CODING ANISOTROPIC ELASTIC PROPERTIES OF SILICON

CENTRE FOR NANO SCIENCE AND ENGINEERING (CENSE)

INDIAN INSTITUTE OF SCIENCE

Guided by - G.K. Ananthasuresh

Chittipolu Santhosh Kumar
M.Tech – 05-16-00-10-51-14-1-11290
CeNSE

Aim

- To code anisotropic elastic properties of silicon and polysilicon
- Software : MAT-LAB

Contents

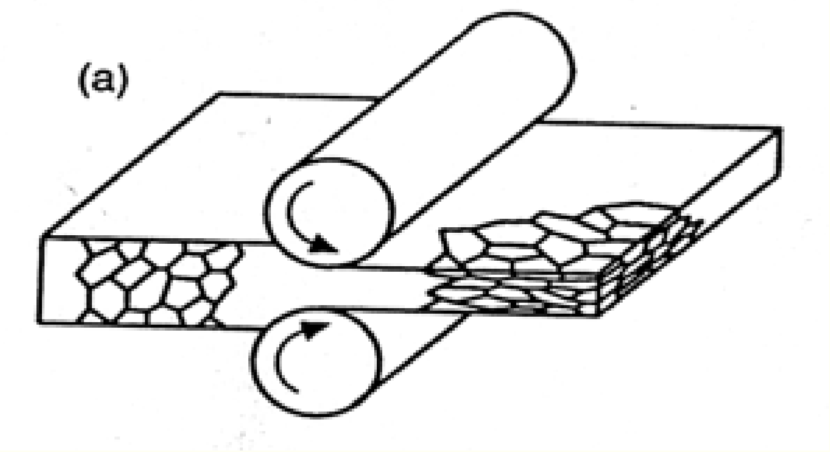
What is Anisotropy?

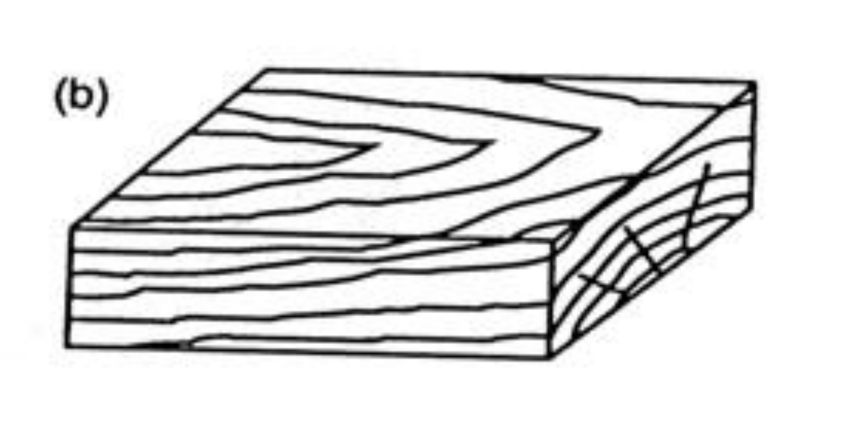
- Anisotropy is the property of being directionally dependent, as opposed to isotropy, which implies identical properties in all directions
- Example wood is the best anisotropic material
- Properties like wood's strength and hardness is different for the same sample measured in different orientations

Image courtesy Wikipedia

What is an Orthotropic material?

- An orthotropic material has three mutually orthogonal twofold axes of rotational symmetry so that its material properties are, in general, different along each axis
- Orthotropic materials are a subset of anisotropic materials; their properties depend on the direction in which they are measured
- Orthotropic materials have three planes/axes of symmetry that means if we choose an orthonormal coordinate system such that the axes coincide with the normals to the three symmetry planes
- An isotropic material, in contrast, has the same properties in every direction
- Examples a) rolled material b) wood



