

What is the Young's Modulus of Silicon?

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Abstract—The Young's modulus (E) of a material is a key parameter for mechanical engineering design. Silicon, the most common single material used in microelectromechanical systems (MEMS), is an anisotropic crystalline material whose material properties depend on orientation relative to the crystal lattice. This fact means that the correct value of E for analyzing two different designs in silicon may differ by up to 45%. However, perhaps, because of the perceived complexity of the subject, many researchers oversimplify silicon elastic behavior and use inaccurate values for design and analysis. This paper presents the best known elasticity data for silicon, both in depth and in a summary form, so that it may be readily accessible to MEMS designers. [2009-0054]

Index Terms—Elastic modulus, elasticity, microelectromechanical systems (MEMS) design, Poisson's ratio, shear modulus, silicon, Young's modulus.

I. INTRODUCTION

THE FIELD of microelectromechanical systems (MEMS), also known as microsystem technology, is an interdisciplinary activity. Researchers from many different backgrounds, including physics, engineering, biology, materials science, and many others, have made significant contributions. Researchers may be tempted to ignore the details of some of the more difficult aspects of areas outside their own background, and use the summaries and conclusions provided by specialists. This is necessary and normal behavior for a generalist, but it must always be accompanied by a cautious assessment of whether the summary provided applies to the case under consideration.

In the case of mechanical design of elastic structures, MEMS technology presents an interesting challenge for engineers. As traditional multipart joints and linkages are difficult to fabricate with microtechnology, most microscale mechanical linkages are constructed using elastic flexures. The design equations which are used to describe elastic flexures, from the basic Hookean relationship between stress and strain to approximations for out-of-plane deflection of a square plate under a point load, all require an effective " E ," the Young's modulus or elastic modulus, to quantify the elastic behavior of the material in question. Additional mechanical behavior is described by other elastic moduli, such as the shear modulus G , the bulk modulus B , and many others.

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Monocrystalline silicon is the single material most widely used in MEMS fabrication, both as a substrate for compatibility with semiconductor processing equipment and as a structural material for MEMS devices. Because silicon is an anisotropic material, with elastic behavior that depends on the orientation of the structure, choosing the appropriate value of E for silicon can appear to be a daunting task. However, the possible values of E for silicon range from 130 to 188 GPa and the choice of E value can have a significant influence on the result of a design analysis. This paper attempts to clarify the correct value of E for a given situation and to show that, while the nuances of fully anisotropic crystal mechanics are a subject for specialists, the symmetry of the cubic structure of silicon makes the complete description of its behavior accessible to the MEMS generalist. In addition, as computing power for finite-element method (FEM) calculations is ever more readily available, calculations using the complete anisotropic material description are increasingly accessible and common. The necessary data for finite-element work are also provided.

While many leading textbooks provide summaries of the material presented here [1]–[3], many others provide oversimplified or incomplete information. Furthermore, the research literature of the past quarter century contains numerous examples of incorrect usage. This appears to be a result of the history of research into silicon, which was initially dominated by the physics community and investigations of the semiconductor behavior by Shockley, Bardeen, Brattain, Smith, Hall, etc. These investigations were predicated on the physical understanding of the material structure provided by quantum theory, as well as X-ray diffraction investigations and other fundamental techniques, and the researchers necessarily understood and used complete (anisotropic) material descriptions. Following shortly thereafter, the early literature of micromachining is also dominated by specialists until the publication of the seminal paper by Petersen in 1982, *Silicon as a Mechanical Material* [4]. Here, Petersen summarizes the state of the art in silicon micromachining and describes the methods by which a wide variety of different silicon devices can be fabricated. In an effort to minimize the complexity of an extraordinarily rich and useful paper (possibly the most cited single paper in MEMS, with well over 1000 citations as of this writing), Petersen gives the Young's modulus of silicon as 1.9×10^{12} dynes/cm² (i.e., 190 GPa), with a footnote that directs readers to a textbook [5] on materials for further information on silicon anisotropy. This value is simply the maximum possible E value for silicon, rounded up. Later in the same paper, as an example of a device made from silicon, he describes a silicon mirror that is suspended with torsional flexures. He uses the value of 190 GPa to calculate the expected resonance frequency of the device as 16.3 kHz, which is a "reasonably accurate" prediction when compared to the

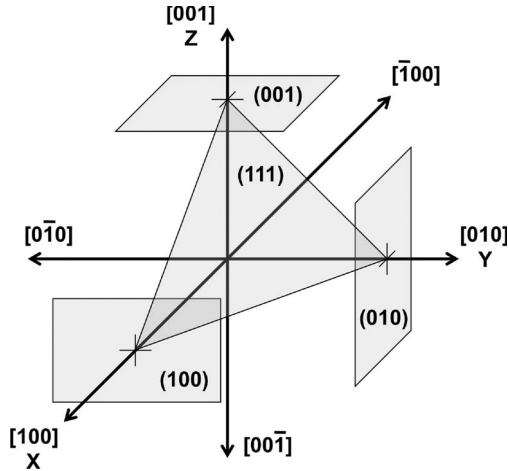


Fig. 1. Miller indices in a cubic crystal. The important planes for silicon are shown. By convention, the directions $[100]$, $[010]$, and $[001]$ are the XYZ Cartesian axes unless otherwise specified.

measured value of 15 kHz. Since then, numerous researchers have cited and used this value of E for silicon, even when their structure is extremely simple (e.g., a beam) and the correct (anisotropic) value is easily determined. Note that using the correct value of E for the example of the torsional mirror, 169 GPa, gives an even more reasonable prediction of 15.4 kHz.

