler [15] reported the stiffness values of silicon as C_{44} is equal to $7.9 \times 10^{10}\,\mathrm{N\,m^{-2}}$, C_{11} is equal to $16.48 \times 10^{10}\,\mathrm{N\,m^{-2}}$; and C_{12} is equal to $6.35 \times 10^{10}\,\mathrm{N\,m^{-2}}$. The transformation relations are given by

$$S_{12} = \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \tag{22}$$

$$S_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})} \tag{23}$$

$$S_{44} = \frac{1}{C_{44}} \tag{24}$$

From above

$$\mathscr{G}_{\mathrm{I}} = 6.66K_{\mathrm{I}}^2 \times 10^{-12}\,\mathrm{m^2\,N^{-1}} \qquad (25)$$

$$\mathscr{G}_{\mathrm{I}} = \frac{3}{8}\,\frac{P^2 W_{\mathrm{m}}^2 S_{44}}{d^4 w} \qquad (26)$$

In Equation 25, K_{I} the stress intensity factor is in $\mathrm{MN\,m^{-3/2}}$. Equations 25 and 26 are general as long as the crack propagation mode is $(1\,1\,0)[\bar{1}\,1\,0]$. If K_{IC}, the critical stress intensity factor, or P_{IC}, the critical fracture load is known, the Equations 25 and 26 can be applied to obtain $\mathscr{G}_{\mathrm{IC}}$, the critical strain energy release rate. The fracture surface energy, γ, is related to $\mathscr{G}_{\mathrm{IC}}$ as follows

$$\mathscr{G}_{\mathrm{IC}} = 2\gamma \qquad (27)$$

Equation 26 is used in calculating $\mathscr{G}_{\mathrm{IC}}$ and P_{IC} is obtained experimentally.

3. Experimental details

Silicon wafer samples used in this investigation were thin. They were 0.0254 m in length and 0.0064 m in width. They were cut from wafers, from Monsanto Co. (St. Louis, Missouri) of 380 μm in thickness. The wafers were of n-type and had a resistivity value of 173 ± 10 ohm m. The orientations of the samples were determined by the X-ray back reflection Laue method using a molybdenum tube operating at 35.5 kV and 27 mA and recording the pattern on type 57 film with an average exposure time of 7 min. The samples were of $\{1\,0\,0\}$ orientation, the planes of the samples are shown in Figs 2 and 3. As-cut samples were lapped with 600 grit SiC and were subsequently etched. Precursor cracks were produced using a standard technique used for brittle ceramics. Lines were scribed on the broad surface of the samples and, with some practice, this technique produced straight long cracks, as shown in Fig. 4. According to Equation 20, the compliance is proportional to the crack length. Experimentally, it was true only when the crack length was between $l/3$ and $2l/3$, where l was the length of the sample. The samples were fractured in mode I. The experimentally obtained value of critical stress intensity factor was near to K_{IC} and was much less as compared to the published K_{IIIC} for silicon. The crack points were continuous, contrary to those in the case of I and III mixed mode fracture. A universal testing machine, model TM, Instron Corp. (Canton, MA) was used in the experiments. The machine was fitted with a compression cage, a double torsion jig and a CM load cell with a maximum capacity of 50 kg. A crosshead speed of $1.27 \times 10^{-4}\,\mathrm{m\,sec^{-1}}$ was used to fracture the samples. When the crack lengths were between $l/3$ and $2l/3$, the P_{IC} values were constant. Equations 26 and 27 were employed to calculate the fracture surface energy for the $\{1\,1\,0\}$ planes in silicon.

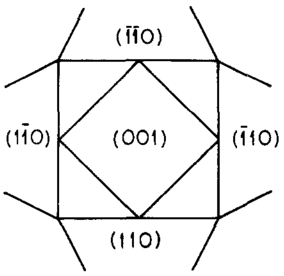

Figure 2 Orientation of (1 0 0) planes with respect to {1 1 0} planes in a diamond cubic structure.

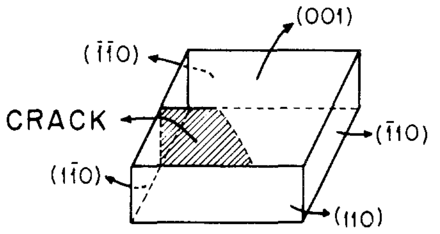

Figure 3 Sketch of the crack plane in the DT specimen of silicon.

4. Results

The fracture surfaces of the silicon samples were determined to be the $\{1\,1\,0\}$ planes. Optical micrographs did not reveal branching of cracks into other planes. The P_{IC} value was found to be 0.650 kg. From Equation 20, $\mathscr{G}_{\mathrm{IC}}$ was calculated to $3.62\,\mathrm{J\,m^{-2}}$ yielding a fracture surface energy of $1.81\,\mathrm{J\,m^{-2}}$ for the $\{1\,1\,0\}$ planes of silicon.