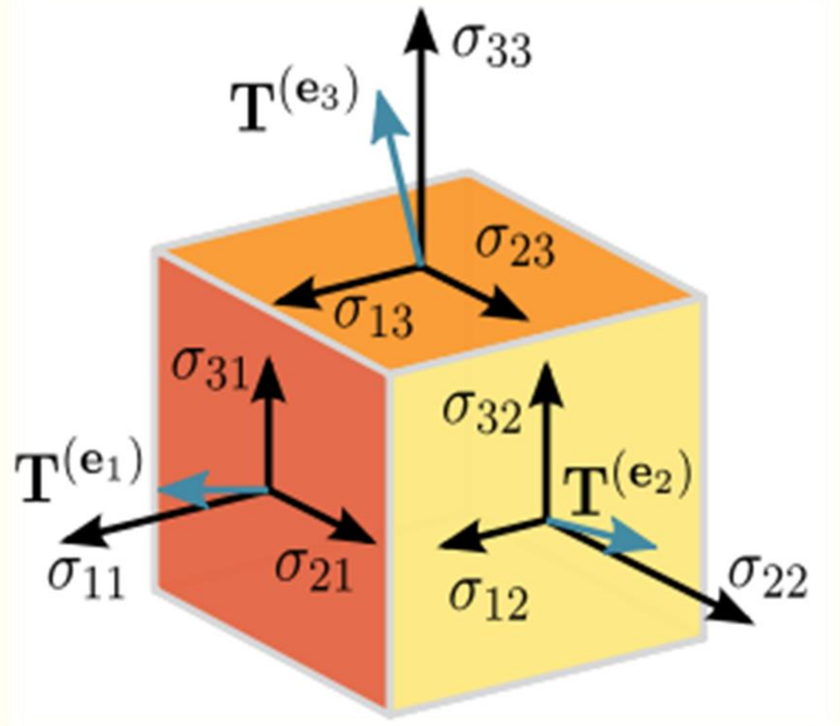


What is a Tensor?

- A tensor can be represented as a multi-dimensional array of numerical values
- The order (also degree) of a tensor is the dimensionality of the array needed to represent it, or equivalently, the number of indices needed to label a component of that array
- Examples are stress and strain. These are 2nd rank tensor and has nine components

$$\sigma_{ij} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix}$$

- The first subscript keeps track of the plane the component acts on (described by its unit normal vector), while the second subscript keeps track of the direction



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Hooke's law for generalized case

- For the generalized case, Hooke's law may be expressed as

$$\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl} \qquad \text{or} \qquad \varepsilon_{ij} = S_{ijkl}\,\sigma_{kl}$$

- Where

  C ⟶ Stiffness (or Elastic constant)
  S ⟶ Compliance

- Both Sijkl and Cijkl are fourth-rank tensor quantities
- Expansion of will produce nine (9) equations, each with nine (9) terms, leading to 81 constants in all
- It is important to note that both σ_{ij} and ε_{ij} are symmetric tensors
- Symmetric tensor Means that the off-diagonal components are equal

$$\sigma_{13} = \sigma_{31}, \; \sigma_{12} = \sigma_{21} \qquad \sigma_{23} = \sigma_{32}$$

- Hence
- Stress tensor

$$\begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix} \equiv \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_{22} & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_{33} \end{pmatrix}$$

