3.2 Elastic constants and moduli of diamond cubic Si

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A INTRODUCTION

This Datareview gives values for the second and third order elastic constants, Sections B and C, the compliances, Section D, the bulk modulus, Section E, and the average elastic moduli in the isotropic approximation, Section F. Finally, in Section G, the dependence of the elastic constants on doping level is summarised.

B SECOND ORDER ELASTIC CONSTANTS

The second order elastic constants or stiffness, as defined by Kittel [1] or Hirth and Lothe [2] relate stresses σ to elastic strains ε, according to Hooke's law. In cubic crystals, three constants C_{11}, C_{12} and C_{44} are sufficient to determine all stress components whatever the state of strain:

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

The ε_{ij} are usually measured by ultrasonic methods. A discussion of current techniques and of theoretical calculations in semiconductors was given by Chen et al [3].

Early data for pure Si were reported by McSkimin and co-workers [4–6]. At room temperature, and atmospheric pressure, the most accurate data seem to be those of Hall [7].

$C_{11} = 1.6564 \times 10^{11}$ Pa
$C_{12} = 0.6394 \times 10^{11}$ Pa
$C_{44} = 0.7951 \times 10^{11}$ Pa

The error in C_{ij} is 0.02%. The values of McSkimin are within 0.1% of Hall's values.

The temperature dependence of C_{ij} was investigated by McSkimin [4] in the range 77–300 K, by Hall [7] in the range 4.2–310 K and by Burenkov and Nikanorov [8] up to 1273 K, but apparently with a lesser accuracy. (Their C_{11} and C_{12} at 293 K are about 5% lower than Hall's values, while their C_{44} agrees with Hall's within 1%).

Below 100 K, the C_{ij} change very little and the extrapolated values at 0 K used in more recent textbooks [3,9] are:

$C_{11} = 1.6772 \times 10^{11}$ Pa
$C_{12} = 0.6498 \times 10^{11}$ Pa
$C_{44} = 0.8036 \times 10^{11}$ Pa

which are 0.1% higher than the data measured by Hall [7] at 4.2 K.

Between 150 and 1000 K the decrease of the C_{ij} with increasing temperature is fairly linear. The measured rates are:

$\left(\frac{1}{C_{11}}\right)\frac{dC_{11}}{dT} = -9.4\times10^{-5}\ K^{-1}$ [9]

$= -9.3\times10^{-5}\ K^{-1}$ [8]

$\left(\frac{1}{C_{12}}\right)\frac{dC_{12}}{dT} = -9.8\times10^{-5}\ K^{-1}$ [9]

$\left(\frac{1}{C_{44}}\right)\frac{dC_{44}}{dT} = -8.3\times10^{-5}\ K^{-1}$ [9]

$= -1.0\times10^{-4}\ K^{-1}$ [8]

$= -7.3\times10^{-5}\ K^{-1}$ [8]

Rates given in [9] were extracted from the $C_{ij}(T)$ data of Hall [7], which cover a limited temperature range compared to that of Burenkov and Nikanorov [8].

C THIRD ORDER ELASTIC CONSTANTS

Measurements of the C_{ij} as functions of applied hydrostatic pressure up to 8 GPa [5,10] show that they are not constant beyond stresses of some hundreds of MPa. Non-linearity effects must be described in terms of higher order elastic constants. The conventional description is due to Thurston and Brugger [11] who used the Lagrangian form of elastic tensors. A summary of elastic theories was given by Nielsen [12].

Cubic crystals have six third-order elastic constants C_{ijk}, which are measured by monitoring the ultrasonic velocities as a function of external static pressure (hydrostatic or uniaxial). Such measurements were performed by McSkimin and Andreatch [6] and by Hall [7]. The data of Hall for pure Si at 298 K are:

$C_{111} = -7.95 \times 10^{11}$ Pa $\pm 0.10 \times 10^{11}$ Pa
$C_{112} = -4.45 \times 10^{11}$ Pa $\pm 0.10 \times 10^{11}$ Pa
$C_{123} = -0.75 \times 10^{11}$ Pa $\pm 0.05 \times 10^{11}$ Pa
$C_{144} = 0.15 \times 10^{11}$ Pa $\pm 0.05 \times 10^{11}$ Pa
$C_{166} = -3.10 \times 10^{11}$ Pa $\pm 0.05 \times 10^{11}$ Pa
$C_{456} = -0.86 \times 10^{11}$ Pa $\pm 0.05 \times 10^{11}$ Pa

The two sets of data [6,7] agree within the estimated error bars, except for $|C_{111}|$ found to be 4% higher by McSkimin.

D COMPLIANCES

The compliances express elastic strains as functions of stresses [1,2]. Using the notations of Hirth and Lothe [2], the compliances are noted S'_{ij} and are given by the relations:

$$S'_{11} = \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}$$

$$S'_{12} = \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}$$

$$S'_{44} = \frac{1}{C_{44}}$$

(These quantities are noted S_{ij} by Kittel [1].)

Using the C_{ij} of Hall [7] we obtain for pure Si:

$S'_{11} = 0.7691 \times 10^{11}$ Pa
$S'_{12} = -0.2142 \times 10^{11}$ Pa
$S'_{44} = 1.2577 \times 10^{11}$ Pa

at 298 K, and atmospheric pressure, with an error of 0.02%.