The example given earlier raises an important point, namely, that the designer may not be concerned with a small improvement in the accuracy of their analysis. We agree that the improvement in this example is not dramatic, but we submit that this improvement was quite easy to achieve and, in other situations, will have more significant effect on the final result. As we shall show, the possible values for Young's modulus range from 130 to 188 GPa, and those for Poisson's ratio range from 0.048 to 0.40. While the simplification of using the highest possible value of Young's modulus was acceptable for the purpose of introducing silicon micromachining to the community 25 years ago, after a generation of MEMS research and the growing availability of computational power, we should do better.

II. CRYSTAL ORIENTATION

In order to describe crystal-orientation-dependent material properties, we first need to describe crystal orientation. Crystallographic planes and directions are described by Miller indices, which are three-integer triples (" hkl "), corresponding to an XYZ coordinate system. The triple can describe either a direction or a plane perpendicular to the direction. The hkl values are the reciprocals of the coordinates of the intercepts on the XYZ -axes, multiplied by the lowest common denominator. Negative values are indicated by a bar. When referring to directions and angles within a cubic crystal, the XYZ -axes are aligned with the $\langle 100 \rangle$ directions unless otherwise specified. The important directions for silicon are shown in Fig. 1. More detailed discussions of crystal orientation can be found in [1], [6], and [7].

In a symmetric crystal lattice, certain directions are equivalent to one another. Groups of equivalent directions or planes are called *families*. For example, in a cubic crystal, directions $[100]$, $[010]$, and $[001]$ are in the $\langle 100 \rangle$ family. Table I lists the

Miller index notation for cubic crystals. The silicon lattice has cubic symmetry, so all directions and planes rotated 90° from each other are equivalent.

III. CRYSTAL ORIENTATION OF A SILICON WAFER

The crystal orientation of the silicon in a silicon wafer has significant effects on the microfabrication properties of the wafer [2], and so, crystal orientation is an important part of wafer specification, as maintained by the industry group SEMI [8]. The crystal orientation is specified in two ways. First, the orientation of the plane of the surface of the wafer is given; for example, an "n-type (100) wafer" has the top surface of the wafer oriented in the (100) plane of the silicon crystal. The second part of the orientation information is given by the location of the wafer primary flat. For the most commonly encountered wafers in research (p- and n-type (100) and (111) wafers), the primary flat is aligned with the $[110]$ direction. The accuracy of the alignment of the wafer flat with the crystal lattice of the silicon material is typically specified to be $\pm 1^\circ$ [8], which corresponds to a variation in the Young's modulus value of much less than 1%. This variation is small compared to other sources of uncertainty and can usually be ignored.

Most MEMS designs are drawn using a computer-based layout editor with an X - Y coordinate space and the layout aligned with the axes in a left-right up-down fashion. Most microfabrication tools use the primary flat of the wafer to orient the wafer for processing, and the conventional orientation is flat "down," i.e., parallel to the floor when the wafer is held up vertically for examination, or toward the operator when inserted horizontally into processing equipment. This means that, in the most common case of fabrication of a MEMS device, namely, a design aligned to the X - Y -axes on a standard (100) silicon wafer, the X - and Y -axes of the design will be aligned with the $\langle 110 \rangle$ silicon crystal directions, as shown in Fig. 2. These directions have equivalent elastic properties.

IV. ANISOTROPIC ELASTICITY

Elasticity is the relationship between stress (σ) and strain (ε). Hooke's law describes this relationship in terms of compliance S or stiffness C

$$\sigma = C\varepsilon \quad \varepsilon = S\sigma. \quad (1)$$

For isotropic uniaxial cases, stiffness C can be represented by a single value of Young's modulus E , and the equation takes the familiar form of $\sigma = E\varepsilon$. In an anisotropic material, a fourth rank tensor with $3^4 = 81$ terms is required to describe the elasticity by relating the second rank tensors of stress and strain. In this case, Hooke's law is written with subscripts which describe the orientation of the face and the vector, shown as

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} \quad \varepsilon_{ij} = s_{ijkl}\sigma_{kl}. \quad (2)$$

Fortunately, in silicon, the combination of cubic symmetry and the equivalence of the shear conditions allow us to specify the fourth rank tensor with only three independent components. The four subscripts can be condensed to two, as given in Table II.

TABLE I
MILLER INDEX NOTATION FOR CUBIC CRYSTALS

Notation	Meaning
$[hkl]$	The direction vector given by hkl
$\langle hkl \rangle$	The family of symmetric direction vectors equivalent to hkl
(hkl)	The crystal plane perpendicular to vector hkl
$\{hkl\}$	The family of planes equivalent to the plane perpendicular to vector hkl

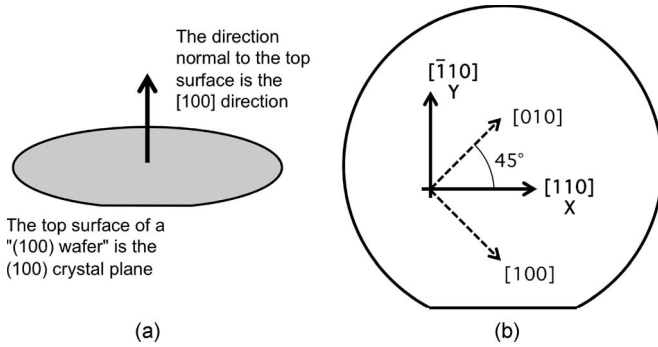


Fig. 2. Crystal orientation in 100-mm-diameter silicon wafers. The natural X- and Y-axes are in the $\langle 110 \rangle$ directions. (a) Orientation of a (100) wafer. (b) Directions and axes in a (100) wafer.

TABLE II
SIMPLIFIED SUBSCRIPTS FOR CUBIC SYMMETRY

Face/Direction	Condensed Numeric Equivalent
xx or 11	1
yy or 22	2
zz or 33	3
yz or 23	4
zx or 31	5
xy or 12	6

Note: Some texts (such as [6]) use numbers instead of letters to indicate faces and directions, with X=1, Y=2, Z=3. The difference between this notation and the simplified equivalents must be inferred from context.