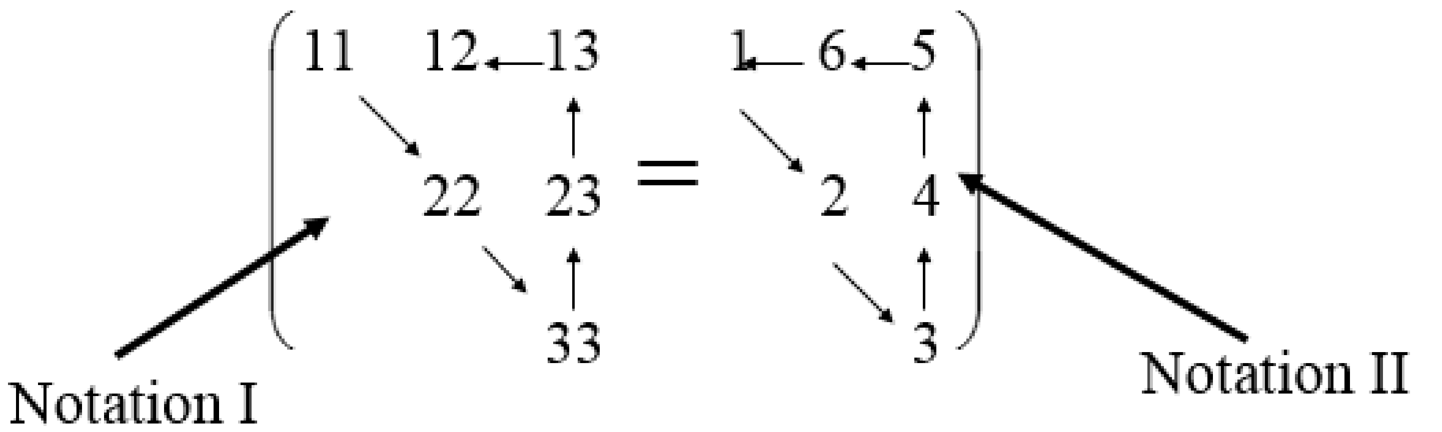
Strain tensor

$$\begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix} \equiv \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{13} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix}$$

- The direct consequence of the symmetry in the stress and strain tensors is that only 36 components of the compliance tensor are independent and distinct terms
- Similarly, only 36 components of the stiffness tensor are independent and distinct terms

- We can replace the indices as follows to put it into matrix form (reference from [John_F_Nye]_Physical_properties_of_crystals)

$$11 \rightarrow 1 \qquad 23 \rightarrow 4$$
$$22 \rightarrow 2 \qquad 13 \rightarrow 5$$
$$33 \rightarrow 3 \qquad 12 \rightarrow 6$$



- Now stress and strain in general form

$$\begin{pmatrix} \sigma_1 & \sigma_6 & \sigma_5 \\ \sigma_6 & \sigma_2 & \sigma_4 \\ \sigma_5 & \sigma_4 & \sigma_3 \end{pmatrix} \; and \; \begin{pmatrix} \varepsilon_1 & \frac{\varepsilon_6}{2} & \frac{\varepsilon_5}{2} \\ \frac{\varepsilon_6}{2} & \varepsilon_2 & \frac{\varepsilon_4}{2} \\ \frac{\varepsilon_5}{2} & \frac{\varepsilon_4}{2} & \varepsilon_3 \end{pmatrix}$$

$$\varepsilon_1 = \varepsilon_{11}, \varepsilon_2 = \varepsilon_{22}$$

$$\varepsilon_3 = \varepsilon_{33}$$

$$\varepsilon_4 = 2\varepsilon_{23} = \gamma_{23}$$

$$\varepsilon_5 = 2\varepsilon_{13} = \gamma_{13}$$

$$\varepsilon_6 = 2\varepsilon_{12} = \gamma_{12}$$

- In matrix format, the stress-strain relation showing the 36 (6 x 6) independent components of stiffness can be represented as

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

- Also denoted as $\sigma_i = C_{ij}\varepsilon_j \ \ and \ \ \varepsilon_i = S_{ij}\sigma_j$

- Symmetry in Stiffness and Compliance matrices requires that

$$C_{ij} = C_{ji} \quad and \quad S_{ij} = S_{ji}$$

- Of the 36 constants, there are six constants where i = j, leaving 30 constants where $i \neq j$
- But only one-half of these are independent constants since Cij = Cji
- Therefore, for the general anisotropic linear elastic solid there are $\frac{30}{2} + 6 = 21$ independent constants
- For cubic there are only three independent elastic constants due to rotation symmetry

Elastic properties of Silicon -> Cubic

- So silicon is a cubic orthotropic(means anisotropic) material

$$
Cij = \begin{bmatrix} 11 & 12 & 12 & 0 & 0 & 0 \\ . & 11 & 12 & 0 & 0 & 0 \\ & . & 11 & 0 & 0 & 0 \\ & . & . & 44 & 0 & 0 \\ & . & . & . & 44 & 0 \\ & . & . & . & . & 44 \end{bmatrix}
$$

- For isotropic materials it reduces to two i.e $C_{44} = \frac{C_{11} - C_{12}}{2}$

Why these properties are important?

