

Stress, Strain, Piezoresistivity, and Piezoelectricity

2.1 STRAIN TENSOR

Strain in crystals is created by deformation and is defined as relative lattice displacement. For simplicity, we use a 2D lattice model in Fig. 2.1 to illustrate this concept, but discuss the general concept in 3D cases. As shown in Fig. 2.1a, we may use two unit vectors \hat{x} , \hat{y} to represent the unstrained lattice, and in a simple square lattice, they correspond to the lattice basis vectors. Under a small uniform deformation of the lattice, the two vectors are distorted in both orientation and length, which is shown in Fig. 2.1b. The new vectors \hat{x}' and \hat{y}' may be written in terms of the old vectors:

$$\hat{x}' = (1 + \varepsilon_{xx})\hat{x} + \varepsilon_{xy}\hat{y} + \varepsilon_{xz}\hat{z}, \quad (2.1)$$

$$\hat{y}' = \varepsilon_{yx}\hat{x} + (1 + \varepsilon_{yy})\hat{y} + \varepsilon_{yz}\hat{z}, \quad (2.2)$$

and in the 3D case, we also have

$$\hat{z}' = \varepsilon_{zx}\hat{x} + \varepsilon_{zy}\hat{y} + (1 + \varepsilon_{zz})\hat{z}. \quad (2.3)$$

The strain coefficients $\varepsilon_{\alpha\beta}$ define the deformation of the lattice and are dimensionless. The 3×3 matrix

$$\bar{\bar{\varepsilon}} = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} \quad (2.4)$$

is called the strain tensor. A tensor is a mathematical notation, usually represented by an array, to describe a linear relation between two physical quantities. A tensor can be a scalar, a vector, or a matrix. A scalar is a zero-rank tensor, a vector is a first-rank tensor, and a matrix is a second-rank tensor, and so on. The strain tensor is a second-rank tensor, which in this book is labeled with two bars over the head. However, in places without confusion, we usually neglect the bars. Suppose a lattice point is originally located

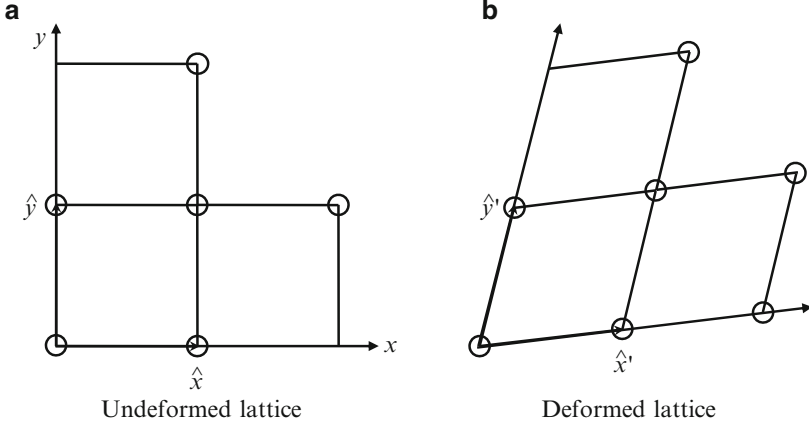


Fig. 2.1. Diagram for (a) an undeformed lattice and (b) a deformed lattice

at $\mathbf{r} = x\hat{x} + y\hat{y} + z\hat{z}$, then with a uniform deformation this point will be at $\mathbf{r}' = x'\hat{x}' + y'\hat{y}' + z'\hat{z}'$. For a general varying strain, the strain tensor may be written as

$$\varepsilon_{\alpha,\beta} = \frac{\partial u_\alpha}{\partial x_\beta}, \quad u_\alpha = u_x, u_y, u_z, \quad x_\beta = x, y, z, \quad (2.5)$$

where u_α is the displacement of lattice point under study along x_α . A strain tensor (2.4) is symmetric, i.e.,

$$\varepsilon_{\alpha\beta} = \varepsilon_{\beta\alpha} = \frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right). \quad (2.6)$$

The antisymmetric part of tensor (2.4) represents a rotation of the entire body.