By using this condensed notation, the three independent components for cubic crystals are 11, 12, and 44. The tensor can then be written in matrix notation as a 6×6 matrix

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} \quad (3)$$

$$\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} = \begin{bmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0 \\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{44} \end{bmatrix} \begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} \quad (4)$$

This matrix representation is given with respect to a specific set of XYZ -axes. In a cubic crystal such as silicon, the $\langle 100 \rangle$ directions are the default XYZ -axes, i.e., X (or 1) is $\langle 100 \rangle$, Y is $\langle 010 \rangle$, and Z is $\langle 001 \rangle$, as shown in Fig. 1. Stress and strain relationships can be calculated from this matrix for directions aligned with the XYZ -axes using normal matrix operations on

(3) and (4) (i.e., solving the simultaneous equations relating σ and ε). However, in order to calculate the stress/strain relationships in an arbitrary direction, the tensor must be rotated so that one of the axes is aligned with the direction of interest. This is a tedious mathematical exercise: See [6] for tensor transformations or [9] and [10] for (relatively) simplified formulas for calculating rotated elasticity components, as well as [7] for a procedure that can be used to perform a rotation on the matrix form of the tensor. However, an explicit tensor rotation is usually unnecessary; shortcut formulas exist for calculating the elastic properties in arbitrary directions for cubic symmetry, as discussed in Section IX.

V. ELASTIC CONSTANTS

So now, the question becomes the following: What are the elastic constants for silicon? Silicon is an important economic material, and it has been studied carefully. The elasticity of a material is a result of the interatomic forces between the constituent atoms. The elasticity values for a crystal can be calculated from quantum theory, as the elastic modulus is simply the strain derivative of the crystal free energy [11], [12], but the calculation is difficult and includes many derived constants and approximations, so those results can be considered a strong guide rather than a rule. The measurement of the elastic constants is best performed using measurements of acoustic wave propagation in the solid, which requires relatively straightforward sample preparation and can be performed with high accuracy since it depends on measurement of a time interval. The measurement methods are described in detail elsewhere, including [12]–[15] and references therein. The values for the elastic constants are given in Table III.

By using the values from Table III, we can now calculate the values for Young's modulus and Poisson's ratio in arbitrary directions with respect to the crystal lattice. Fig. 3 reproduces some plots from [9], showing the variation of Young's modulus and Poisson's ratio in the (100) plane. These plots apply, for example, to the typical (100) wafer described in Section III.

Although the effective moduli resulting from these constants can be calculated, it is worthwhile to measure them experimentally for verification and to investigate conditions in actual use, such as the difference between bulk and thin-film properties. In [18], Sharpe tabulates a large number of measurements of the Young's modulus of silicon for MEMS applications. As expected, the results converge on the values calculated from acoustic wave propagation in bulk samples. Experimental values do diverge from the crystal properties at the nanoscale (sample dimensions less than $0.1 \mu\text{m}$), where lattice defects and surface effects dominate the mechanical response of the sample. See, for example, [19]–[21].

TABLE III
ELASTIC CONSTANTS OF SILICON. VALUES FOR 298 K, FROM HALL [12]

c: 10 ⁹ Pa s: 10 ⁻¹² Pa	c ₁₁	c ₁₂	c ₄₄	s ₁₁	s ₁₂	s ₄₄
Silicon	165.6	63.9	79.5	7.68	-2.14	12.6

Note: Values from Mason [16] are often cited in the literature. The measurements performed a decade later by Hall report slightly better accuracy, although the differences between the two are not significant. Additional references: [9], [13], [14], [17]

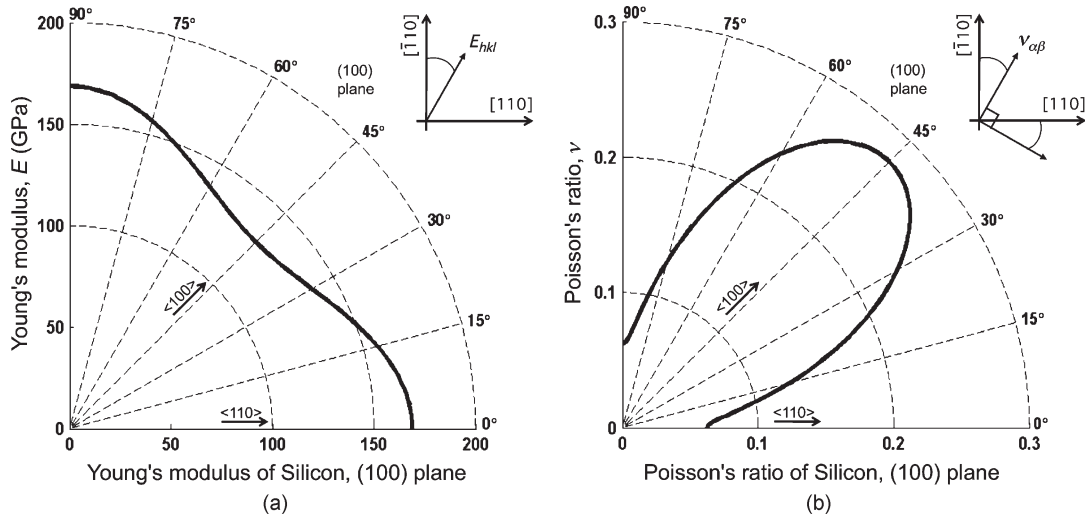


Fig. 3. Value of Young's modulus and Poisson's ratio versus orientation in silicon. Values are for the (100) plane, calculated using the constants in Table III. The plot axes align with the orientation of a typical wafer flat, as shown in Fig. 2(b). (a) Young's modulus. (b) Poisson's ratio.