- In the field of microelectromechanical systems (MEMS) mono crystalline silicon is the most widely used in MEMS fabrication, both as substrate for compatibility with semiconductor processing equipment and as a structural material for MEMS device
- 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 Y for silicon range from 130 to 188 GPa and the choice of Y value can have a significant influence on the result of a design analysis

Elastic constants for arbitrary coordinate system as function of Direction Cosines

- for xi'=lix1+mix2+nix3 where xi' is the transformed coordinates
- where li, mi, ni i = 1,2,3 are direction cosines
- Here one is normal to cut plane and other two are orthogonal to these two and in the plane .
- Let u be vector - direction ratios along normal and v,w are vectors in the plane perpendicular to each other
- Hence equations to solve are u.v=0 u.w=0 v.w=0 and v x w should be parallel to u and find direction cosines for the obtained direction ratios
- Apply those direction cosines in the following equaation to find new constants in the transformed coordinates
- c11' = c11 +Cc*(l^4+ m^4+n^4 - 1)
- c12' = c12+Cc*(l1^2*l2^2+m1^2*m2^2+n1^2*n2^2)
- c44' = c44+Cc*(l2^2*l3^2+m2^2*m3^2+n2^2*n3^2)
- Cc = c11 -c12 -2*c44

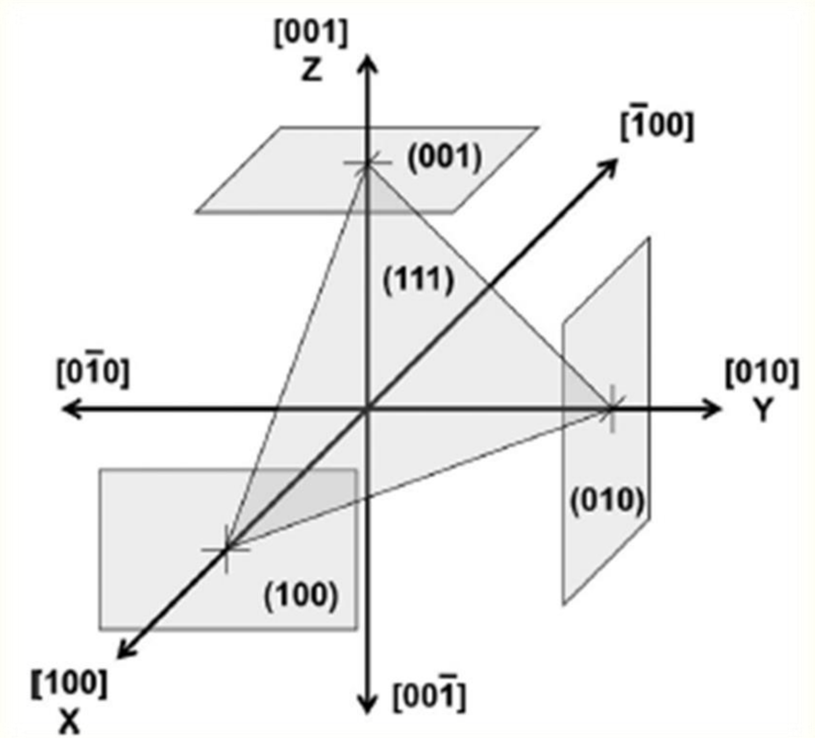


Image courtesy reference paper : What is the Young's Modulus of Silicon? Matthew A. Hopcroft, Member, IEEE, William D. Nix, and Thomas W. Kenny

