Basic Mechanical and Thermal Properties of Silicon

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A Introduction

This paper outlines some of the basic mechanical and thermal properties of silicon.

B Crystalline Structure and Elastic Properties

Three values for the lattice parameter of pure Silicon at 22.500 °C are given below. The values were determined in independent studies through X-ray and optical interferometry (XROI).

a= 543102.032 +/- 0.033 fm [2]
a= 543102.044 +/- 0.017 fm [3]
a= 543101.99 +/- 0.09 fm [4]

The value of the linear thermal expansion coefficient ($\alpha(T)$) is given by the following expression:

$$\alpha(T) = (3.725\{1- \exp[-5.88 \times 10^{-3} (T - 124)]\} + 5.548 \times 10^{-3} T) \times 10^{-3}\ K^{-1} \quad [1]$$

where T is the absolute temperature expressed in Kelvin and valid for values of T between 120 K and 1500 K. At 25.0 °C the recommended value is

$$\alpha_{298.2} = (2.59 \pm 0.05) \times 10^{-6}\ K^{-1}$$

The lattice parameter at T K is given by

$$a(T) = a_0 \left(\int_{295.7}^{T} \alpha(T)\, dT + 1 \right) \quad [1]$$

where a_0 is the lattice parameter at 295.7 K.

The second order lattice constants are related by [5]

$$\sigma_{ii} = C_{11}\, \varepsilon_{ii} + C_{12} (\varepsilon_{jj} + \varepsilon_{kk})$$
$$\sigma_{ii} = 2C_{44}\, \varepsilon_{ij} \qquad (i \neq j)$$

where σ represents stresses and ε represents elastic strains. The three constants at room temperature and atmospheric pressure are given below [6]

$C_{11} = 1.6564 \times 10^{11}$ Pa
$C_{12} = .6394 \times 10^{11}$ Pa
$C_{44} = .7951 \times 10^{11}$ Pa

Between 150 K and 1000 K the decrease of the C_{ij} with increasing temperature is fairly linear and follows these rates:

$$\left(\frac{1}{C_{11}}\right)\frac{dC_{11}}{dT} = -9.4 \times 10^{-5}\ K^{-1} \quad [7]$$
$$= -9.3 \times 10^{-5}\ K^{-1} \quad [8]$$

$$\left(\frac{1}{C_{12}}\right)\frac{dC_{12}}{dT} = -9.8 \times 10^{-5}\ K^{-1} \quad [7]$$

$$\left(\frac{1}{C_{44}}\right)\frac{dC_{44}}{dT} = -8.3 \times 10^{-5}\ K^{-1} \quad 7]$$
$$= -1.0 \times 10^{-4}\ K^{-1} \quad [8]$$
$$= -7.3 \times 10^{-5}\ K^{-1} \quad [8]$$

For further information on third order elastic constants and the effects of doping see [6].

C Thermal Properties

Table 1 Thermal Expansion Coefficient [1]

T (K)	α (10^{-6} K^{-1})	T (K)	α (10^{-6} K^{-1})	T (K)	α (10^{-6} K^{-1})
5	0.6×10^{-4}	180	1.061	700	4.016
10	0.48×10^{-3}	200	1.406	800	4.151
20	-0.29×10^{-2}	220	1.715	900	4.185
40	-0.164	240	1.986	1000	4.258
60	-0.400	260	2.223	1100	4.323
80	-0.472	280	2.432	1200	4.384
100	-0.330	300	2.616	1300	4.442
120	-0.057	400	3.253	1400	4.500
140	0.306	500	3.614	1500	4.556
160	0.689	600	3.842	1600	4.612

Table 2 Melting Temperatures [1]

Temperature (°C)	1408	1410	1412	1414	1416
Number or Reports	1	1	7	8	3

Table 2 summarizes the reported melting points since 1948 of silicon. The melting point is extremely difficult to determine due to the calibration of the machinery and also the fact that molten silicon is highly reactive and most impurities serve to depress the melting point. The mean of the data given above is 1413.2 °C with a standard error of 0.31 degrees. Since the error in these measurements is negative, the best value to use would be one slightly higher than the mean, such as 1414.0 °C. [1]

Table 3 Thermal Conductivity Values (Above 200 K) [9]

T (K)	K (W cm^{-1} K^{-1})	T (K)	K (W cm^{-1} K^{-1})
200	2.66	1000	0.31
300	1.56	1100	0.28
400	1.05	1200	0.26
500	0.80	1300	0.25
600	0.64	1400	0.24
700	0.52	1500	0.23
800	0.43	1600	0.22
900	0.36	1681	0.22

Table 4 Thermal Conductivity Values (Below 200 K) [10]

T (K)	K (W cm^{-1} K^{-1})	T (K)	K (W cm^{-1} K^{-1})
150	4.10	20	47.7
100	9.13	10	24.0
50	28.0	8	16.4
40	36.6	6	8.99
30	44.2	4	3.11
		2	0.44

Table 4 Maximum Thermal Conductivity Versus Concentration of Boron Impurities [1][10]

	Thermal Conductivity		
Boron Concentration (cm^{-3})	Maximum (W cm^{-1} K^{-1})	Temperature (K)	Sample cross-section (mm^2)
1.0×10^{13}	48	22	6.03 x 6.07
4.2×10^{14}	43	25	6.17 x 6.32
4.2×10^{14}	38	26	3.45 x 3.50

1.0 x 10^{15}	43	25	6.19 x 6.32
4.0 x 10^{15}	33	27	5.86 x 5.86
4.0 x 10^{16}	18	37	6.24 x 6.27

Table 5 Thermal Diffusivity (Above 300 K) [11]

T (K)	D(cm^2 s^{-1})	T(K)	D(cm^2 s^{-1})
300	0.86	800	0.19
400	0.52	900	0.16
500	0.37	1000	0.14
600	0.29	1200	0.12
700	0.24	1400	0.12

Table 6 Thermal Diffusivity (Below 300 K) [12]

T (K)	D(cm^2 s^{-1})	T(K)	D(cm^2 s^{-1})
50	63.5	100	11.3
60	37.6	150	4.24
70	24.8	200	2.23
80	17.1	250	1.23
90	14.4		

For information on the heat for fusion for silicon, see [13][14]
For information on the surface tension of liquid silicon, see [15]

D Conclusion
This paper contained information on basic mechanical and thermal properties of silicon.

E References

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