VI. ELASTICITY OF DOPED SILICON

Most silicon wafers are not pure silicon; a certain amount of chemical impurities is usually added to control the wafer's electrical properties. This is called "doping." The volumetric effect of adding the mass of the dopant atoms to the crystal lattice is negligible, but the effect of doping on crystalline semiconductor elastic behavior through electrical interaction can be predicted from the strain energy of the crystal using the standard "many-valleys" model, and measurements align well with the theoretical predictions [11], [12], [22]–[24]. The changes are typically a 1%–3% decrease for heavy doping levels and are usually ignored for engineering calculations.

VII. ORTHOTROPIC ELASTICITY

The matrix representation of the anisotropic elasticity tensor in (3) is created by simplifying the complete anisotropic fourth rank elasticity tensor. Because silicon has cubic symmetry, it is also possible to give the elastic properties in terms of *orthotropic* material constants. An orthotropic material is

one which has at least two orthogonal planes of symmetry, and silicon, with cubic symmetry, can be described this way. Orthotropic elasticity is described with a matrix that looks quite similar to (3), except that the values for each entry are derived from the "fundamental" elasticity quantities of Young's modulus (*E*), Poisson's ratio (*ν*), and the shear modulus (*G*) in the axes of interest (*x, y, z*); see (5) shown at the bottom of the page where

$$\Delta = \frac{1 - \nu_{xy}\nu_{yx} - \nu_{yz}\nu_{zy} - \nu_{zx}\nu_{xz} - 2\nu_{xy}\nu_{yz}\nu_{zx}}{E_x E_y E_z}$$

and

$$\begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{zx} \\ \epsilon_{xy} \end{bmatrix} = \begin{bmatrix} \frac{1}{E_x} & -\frac{\nu_{yx}}{E_y} & -\frac{\nu_{zx}}{E_z} & 0 & 0 & 0 \\ -\frac{\nu_{xy}}{E_x} & \frac{1}{E_y} & -\frac{\nu_{zy}}{E_z} & 0 & 0 & 0 \\ -\frac{\nu_{xz}}{E_x} & -\frac{\nu_{yz}}{E_y} & \frac{1}{E_z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{yz}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{zx}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{xy}} \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} \quad (6)$$

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} \frac{1 - \nu_{yz}\nu_{zy}}{E_y E_z \Delta} & \frac{\nu_{yx} + \nu_{yz}\nu_{zy}}{E_y E_z \Delta} & \frac{\nu_{zx} + \nu_{yx}\nu_{zy}}{E_y E_z \Delta} & 0 & 0 & 0 \\ \frac{\nu_{xy} + \nu_{xz}\nu_{zy}}{E_z E_x \Delta} & \frac{1 - \nu_{zx}\nu_{xz}}{E_z E_x \Delta} & \frac{\nu_{zy} + \nu_{xz}\nu_{xy}}{E_z E_x \Delta} & 0 & 0 & 0 \\ \frac{\nu_{xz} + \nu_{xy}\nu_{yz}}{E_x E_y \Delta} & \frac{\nu_{yz} + \nu_{xz}\nu_{yx}}{E_x E_y \Delta} & \frac{1 - \nu_{xy}\nu_{yx}}{E_x E_y \Delta} & 0 & 0 & 0 \\ 0 & 0 & 0 & G_{yz} & 0 & 0 \\ 0 & 0 & 0 & 0 & G_{zx} & 0 \\ 0 & 0 & 0 & 0 & 0 & G_{xy} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ \epsilon_{yz} \\ \epsilon_{zx} \\ \epsilon_{xy} \end{bmatrix} \quad (5)$$

The advantage of the orthotropic description is that the values can be used without a lot of tedious discussions of crystal orientation and tensor rotation; the elastic quantities for the orientation of interest are simply given, and the stress/strain relationships can be calculated from the matrix. The elasticity quantities for a given orientation can be derived from the full anisotropic expressions using the values given in Section V. For example, the orthotropic stiffness matrix for silicon with three axes at [100], [010], and [001] is

$$\begin{aligned}
 E_x = E_y = E_z &= 130 \text{ GPa} \\
 \nu_{yz} = \nu_{zx} = \nu_{xy} &= 0.28 \\
 G_{yz} = G_{zx} = G_{xy} &= 79.6 \text{ GPa}
 \end{aligned}$$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} 165.7 & 63.9 & 63.9 & 0 & 0 & 0 \\ 63.9 & 165.7 & 63.9 & 0 & 0 & 0 \\ 63.9 & 63.9 & 165.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 79.6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 79.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 79.6 \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix}. \quad (7)$$

This is, of course, identical to (3) with the constants from Table III.

The most common use of the orthotropic expressions for silicon is to provide the elasticity values in the frame of reference of a standard (100) silicon wafer (see Section III), which is [110], $[\bar{1}10]$, [001]

$$\begin{aligned}
 E_x = E_y &= 169 \text{ GPa} & E_z &= 130 \text{ GPa} \\
 \nu_{yz} &= 0.36 & \nu_{zx} &= 0.28 & \nu_{xy} &= 0.064 \\
 G_{yz} = G_{zx} &= 79.6 \text{ GPa} & G_{xy} &= 50.9 \text{ GPa}
 \end{aligned}$$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} 194.5 & 35.7 & 64.1 & 0 & 0 & 0 \\ 35.7 & 194.5 & 64.1 & 0 & 0 & 0 \\ 64.1 & 64.1 & 165.7 & 0 & 0 & 0 \\ 0 & 0 & 0 & 79.6 & 0 & 0 \\ 0 & 0 & 0 & 0 & 79.6 & 0 \\ 0 & 0 & 0 & 0 & 0 & 50.9 \end{bmatrix} \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{bmatrix} \quad (\text{in GPa}). \quad (8)$$

When ‘‘orthotropic silicon’’ properties are used, it is essential to know what reference axes are used for the matrix. In general, use of the anisotropic matrix of (3) and the expressions given in Section IX is recommended, as the direction must be stated explicitly, so there is less chance for confusion. Moreover, the generalized shortcut formulas in Section IX are not applicable to the values in an orthotropic matrix.

