ISBN: 978-3-95450-229-5 ISSN: 2673-5520 doi:10.18429/JACoW-MEDSI2020-WEPC09

TEMPERATURE-DEPENDENT ELASTIC CONSTANTS AND YOUNG'S MODULUS OF SILICON SINGLE CRYSTAL*

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Abstract

Silicon crystals have been widely used for x-ray monochromators. It is an anisotropic material with temperature-dependent properties. Values of its thermal properties from cryogenic to high temperature are available in the literature for expansion, conductivity, diffusivity, heat capacity, but neither elastic constants nor Young's modulus. X-ray monochromators may be liquid-nitrogen cooled or water cooled. Finite Element Analysis (FEA) is commonly used to predict thermal performance of monochromators. The elastic constants and Young's modulus over cryogenic and high temperature are now collected and derived from literature, with the purpose of assisting in providing accurate FEA predictions.

INTRODUCTION

Silicon single crystals have been widely used for x-ray monochromators [1], in addition to application in MEMS fabrication, both as a substrate for compatibility with semiconductor processing equipment and as a structural material for MEMS devices [2-4]. It is an anisotropic material with temperature-dependent properties, such as thermal conductivity [5, 6], thermal expansion coefficients [7-9], and elastic constants [10] or Young's modulus [11, 12]. At room temperature, Young's modulus varies from 130 GPa in the <100> directions to 190 GPa in the <111> directions.

Burenkov *et al*. [13] and Kury *et al*. [14] studied the temperature dependence of Young's modulus $E_{<ijk>}$ for Si and Ge. Polynomial expressions for the dependence on temperature between room temperature and 1000˚C of the bi-axial Young's modulus $E_{<ijk>}/(1-v)$, with v the Poisson's ratio, were developed. Vanhellemont *et al*. reported temperature-dependent Young's modulus of silicon by means of impulse excitation technique [12]. The data $E_{<ijk>}$ along <100>, <110>, and <111> directions are available from room temperature to 1400˚C.

McSkimin measured elastic constants C_{11}, C_{12}, C_{44} of silicon single crystal at low temperatures by means of ultrasonic waves [10]. The data are valid from 78 K to 300 K.

This report derives Young's modulus at low temperatures from elastic constants C_{11}, C_{12}, C_{44} of silicon single crystal in ref. [10], and elastic constants at high temperatures from Young's modulus in ref. [12]. Therefore, complete sets of Young's modulus and elastic constants are provided from -196˚C up to 1400˚C, or ~78 K to ~1673 K. Further, users may derive temperature-dependent Young's modulus or elastic constants at any arbitrary orientations.

* This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility at Argonne National Laboratory and is based on research supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
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ELASTIC CONSTANTS

The stiffness coefficients C_{ijkl} and the compliance coefficients S_{ijkl} are defined as the proportionality constants between stress σ and strain ε tensors in the form of generalized Hooke's law:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \text{ and } \varepsilon_{ij} = S_{ijkl}\sigma_{kl}. \quad (1)$$

In the Coordinate System of a Cubic Crystal

Figure 1 shows the coordinate system with "X,Y,Z"-axes in the <100>,<010>, and <001> directions of a cubic structure. Because of its orthogonality, this coordinate system is actually a Cartesian coordinate system. An arbitrary orientation <hkl> rotating with respect to those three directions is also illustrated.