E BULK MODULUS

The bulk modulus B is defined as $B = -V(dP/dV)$ where V is the volume and P the hydrostatic pressure.

The compressibility K is defined as $K = 1/B$.

In cubic crystals, B is given by the following linear combination of elastic constants:

$$B = \frac{C_{11} + 2C_{12}}{3}$$

Using the C_{ij} measured by Hall [7] we obtain at 298 K and atmospheric pressure:

$B = 0.9784 \times 10^{11}$ Pa
$K = 1.0221 \times 10^{-11}$ Pa^{-1}

(The error in B, K is 0.02%.)

When non-linear effects become noticeable, the bulk modulus changes with pressure as

$$B(P) = B(0) - B'P$$

where the dimensionless $B' = -(dB/dP)$ is expressed in terms of third-order elastic constants as:

$$B' = -(C_{111} + 6\,C_{112} + 2\,C_{123}) / 9B$$

in the framework of Lagrangian elastic theory. With Hall's values for the C_{ijk}, we obtain:

$B' = 4.11$

at 298 K, and atmospheric pressure. The error in B' is about 2%.

F AVERAGE ELASTIC MODULI IN THE ISOTROPIC APPROXIMATION

Silicon is not elastically isotropic. The anisotropy of cubic solids is conveniently characterised by the anisotropy ratio, $A = 2\,C_{44} / (C_{11} - C_{12})$ and the anisotropy factor, $H = 2\,C_{44} + C_{12} - C_{11}$.

In pure Si, at ambient temperature and pressure:

$A = 1.56$
$H = 5.74 \times 10^{11}$ Pa

In view of the difficulties of exact calculations in anisotropic media, one is often satisfied with the isotropic approximation. In isotropic solids, two quantities are sufficient to relate stresses and strains. General use is made of the shear modulus μ, such as $\sigma_{ij} = 2\,\mu\,\varepsilon_{ij}$, and of the Poisson's ratio ν, the ratio of transverse contraction to elongation in simple tension. Also commonly used is the Young's modulus, E, the ratio of simple tensile stress to strain.

There are two ways to define these average quantities in real solids. The Voigt average is over the elastic constants C_{ij} and is appropriate for a polycrystalline material in which the grains of different orientations have the same stress. The Voigt average is also better to deal with local strains around dislocations. In contrast, the Reuss average is over the compliances S'_{ij} and is better when the grains have the same state of strain or in cases involving long-range internal stress-fields.

In cubic crystals, average moduli are defined as follows:

Voigt average

shear modulus $$\mu = C_{44} - \frac{1}{5}H$$

Poisson's ratio $$\nu = \frac{C_{12} - H/5}{2(C_{12} + C_{44} - 2H/5)}$$

Young's modulus $$E = 2\mu\,(1 + \nu)$$

Reuss average

shear modulus $$\mu_R = \left(S'_{44} + \frac{4}{5}J\right)^{-1}$$

Poisson's ratio $$\nu_R = \left(-S'_{12} - \frac{J}{5}\right)\left(S'_{11} - \frac{2J}{5}\right)^{-1}$$

Young's modulus $$E_R = \left(S'_{11} - \frac{2}{5}J\right)^{-1}$$

with $J = S'_{11} - S'_{12} - \frac{S'_{44}}{2}$

Using the C_{ij} of Hall [7] we obtain, for pure Si at ambient temperature and pressure:

$\mu = 6.80 \times 10^{11}$ Pa
$\nu = 0.218$
$E = 16.56 \times 10^{11}$ Pa
$\mu_R = 6.49 \times 10^{11}$ Pa
$\nu_R = 0.228$
$E_R = 15.94 \times 10^{11}$ Pa

G DOPING DEPENDENCE OF ELASTIC CONSTANTS

As explained by Keyes [13], the elastic properties of semiconductors depend on the carrier concentration, so that the elastic constants are expected to change significantly with electronic doping.

Second-order elastic constants were measured in heavily doped n-type Si by Hall [7], for a carrier concentration $n = 2.0 \times 10^{19}$ cm^{-3} (phosphorus) in the range 4.2–310 K, and by Beilin et al [14] for $n = 4.8 \times 10^{19}$ cm^{-3} (arsenic) at 78 and 295 K. Hall also measured the C_{ijk}. Heavily doped p-type Si was investigated by Mason and Bateman [15] for various concentrations from 5×10^{17} to 3×10^{19} cm^{-3} (boron and gallium). Theoretical approaches were given by Keyes [13], Kim [16] and Khan and Allen [17] (see also [3]). The typical effect of heavy doping is to decrease the C_{ij} by 1–3% and to modify the temperature dependences. The C_{ijk} can be changed in much larger proportions.

H CONCLUSION

Second order elastic constants, or stiffness, relate stresses to strains and this Datareview has summarised their values and variation with temperature. Third order elastic constants are required to describe the pressure dependence, above a few hundred MPa. Values are also given for the compliances, at ambient temperature and pressure, and the bulk modulus, at ambient temperature and pressure and at higher pressure. Silicon is not elastically isotropic and an approximation is needed, via the Voigt and Reuss averages, using the shear modulus, Poisson's ratio and Young's modulus. Elastic constants change markedly on doping with P, As, B and Ga.

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