VIII. ELASTICITY IN FINITE-ELEMENT SIMULATIONS

The detailed calculation of anisotropic elasticity can be tedious, and the problem is well suited to solving by computer. However, it is important to note that many FEM computer programs do not use the anisotropic elasticity formulas by default (this is intended to reduce the computation complexity). Moreover, the ‘‘anisotropic’’ setting typically requires the

user to enter the elastic constants from Table III or the orthotropic values. Note also that the orientation of the simulation workspace may not be the same as the layout of your design. From Section III, the X – Y -axes of a typical (100) wafer (the $\langle 110 \rangle$ directions) are not aligned with the X – Y -axes of the fundamental elasticity matrix (the $\langle 100 \rangle$ directions). In this case, if you enter the values from Table III, the FEM results will reflect a device oriented on the $\langle 100 \rangle$ directions, not the $\langle 110 \rangle$. Either rotate your elasticity matrix, rotate your design in the workspace, or use the appropriate orthotropic elasticity values [in most cases, (8)]. See Section XI for an example.

IX. ELASTICITY IN DESIGN CALCULATIONS

The appropriate values of Young’s modulus and Poisson’s ratio for silicon depend on the crystal orientation of the structure and the type of loads that will be encountered. Seven common cases are described here. The choice of analytical expression that best describes a given mechanical structure is left to the judgment of the designer. See, for example, [25].

A. Uniaxial Tension/Compression

Use the appropriate E value for the direction of tension/compression. E can be calculated from the tensor in (3) or by using the simplified formula for cubic crystals [6]

$$\frac{1}{E_{hkl}} = s_{11} - 2 \left[(s_{11} - s_{12}) - \frac{1}{2} s_{44} \right] (m^2 n^2 + n^2 p^2 + m^2 p^2). \quad (9)$$

The terms m , n , and p are the ‘‘direction cosines’’ the cosine of the angle between the direction of interest $[hkl]$ and the X -, Y -, and Z -axes (the $\langle 100 \rangle$ directions). The most common cases simplify as

$$\begin{aligned}
 \frac{1}{E_{100}} &= s_{11} \\
 \frac{1}{E_{110}} &= s_{11} - \frac{1}{2} \left[(s_{11} - s_{12}) - \frac{1}{2} s_{44} \right] \\
 \frac{1}{E_{111}} &= s_{11} - \frac{2}{3} \left[(s_{11} - s_{12}) - \frac{1}{2} s_{44} \right]. \quad (10)
 \end{aligned}$$

For example, in the surface plane of a (100) silicon wafer, the following values are appropriate.

- 1) For the ‘‘ X - or Y -axis’’ direction (parallel/perpendicular to flat), use $E_{110} = 169$ GPa.
- 2) For the ‘‘off-axis’’ direction (45° diagonal to flat), use $E_{100} = 130$ GPa.

The maximum E value in silicon is 188 GPa, which occurs in the $\langle 111 \rangle$ direction, and the minimum value is 130 GPa, in the $\langle 100 \rangle$ direction.

B. Small Deflection of a Long Thin Beam

The deflection of long thin beams, as approximated by the Euler–Bernoulli equation, is governed by axial tension and compression, so use the E_{hkl} value for the orientation of the neutral axis, as given earlier. Small deflection of a beam is

defined as deflection less than 10% of the length of the beam. For accuracy, a beam should have a length L , along the axis of bending, greater than five times its width w (see [25]–[27] for further discussion of beam-bending approximations). For $L < 5w$, use the plate expressions (below). The thickness of a beam should be small compared to the width.

C. Small Deflection of a Short Wide Beam

Deflections of short wide beams (i.e., a plate or slab where $L < 5w$) are reduced compared to corresponding beams of lesser width because the transverse bending is restricted (see [25] for further explanation). For these structures, use a “plate modulus” E' for the major axis of bending. The plate modulus is

$$E'_{hkl} = \frac{E_{hkl}}{(1 - \nu_{\alpha\beta}^2)} \quad (11)$$

where $\nu_{\alpha\beta}$ is Poisson’s ratio, the ratio of strain between two orthogonal directions α and β . For plate bending, α is the direction of the plate curvature, and β is in the plane of the plate. Poisson’s ratio can be computed for arbitrary directions in a cubic crystal with a relation similar to (9) [17]

$$\nu_{\alpha\beta} = \frac{s_{12} + (s_{11} - s_{12} - \frac{1}{2}s_{44})(m_{\alpha}^2 m_{\beta}^2 + n_{\alpha}^2 n_{\beta}^2 + p_{\alpha}^2 p_{\beta}^2)}{s_{11} - 2(s_{11} - s_{12} - \frac{1}{2}s_{44})(m_{\alpha}^2 n_{\alpha}^2 + n_{\alpha}^2 p_{\alpha}^2 + m_{\alpha}^2 p_{\alpha}^2)} \quad (12)$$

Poisson’s ratio for silicon between the $\langle 110 \rangle$ directions in the (100) plane is 0.064, and it increases to 0.28 for the $\langle 100 \rangle$ directions [see Fig. 3(b)].