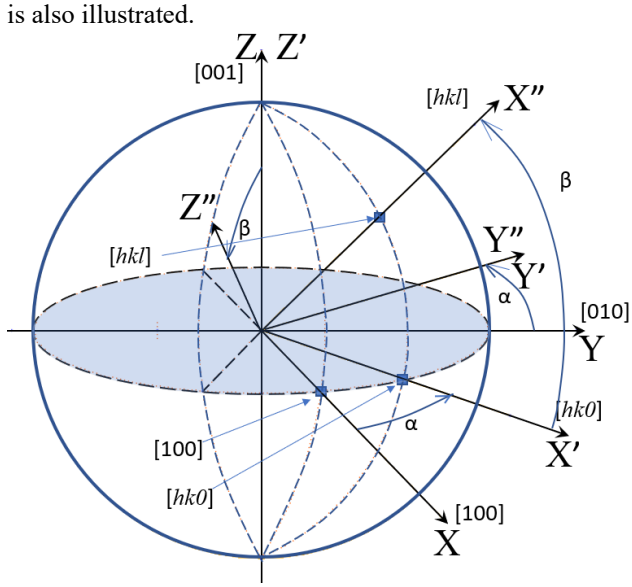

Figure 1: Illustration of coordinate system transformation with respect to the primary directions of a cubic structure.

For a cubic crystal such as silicon, the combination of cubic symmetry and the equivalence of the shear conditions enables specifying the fourth rank tensor with only three independent elastic constants. With respect to a specific basis that is commonly given for the <100> directions of the cubic structure, these tensors are given as [15, 16]:

$$\sigma_{ii} = C_{11}\varepsilon_{ii} + C_{12}\left(\varepsilon_{jj} + \varepsilon_{kk}\right), \text{ and } \sigma_{ij} = C_{44}\varepsilon_{ij}. \quad (2)$$

The stiffness matrix can be shortened as C_{pq} or:

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{bmatrix}. \quad (3)$$

The compliance matrix can be written in a similar form, which is the inverse of the stiffness matrix. The second-order elastic compliances S_{pq} can be expressed as:

ISBN: 978-3-95450-229-5 ISSN: 2673-5520 doi:10.18429/JACoW-MEDSI2020-WEPC09

$$S_{11} = (C_{11} + C_{12})/[(C_{11} - C_{12})(C_{11} + 2C_{12})],$$
$$S_{12} = -C_{12}/[(C_{11} - C_{12})(C_{11} + 2C_{12})],$$
$$S_{44} = 1/C_{44}. \quad (4)$$

To obtain Eq. (4), the following relation is applied [17]:

$$2C_{11}(C_{11} + C_{12}) = (C_{11} - C_{12})(C_{11} + 3C_{12}) \quad (5)$$

In an Arbitrary Orientation of a Cubic Crystal

In an arbitrary orientation <hkl> as shown in Fig. 1, the corresponding elastic constants C_{pq}' and S_{pq}' can be calculated through a transformation [11, 18]. The results of such a transformation are listed in Table 1. The transformation from the crystal axes x_i (unprimed) to the arbitrary system x_i" (primed) is expressed by:

$$x_i'' = l_i x_1 + m_i x_2 + n_i x_3, \quad i = 1,2,3 \quad (6)$$

with l, m, n being the direction cosines of the rotational transformation.

Table 1: Stiffness and Compliance Coefficients of Transformation for Rotated Axes in Cubic Crystals

Coefficient transformation[1]	Analogous[2] coefficients
$C_{11}' = C_{11} + C_c(l_1^4 + m_1^4 + n_1^4 - 1)$	C_{22}', C_{33}'
$C_{12}' = C_{12} + C_c(l_1^2 l_2^2 + m_1^2 m_2^2 + n_1^2 n_2^2)$	C_{13}', C_{23}'
$C_{14}' = C_c(l_1^2 l_2 l_3 + m_1^2 m_2 m_3 + n_1^2 n_2 n_3)$	$C_{15}', C_{16}', C_{24}', C_{25}', C_{26}', C_{34}', C_{35}', C_{36}' C_{45}', C_{46}', C_{56}'$
$C_{44}' = C_{44} + C_c(l_2^2 l_3^2 + m_2^2 m_3^2 + n_2^2 n_3^2)$	C_{55}', C_{66}'
$S_{22}' = S_{11} + S_c(l_2^4 + m_2^4 + n_2^4 - 1)$	S_{11}', S_{33}'
$S_{13}' = S_{12} + S_c(l_1^2 l_3^2 + m_1^2 m_3^2 + n_1^2 n_3^2)$	S_{12}', S_{23}'
$S_{14}' = 2S_c(l_1^2 l_2 l_3 + m_1^2 m_2 m_3 + n_1^2 n_2 n_3)$	$S_{15}', S_{16}', S_{24}', S_{25}' S_{26}', S_{34}', S_{35}', S_{36}'$
$S_{56}' = 4S_c(l_1^2 l_2 l_3 + m_1^2 m_2 m_3 + n_1^2 n_2 n_3)$	S_{45}', S_{46}'
$S_{55}' = S_{44} + 4S_c(l_1^2 l_3^2 + m_1^2 m_3^2 + n_1^2 n_3^2)$	S_{44}', S_{66}'