Elastic constants

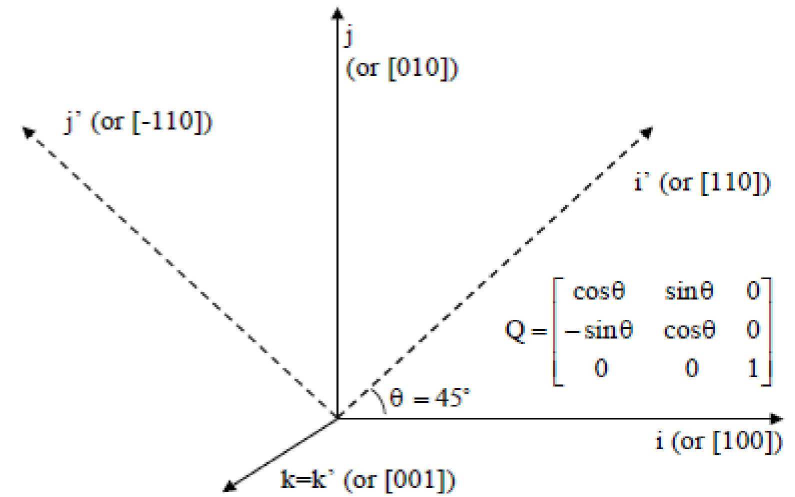
- Now we have C' matrix . Take inverse of this C' gives S' matrix.
- Hence young's modulus is given as Y = $1/S'_{ii}$ where i=1,2 & 3 (one along normal direction which is considered as young's modulus and remaining are orthogonal directions as discussed for orthotropic material)
- Shear modulus G = $1/S'_{jj}$ where j = 4,5 & 6 (again orthotropic directions and one along normal)
- Poisson's ratio = $-S'_{ij}/S'_{ii}$ where Ii$\neq$ j

How to find these constants for polysilicon?

- Polysilicon is a material with texture or grain boundaries each may orient in any direction
- We have to check all the possibilities of random orientations and calculate angular average of those constants
- That means we are finding effective constants

$$C'_{ijkl} = \sum_{p=1}^{3}\sum_{q=1}^{3}\sum_{r=1}^{3}\sum_{s=1}^{3} Q_{pi}Q_{qj}Q_{rk}Q_{sl}C_{pqrs}$$

- Here θ varies from $-\pi$ to $+\pi$ and take avg of C'_{ijkl}
- Then constants are obtained using previous formulas



Axis rotation using rotation matrix **Q**. *The new axes is obtained with* $\mathbf{x}' = \mathbf{Q}\mathbf{x}$

Image courtesy : Ville Kaajakari

Single crystal silicon elastic constants for different planes

NE211 Mini Project

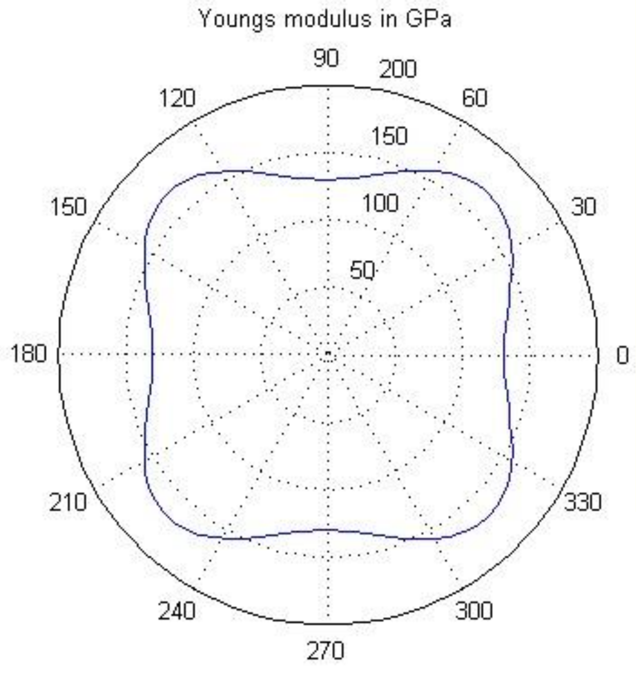
Chittipolu Santhosh Kumar M.Tech Sr-no: 11290