D. Stress/Strain Calculations for Symmetric Loading Conditions or Bending Substrate (Including Stoney’s Equation)

Some membranes have symmetric boundary conditions along the equivalent orthogonal axes, such as the curvature of a wafer induced by thin-film stress, which is typically calculated with Stoney’s equation [28], or the deformation of membranes under pressure. Another example is the strain in a square block compressed equally on all sides (see, e.g., [29]). Elastic deformations of these structures can be computed using the symmetric biaxial modulus B_{hkl} for the appropriate symmetric crystal plane, either (100) or (111). The (110) plane is not symmetric and cannot be treated with a single value. The biaxial moduli are given by

$$B_{100} = c_{11} + c_{12} - \frac{2c_{12}^2}{c_{11}} \quad B_{111} = \frac{6c_{44}(c_{11} + 2c_{12})}{c_{11} + 2c_{12} + 4c_{44}} \quad (13)$$

For silicon, $B_{100} = 180$ GPa.

E. Stress Concentrations or Multidirectional Polycrystalline Situations

Use a Voigt or Reuss volume average for stress concentration calculations or estimates for multidirectional polycrystalline

TABLE IV
TEMPERATURE COEFFICIENTS OF THE ELASTIC CONSTANTS. FROM [38]

Elastic Constant Temp. Coeff.	p-type (4 Ω -cm, B)	n-type (0.05 Ω -cm, Ph)
	First order $\times 10^{-6}/^{\circ}\text{C}$	
TS_{11}	64.73 \pm 0.29	63.60 \pm 0.60
TS_{12}	51.48 \pm 1.5	45.79 \pm 2.8
TS_{44}	60.14 \pm 0.20	57.96 \pm 0.17
TC_{11}	-73.25 \pm 0.49	-74.87 \pm 0.99
TC_{12}	-91.59 \pm 1.5	-99.46 \pm 3.5
TC_{44}	-60.14 \pm 0.20	-57.96 \pm 0.17
	Second order $\times 10^{-9}/^{\circ}\text{C}^2$	
TS_{11}	61.19 \pm 1.1	60.51 \pm 0.35
TS_{12}	72.26 \pm 5.1	75.70 \pm 6.1
TS_{44}	54.90 \pm 1.7	57.31 \pm 1.4
TC_{11}	-49.26 \pm 4.8	-45.14 \pm 1.4
TC_{12}	-32.70 \pm 10.1	-20.59 \pm 11.0
TC_{44}	-51.28 \pm 1.9	-53.95 \pm 1.8

structures [30]. The Voigt average modulus E_V (isostrain assumption) and Reuss average modulus E_R (isostress assumption) values will give the upper and lower theoretical bounds on the true value. For a cubic crystal, these values can be calculated as [31]

$$E_V = \frac{(c_{11} - c_{12} + 3c_{44})(c_{11} + 2c_{12})}{2c_{11} + 3c_{12} + c_{44}}$$

$$E_R = \frac{5}{3s_{11} + 2s_{12} + s_{44}} \quad (14)$$

For silicon, $E_V = 166$ GPa and $E_R = 159$ GPa. The E_R value is sometimes presented as an “average” value for silicon (see, e.g., [32]).

For a polysilicon film, i.e., a layer of silicon that has been deposited by chemical vapor deposition or other low-temperature process such that it is composed of distinct grains of silicon, the modulus will be further affected by the prevalence of grain boundaries, impurities, and dislocations. A polysilicon structure will be isotropic unless the growth conditions have created a crystallographic texture. The actual elastic value of such films will vary widely between fabrication facilities and with different deposition conditions (see, e.g., [33]). Sharpe tabulates a large number of experimental measurements of polysilicon films in [18] and concludes that, for polysilicon designs, the values of $E_{\text{poly}} = 160$ GPa and $\nu_{\text{poly}} = 0.22$ are appropriate.

F. Hydrostatic Loads

For calculating volume change due to hydrostatic (uniform pressure) loads, use the Bulk modulus B which, for cubic crystals, is given by [13]

$$B = \frac{c_{11} + 2c_{12}}{3} \quad (15)$$

For silicon, $B = 97.8$ GPa. The symbol for the Bulk modulus B should not be confused with the symbol for biaxial modulus B_{hkl} .

G. Shear Modulus

The shear modulus G (sometimes called “Rigidity modulus”) is a relationship between shear stress and strain in two

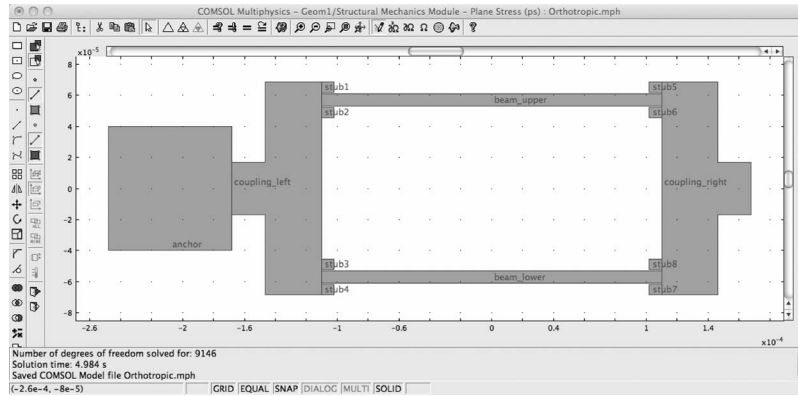


Fig. 4. DETF resonator model drawn in COMSOL. The anchor is the large block at the left, and the tuning fork beams are the two long narrow horizontal rectangles. The X – Y coordinate axes are displayed along the bottom and left edges of the drawing space.

orthogonal directions. This value is often used for estimating twisting under torque or shear loads. In an anisotropic crystal

$$G_{ij} = \frac{1}{s_{ijij}}, \quad \text{for } i \neq j. \quad (16)$$

Expanded expressions for G in a cubic crystal are given in [9], [10], [34], and [35]. The value of G is 79.6 GPa between the [100] direction and any other direction in the (100) plane. G is approximately 50.9 GPa between the $\langle 110 \rangle$ directions in the (100) plane (i.e., twisting a beam that lies in the plane of a wafer).