Usually people work with the other set of strain components, which are defined as

$$e_{xx} = \varepsilon_{xx}; \quad e_{yy} = \varepsilon_{yy}; \quad e_{zz} = \varepsilon_{zz}, \quad (2.7)$$

which describe infinitesimal distortions associated with a change in volume, and the other strain components e_{xy} , e_{yz} , and e_{zx} are defined in terms of changes of angle between the basis vectors. Neglecting the terms of order ε^2 in the small strain approximation, they are

$$\begin{aligned} e_{xy} &= \hat{\mathbf{x}}' \cdot \hat{\mathbf{y}}' = \varepsilon_{xy} + \varepsilon_{yx}, \\ e_{yz} &= \hat{\mathbf{y}}' \cdot \hat{\mathbf{z}}' = \varepsilon_{yz} + \varepsilon_{zy}, \\ e_{zx} &= \hat{\mathbf{z}}' \cdot \hat{\mathbf{x}}' = \varepsilon_{zx} + \varepsilon_{xz}. \end{aligned} \quad (2.8)$$

These six coefficients completely define the strain. We can write these six strain coefficients in the form of an array as $\mathbf{e} = \{e_{xx}, e_{yy}, e_{zz}, e_{yz}, e_{zx}, e_{xy}\}$. The introduction of this set of notation for the strain components is merely for the convenience of describing the relations between strain and the other strain-related physical quantities. The relation between two second-rank tensors

must be described by a fourth-rank tensor, which is very complicated; while after transforming the second-rank tensors to first-rank, only a second-rank tensor is required.

The crystal dilation under deformation can be evaluated through calculating the volume defined by $\hat{\mathbf{x}}'$, $\hat{\mathbf{y}}'$, and $\hat{\mathbf{z}}'$,

$$V' = \hat{\mathbf{x}}' \cdot \hat{\mathbf{y}}' \times \hat{\mathbf{z}}' = 1 + e_{xx} + e_{yy} + e_{zz}, \quad (2.9)$$

and the dilation δ then is given by

$$\delta = \frac{\delta V}{V} = e_{xx} + e_{yy} + e_{zz}, \quad (2.10)$$

which is the trace of the strain tensor. The dilation is negative for hydrostatic pressure.

2.2 STRESS TENSOR

Crystal deformations can be induced by externally applied forces, or in other words, a solid resists deformations, thus deformations will generate forces. Stress is defined as the force in response to strain in a unit area. Stress has nine components and is a second-rank tensor, which we write as $\tau_{\alpha\beta}$, $\alpha, \beta = x, y, z$. On the surface of an infinitesimal volume cube, the stress distribution is illustrated in Fig. 2.2, where τ_{xx} represents a force applied in the x direction to a unit area of the plane whose outward-drawn normal lies in the x direction, and τ_{xy} represents a force applied in the x direction to a unit area of the

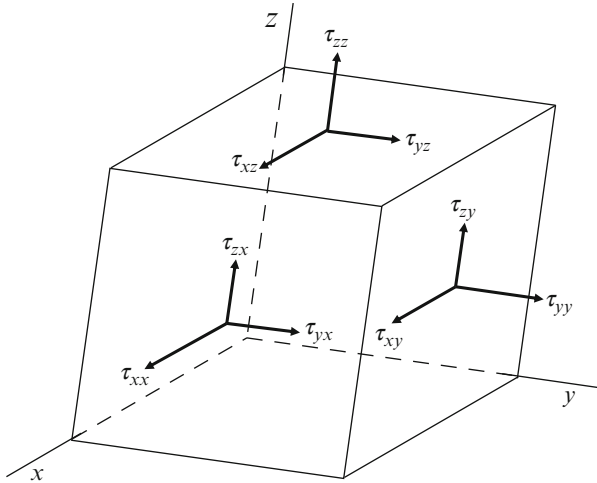


Fig. 2.2. Illustration for stress components on the surfaces of an infinitesimal cube

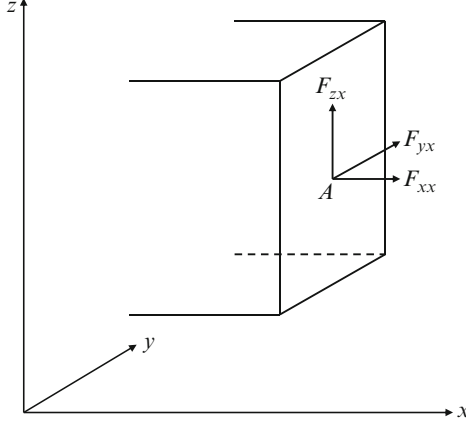


Fig. 2.3. Illustration of the forces applied on one surface with area of A of the cube shown in Fig. 2.2

plane whose outward-drawn normal lies in the y direction. The stress tensor is symmetric just as the strain tensor. The antisymmetric part of the stress tensor represents a torque, and in a state of equilibrium, all torques must vanish inside a solid.