Note:
1. $C_{ij}' = C_{ji}'$, $S_{ij}' = S_{ji}'$;
$C_c = C_{11} - C_{12} - 2C_{44}$, $S_c = S_{11} - S_{12} - \frac{1}{2}S_{44}$
2. The subscript on a direction cosine, as well as on a coefficient, represents two subscripts: (1→11, 2→22, 3→33, 6→12, 5→13, 4→23).

YOUNG'S MODULUS, SHEAR MODULUS, AND POISSON'S RATIO

Young's modulus is defined as a proportional constant of stress over its corresponding strain of a normal deformation, while the shear modulus is defined as stress over the corresponding strain of a transverse deformation:

$$E_i = \sigma_i/\varepsilon_i, \quad i = 1,2,3$$
$$G_i = \sigma_i/\varepsilon_i, \quad i = 4,5,6. \quad (7)$$

The Poisson's ratio is defined as

$$v_{ij} = -\varepsilon_j/\varepsilon_i, \quad i,j = 1,2,3, i \neq j. \quad (8)$$

By comparing the definitions of these moduli and stiffness, it can readily be shown that

$$E_i(or\ G_i) = 1/S_{ii}, \text{ and } v_{ij} = -S_{ji}/S_{ii}. \quad (9)$$

The Young's modulus E_{hkl} can be calculated from the general formulae for cubic crystal as [15, 16, 19]:

$$\frac{1}{E_{hkl}} = S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2S_{44}}\right)(l^2m^2 + m^2n^2 + l^2n^2). \quad (10)$$

The corresponding Poisson's ratio and shear modulus in the cubic configuration can be expressed as:

$$v_{\alpha\beta} = \frac{S_{12} + \left(S_{11} - S_{12} - \frac{1}{2S_{44}}\right)(l_\alpha^2 l_\beta^2 + m_\alpha^2 m_\beta^2 + n_\alpha^2 n_\beta^2)}{S_{11} - 2\left(S_{11} - S_{12} - \frac{1}{2S_{44}}\right)\left(l_\alpha^2 m_\alpha^2 + m_\alpha^2 n_\alpha^2 + l_\alpha^2 n_\alpha^2\right)} \quad (11)$$

$$G_{ij} = 1/S_{ij}', (S_{ij}' \text{ as shown in Table 1}) \quad (12)$$

with α and β being the two orthogonal directions, and l_γ, m_γ, n_γ are the directional cosines of the angles between the γ direction and basis axes.

By substituting Eq. (4) into Eq. (10), one obtains

$$\frac{1}{E_{hkl}} = \frac{C_{11}+C_{12}}{(C_{11}-C_{12})(C_{11}+2C_{12})} - 2\left(\frac{C_{11}+C_{12}}{C_{11}-C_{12}} - \frac{C_{44}}{2}\right)(l^2m^2+m^2n^2+l^2n^2). \quad (13)$$

Young's moduli in the <100>, <110>, and <111> crystallographic directions can be derived as [20]:

$$E_{[100]} = (C_{11} - C_{12})(C_{11} + 2C_{12})/(C_{11} + C_{12}),$$
$$E_{[110]} = 2/\left\{\frac{C_{11}}{(C_{11}-C_{12})(C_{11}+2C_{12})} + \frac{1}{2C_{44}}\right\},$$
$$E_{[111]} = 3/\left(\frac{1}{C_{11}+2C_{12}} + \frac{1}{C_{44}}\right). \quad (14)$$

Inversely stiffness coefficients C_{11}, C_{12}, and C_{44} can be obtained from Eq. (14).