X. TEMPERATURE EFFECTS ON ELASTICITY OF SILICON

The Young's modulus of silicon changes with temperature; this is called the temperature coefficient of Young's modulus (TCE). As with E , the temperature behavior of elasticity is more properly described by the temperature coefficients of the individual components of the elasticity tensor: Tc_{11} , Ts_{12} , etc. A class m3m crystal such as silicon will experience uniform thermal expansion in all directions [6] (2.6 ppm/K at room temperature [36]) and also a uniform change in elasticity in all directions, at least to first order. Several different measurements of the temperature coefficients of elasticity are reported in the literature, and so, their values cannot be given definitively. Furthermore, there is some indication that the TCE is affected by very high levels of doping [37]. However, the value of silicon TCE for typical axial loading situations is nearly identical in all crystal orientations and equal to approximately -60 ppm/ $^{\circ}\text{C}$ near room temperature. The results given by Bourgeois *et al.* [38] are the most carefully performed experiments that we are aware of, and those values agree with recent experimental results [39]. The results from [38] are reproduced in Table IV. Note that the temperature coefficients are not simple linear quantities. By using the values from [38], the TCE of silicon in uniaxial-load cases is about -64 ppm/ $^{\circ}\text{C}$ at room temperature (25 $^{\circ}\text{C}$) and -75 ppm/ $^{\circ}\text{C}$ at 125 $^{\circ}\text{C}$. Additional references for the silicon temperature coefficient of elasticity are: [12], [13], [40].

XI. DESIGN EXAMPLE

Let us consider a recently published MEMS resonator design as an example of elasticity calculations [41], [42]. The device

is a double-ended tuning fork (DETF) resonator. A DETF consists of two matched fixed-fixed rectangular beams, and the frequency of resonance can be estimated by considering the response of a single beam, using the following expression [43]:

$$f = \frac{\beta^2}{2\pi L^2} \sqrt{\frac{EI}{\rho A}} \quad (17)$$

where L is the beam length, ρ is the density (2330 kg/ m^3 [12]), I is the second moment of inertia of the beam, A is the beam cross-sectional area, and β is the mode constant, equal to 4.73 for the first mode of a fixed-fixed beam. For small deflections of the beam, the elastic behavior is essentially uniaxial loading along the direction of the beam. Let us consider a DETF whose beams have width in the direction of bending of 8 μm , height of 20 μm , and length L of 220 μm . If the layout of the device is oriented along the x -axis of the wafer (a $\langle 110 \rangle$ direction), then from Section IX, we should use $E = 169$ GPa, and the predicted resonance frequency from (17) is $f = 1.45$ MHz. However, fabricated silicon resonators with these dimensions exhibit measured resonance frequencies of approximately 1.3 MHz.

We can use FEM simulations to investigate further. For this example, we will use the COMSOL FEM software [44] and solve for the eigenfrequencies of the structure in order to predict its first symmetric mode resonance frequency. The 2-D geometry of the device is drawn in COMSOL, as shown in Fig. 4. Note that the resonator beams are aligned with the x -axis of the drawing space, as it seems natural. Now, we specify the material properties of the structure (Fig. 5). We have three choices for linear materials: isotropic, orthotropic, and anisotropic. If we choose isotropic, we are asked to supply single values for E , ν , α , etc. No matter what values we choose, the predicted resonance is lower than what (17) suggests, because the compliance of the coupling bars is taken into account.

To increase the prediction accuracy further, we can use an anisotropic elasticity model for the structural material. In COMSOL, select "Anisotropic material," and enter the values from Table III. The simulation now predicts a suspiciously low frequency of 1.18 MHz. This is because the X – Y drawing plane is, by default, oriented to the $\langle 100 \rangle$ directions, and the simulation is now predicting the frequency of a device with the beams oriented along the silicon [100] direction, where the

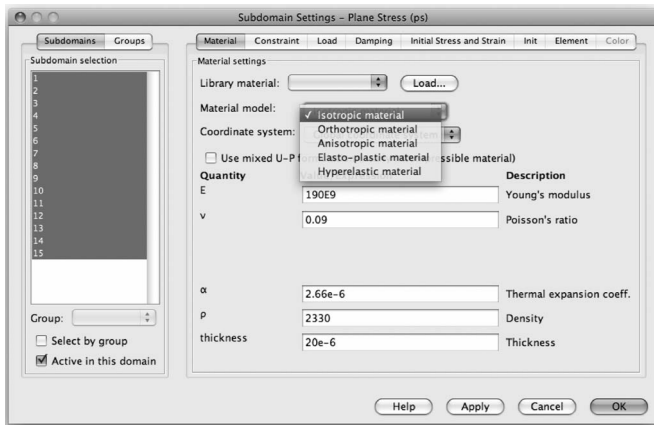


Fig. 5. Dialog box for specifying material properties in COMSOL. The choices for the type of linear material model are isotropic, orthotropic, and anisotropic.

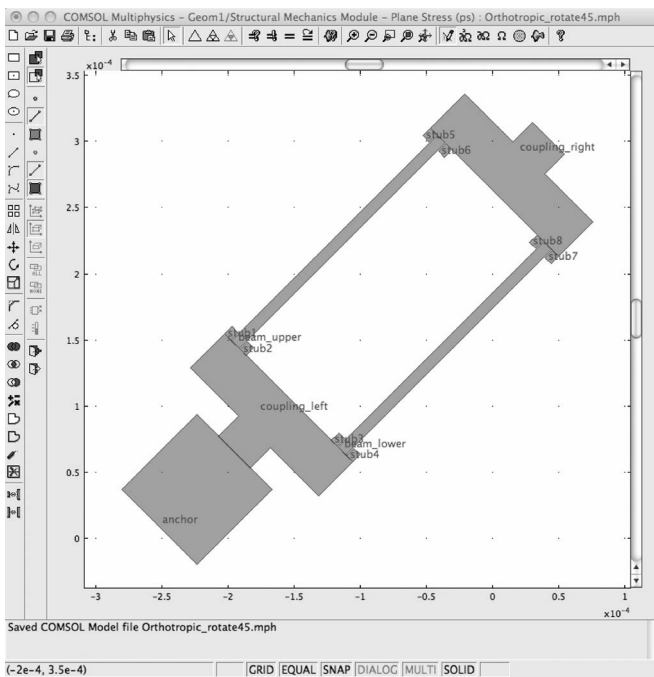


Fig. 6. DETF resonator model drawn in COMSOL, rotated 45° . The structure shown in Fig. 4 was simply rotated 45° counterclockwise.