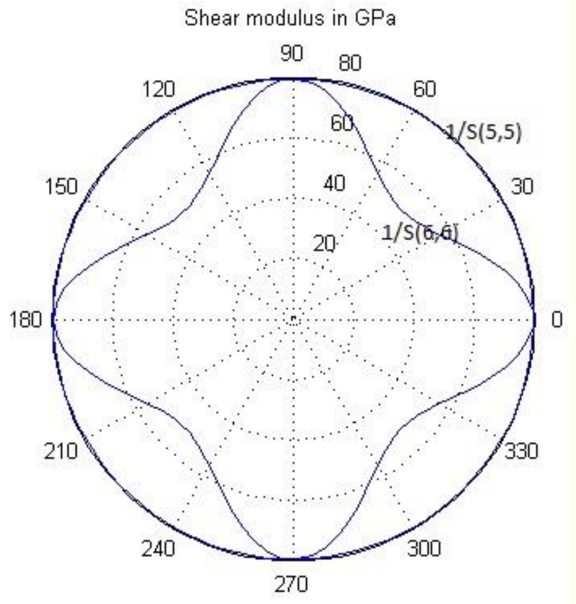
Results Tabulated : Anisotropy Elastic constans in different directions for Silicon

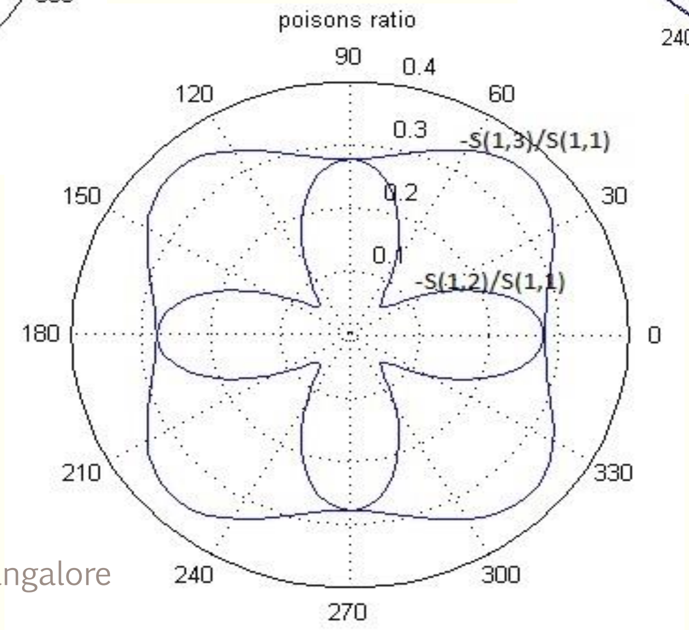
Planes	Youngs's Modulus in Gpa			Shear Modulus in Gpa			Poisson's Ratio		
100	130.132	130.132	130.132	79.6	79.6	79.6	-1	0.2783	0.2783
							0.2783	-1	0.2783
							0.2783	0.2783	-1
010	130.132	130.132	130.132	79.6	79.6	79.6	-1	0.2783	0.2783
							0.2783	-1	0.2783
							0.2783	0.2783	-1
001	130.132	169.101	169.1012	50.9	79.6	79.6	-1	0.2783	0.2783
							0.3617	-1	0.0622
							0.3617	0.0622	-1
110	169.101	130.132	169.1012	79.6	50.9	79.6	-1	0.3617	0.0622
							0.2783	-1	0.2783
							0.0622	0.3617	-1
101	169.101	187.853	169.1012	57.853	67.0062	57.853	-1	0.162	0.2618
							0.18	-1	0.18
							0.2618	0.162	-1
011	169.101	187.853	169.1012	57.853	67.0062	57.853	-1	0.162	0.2618
							0.18	-1	0.18
							0.2618	0.162	-1
111	187.853	169.101	169.1012	67.0062	57.853	57.853	-1	0.18	0.18
							0.162	-1	0.2618
							0.162	0.2618	-1
21 21 20	187.767	166.902	169.1012	67.6912	57.3519	58.396	-1	0.1874	0.1728
							0.1666	-1	0.2647
							0.1556	0.2682	-1

Polysilicon results

- Youngs modulus of polysilicon in GPa is
- 151.2643   151.2643   130.0018
- Shear modulus of polysilicon in GPa is
- 79.5204   79.5204   65.1848
- Poissons Ratio of polysilicon is
- -1.0000 0.1603 0.3238
- 0.1603 -1.0000 0.3238
- 0.2783 0.2783 -1.0000







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Thank you