TEMPERATURE-DEPENDENT ELASTIC CONSTANTS AND YOUNG'S MODULUS

The temperature-dependent Young's modulus of silicon $E_{<100>}$, $E_{<110>}$, and $E_{<111>}$ are available from room temperature to 1400˚C [12]. The corresponding stiffness coefficients C_{11}, C_{12}, and C_{44} can be calculated with Eq. (14) if one is interested in the coefficients at high temperature.

Data of measured stiffness coefficients C_{11}, C_{12}, and C_{44} of silicon single crystal are valid from 78 K to 300 K [10]. The data can be converted to the Young's modulus, Poisson's ratio, and shear modulus by using Eqs. (4, 10-12) when needed. For example, ANSYS Workbench takes temperature dependent data of orthogonal elasticity in terms of Young's modulus, Possion's ratio, and shear modulus.

By combining data at low and high temperatures, Fig. 2 shows Young's modulus $E_{<100>}$, $E_{<110>}$, and $E_{<111>}$ from 4 to 1400 K, and Fig. 3 shows stiffness coefficients C_{11}, C_{12}, and C_{44} from 4 to 1400 K. The data below 80 K are artificial for curve fitting purposes.

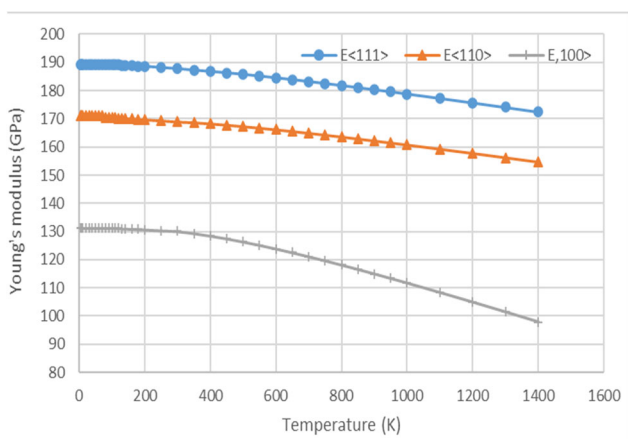

Figure 2: Young's modulus of silicon single crystal.

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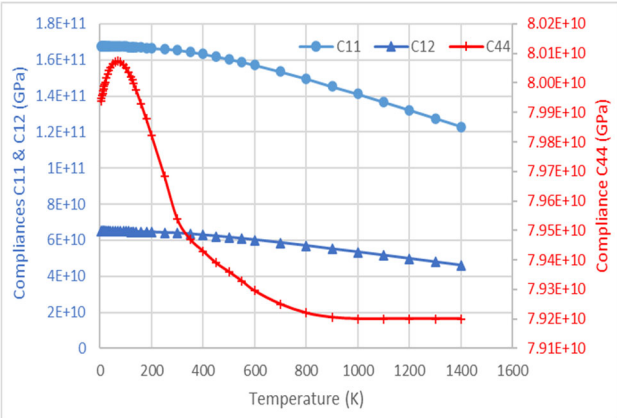

Figure 3: Stiffness coefficients of silicon single crystal.

CONCLUSION

For cubic crystals such as silicon, conversion equations between elastic constants and Young's modulus along crystallography axes are summarized. Based on the available amount of measured data of Young's modulus from room temperature to melting temperature and stiffness coefficients from room temperature to cryogenic temperature, complete sets of data of both Young's modulus and stiffness coefficients from cryogenic temperature to 1400 K are presented.

ACKNOWLEDGEMENTS

Thanks to Xianbo Shi for his advisory assistance with information on the coordinate transformation for silicon crystals.

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