5. Discussion

This study brought out some interesting points regarding the fracture surface energies of $\{1\,1\,0\}$ type planes in silicon. The different surface energy values from the literature are tabulated in Table I. Chen and Leipold's [5] experimental value was extracted from their K_{IC} value with the help of Equation 25. Following Jaccodine's idea [2], it was noted that the fracture surface energies of two surfaces are proportional to their planar bond densities. The planar bond density on a $\{1\,1\,1\}$ plane is given as $4/3^{1/2}a_0^2$ and that on the $\{1\,1\,0\}$ plane is $2(2)^{1/2}a_0^2$, where a_0 is the crystal lattice parameter of silicon. The ratio of the number of bonds on $\{1\,1\,1\}$ to that on $\{1\,1\,0\}$ is, therefore, 0.816. From

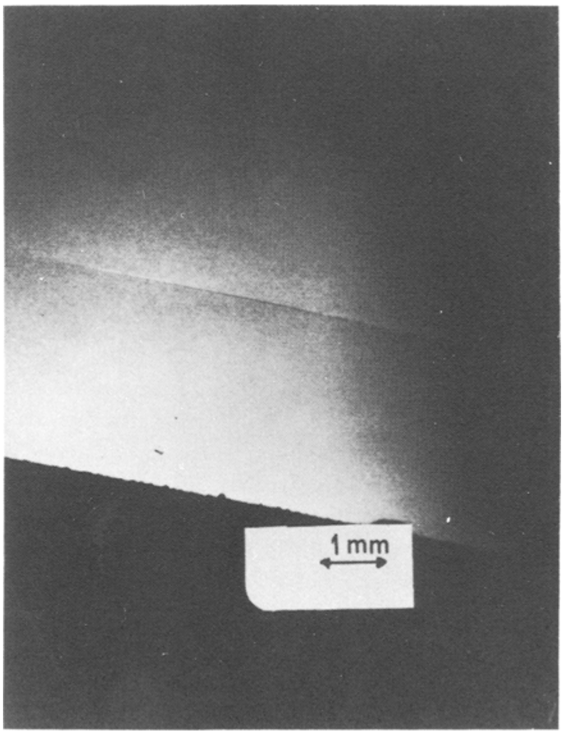

Figure 4 Silicon specimen with a precursor crack.

TABLE I Experimentally determined fracture surface energies of silicon

Plane orientation	Surface fracture energy (J m^{-2})	Reference	Comments
{1 1 1}	1.24	Gilman [1]	Precracked DCB specimens
{1 1 1}	1.23	Jaccodine [2]	DCB specimen
{1 1 1}	2.50	St. John [3]	Tapered DCB specimen
{1 1 1}	1.14	Messmer [4]	Edge crack tension
{1 1 0}	1.9	Messmer [4]	
{1 1 0}	1.81	Present study	DT specimen
{1 1 0}	2.69	Chen and Leipold [5]	Controlled flaw 4 point blend specimen

our experimental data, the fracture surface energy of {1 1 1} type planes was calculated to be 1.47 J m^{-2}, a value slightly higher than the figures reported by Gilman [1], Jaccodine [2] and Messmer [4]. Gilman and Jaccodine did not perform any experiments on {1 1 0} planes. Messmer's [4] experimental value of 1.90 J m^{-2} for {1 1 0} planes is equivalent to 1.55 J m^{-2} for {1 1 1} planes. This result is higher than his own experimental value of 1.14 J m^{-2} for {1 1 1} planes [16]. Thus Messmer's data shows a discrepancy to Jaccodine's idea. Careful scrutiny revealed that his samples were thicker ($\sim$ 1 mm) than the usual samples. Therefore, there was a possibility that the cracks initiated on the {1 1 0} planes of his samples could branch out to the {1 1 1} planes. Messmer actually saw river markings on the fractured surfaces, which could be due to the transfer of the crack plane from the {1 1 0} to the {1 1 1} plane. Also, Chen and Leipold [5] observed branching of cracks from {1 1 0} planes into the {1 1 1} planes. This is the reason they obtained a very high fracture surface energy of 2.69 J m^{-2}. In the present case, the fractured surfaces were carefully examined by using an X-ray back reflection Laue technique and optical microscopy. No crack branching or deviation of the crack planes were observed. Thus, the present data represent data of {1 1 0} planes only.

The present experimental values are also compared with theoretical calculations. Sinclair and Lawn [17] and Cahn and Hanneman [18] assumed the force laws for the diamond structure and determined the surface energies of different crack planes. Their estimate for the {1 1 1} type planes was 1.41 J m^{-2} equivalent to 1.74 J m^{-2} for {1 1 0} planes. This was close to our experimental results of 1.81 J m^{-2} for {1 1 0} planes. Our results could be also viewed with respect to the lattice trapping theory [19]. This theory predicted that the surface energy varies periodically with the propagation of the crack. The present experiments were performed with ambient environment and the conditon of the lattice trapping theory was not fulfilled in our experiments. Therefore, no variation of surface energy was observed. Rice [20] extended the thermodynamic approach of crack growth theory from the Griffith theory. He extended the expression of surface energy by adding terms in the case of adsorption of fluid phases at the freshly cracked surface. The strain energy release rate was found to be $2\int_{\infty}^{\mu} \Gamma'(\mu')\mathrm{d}\mu'$ where Γ' is the surface energy isotherm at a particular temperature, and μ the chemical potential of the adsorbed fluid phase. The lower limit was for the extremely dilute case or the vacuum case. Rice's treatment showed that with the presence of more adsorbed species the difference between the intrinsic surface energy and that of the case with adsorbed species increases. This suggests that the experimental value might, in fact, be quite different from the true fracture surface energy despite its being quite near to the theoretical calculations.

6. Conclusions

The fracture surface energy of {1 1 0} planes of silicon were determined by the double torsion method. For thin samples, controlled precursor cracks could be easily produced and cracks propagated all along {1 1 0} type planes. To calculate the fracture surface energy, the double torsion formulae were modified taking into account the elastic anisotropy. The experimentally determined value of 1.81 J m^{-2} compared well with other data presented in the literature.

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