effective modulus is 23% lower (130 GPa). If we rotate the drawing in the COMSOL drawing layout by 45° (Fig. 6), the simulation predicts a resonance frequency of 1.32 MHz. Similar results are obtained using an orthotropic elasticity description: using values for the $\langle 100 \rangle$ orientation [i.e., [100], [010], [001]; see (7)]; again, the predicted frequency reflects a device oriented to the [100] direction. Rotating the drawing or using orthotropic values for the standard wafer orientation [see (8)] corrects the situation.

In conjunction with the work described in [41] and [42], MEMS DETF resonators were fabricated on (100) silicon wafers at both 0° and 45° orientations with respect to the $\langle 110 \rangle$ directions. The results of the predictions and measurements are summarized in Table V. The predicted resonance frequencies vary by almost 30%, and the correct use of anisotropic elas-

TABLE V
PREDICTED DETF RESONANCE FREQUENCY (MHz)

Resonance Frequency Prediction Method	Design orientation with respect to x-axis	
	0°	45°
Expression (17), $E = 190$ (value from [4])	1.53	
Expression (17), $E = 169$ ($\langle 110 \rangle$ value)	1.45	
Expression (17), $E = 160$ ("average" value)	1.41	
Expression (17), $E = 130$ (min. value)	1.27	
FEM, Isotropic, $E = 190$, $\nu = 0.09$	1.41	1.41
FEM, Isotropic, $E = 169$, $\nu = 0.064$	1.33	1.33
FEM, Anisotropic, from (3) and Table 3	1.18	1.32
FEM, Orthotropic, "standard" values (7)	1.18	1.32
FEM, Orthotropic, "wafer" values (8)	1.33	1.18
Measurements (room temperature)	1.31	1.15

Note: Measured resonance frequencies are expected to be lower than the eigenmode solutions due to the electrostatic measurement methods and reduction in beam width due to the silicon etch process.

ticity values with FEM simulations provides the most accurate prediction of the measured results.

The FEM simulation significantly refines the prediction of the resonance frequency, but only when attention is paid to the orientation of the device with respect to the anisotropic material. In this example, the difference between isotropic and anisotropic FEM results is small because the structure is composed of rectangles aligned with the orthogonal axes. In cases where a structure is constructed with curves or angled members, the difference will be significant. Since the savings in computation time are typically negligible for a modern computer, it is strongly recommended to use the anisotropic elasticity descriptions for silicon in FEM work.

XII. SUMMARY

The appropriate elastic modulus values for silicon for the most common load cases in MEMS are summarized in Table VI.

For polysilicon structures, the "average" values of $E = 160$ GPa, $\nu = 0.22$, and $G = 65$ GPa [18], [45] are appropriate, although it should be noted that the actual material properties of polysilicon depend strongly on the deposition conditions.

XIII. CONCLUSION

The anisotropic values of Young's modulus, Poisson's ratio, and other elasticity quantities for the design and analysis of silicon structures have been fully described. For design calculations and analytic expressions where a single isotropic elasticity value is called for, the choice depends on the orientation and loading of the structure. The crystal structure of silicon has cubic symmetry, so calculations for devices with orthogonal shapes and loads will be reasonably accurate, as long as the appropriate elasticity value for the direction family is used. We can estimate the effect of using the correct elasticity values by taking the derivative of an expression with respect to Young's modulus, and for most design calculations, the relative change in the quantity of interest is equal to or less than the relative change in Young's modulus. This difference may be a little as 5% (using 160 GPa instead of 169 GPa) or as much as 46% (using 190 GPa instead of 130 GPa). For finite-element

TABLE VI
ELASTIC MODULUS VALUES FOR SILICON

Load Case	Symbol	Appropriate Value for Silicon
Axial or narrow beam bending loads <110> directions ("X" or "Y" axis) <100> directions ("45° off-axis")	E	169 GPa 130 GPa
Plate bending, $\nu = 0.064$ for <110> in (100)	E'_{110}	170 GPa
Thin film biaxial stress/strain, (100) plane	B_{100}	180 GPa
Shear load, twisting a <110> ("X" or "Y") beam	G	50.9 GPa
Stress concentrations	E_V	166 GPa
Hydrostatic loads	B	97.8 GPa
Temperature Coefficient of E	TCE	~ -60 ppm/°C
Orthotropic material model properties for a standard (100) silicon wafer	$E_x = E_y = 169$ GPa, $E_z = 130$ GPa $\nu_{yz} = 0.36$, $\nu_{zx} = 0.28$, $\nu_{xy} = 0.064$ $G_{xy} = G_{zx} = 79.6$ GPa, $G_{xy} = 50.9$ GPa	

calculations, the use of the full anisotropic description of elasticity can have significant benefits for the accuracy of the results, particularly for more complex designs with off-axis orientations or nonrectilinear structures, and there is no reason not to use the complete elastic matrix when doing computer calculations. Moreover, the use of the correct values is quite accessible to nonspecialists.

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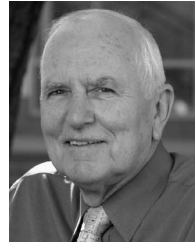
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