The stress and force relation is better illustrated in Fig. 2.3 where we show a force applied on an infinitesimal plane whose normal is along x and has an area A . In such a case, we resolve the force into components along the coordinate axes, i.e., F_{xx} , F_{yx} , and F_{zx} . The stress components in this plane are

$$\tau_{xx} = \frac{F_{xx}}{A}, \tau_{yx} = \frac{F_{yx}}{A}, \tau_{zx} = \frac{F_{zx}}{A}. \quad (2.11)$$

We now study some simple stress cases to determine the stress tensors.

1. Hydrostatic pressure:

Under a hydrostatic pressure P , all shear stress is zero. Stress along any principle direction is $-P$, namely,

$$\tau = \begin{pmatrix} -P & 0 & 0 \\ 0 & -P & 0 \\ 0 & 0 & -P \end{pmatrix}. \quad (2.12)$$

Here the sign convention is that tensile stress is positive and compressive stress is negative.

2. Uniaxial stress T along the $[001]$ direction:

For a uniaxial stress T along the $[001]$ direction, all stress components but τ_{zz} are zero, and $\tau_{zz} = T$. So

$$\tau = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & T \end{pmatrix}. \quad (2.13)$$

3. Uniaxial stress T along the $[110]$ direction:

The case for a uniaxial stress along the $[110]$ direction is a little more complicated. Generally when we talk about a stress T along the $\langle 110 \rangle$ direction, it refers to the force exerted along the $\langle 110 \rangle$ direction divided by the cross section of the (110) surface, but not necessarily equal to any of the stress tensor elements. To find the stress elements, we can use two methods. First is to resolve the force into three coordinate axes. For $[110]$ uniaxial stress T as shown in Fig. 2.4a, the force along the $[110]$ direction is $F = Ta^2$. Its component along $[001]$ is zero. Along both x and y direction, the force is $F/\sqrt{2}$. However, the cross area for the force along $[110]$ shown in Fig. 2.4a is a^2 and is $\sqrt{2}a^2$ for the forces along the x and y direction. Thus, the stress along both x and y is $F/2a^2 = T/2$. The shear stress on both $[100]$ and $[010]$ planes is also $T/2$. The second method to obtain the stress components is through the coordinate transformation method. Suppose in an unprimed coordinate system, stress T is along the x direction, and thus $\tau_{xx} = T$, and all the other stress components are zero. We can rotate the x and y axes 45° clockwise, and then an original $[100]$ uniaxial stress that only has one nonvanishing component $\tau_{xx} = T$ now corresponds to a $[110]$ uniaxial stress in a primed coordinate system, as shown in Fig. 2.4b. The stress elements in the primed coordinate system are given by the transformation,

$$\tau'_{ij} = \sum_{mn} \tau_{mn} \frac{\partial x'_i}{\partial x_m} \frac{\partial x'_j}{\partial x_n}, \quad (2.14)$$

where $\frac{\partial x'_i}{\partial x_m}$, etc. represent the directional cosines of the transformed axes made to the original axes. This equation results from the general tensor transformation of S to S' under an orthogonal coordinate transformation A ,

$$S' = ASA^T, \quad (2.15)$$

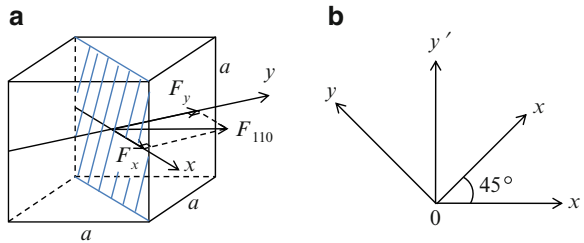


Fig. 2.4. (a) The decomposition of a force along the $[110]$ direction along the x and y directions, and their stress relations. Please note that in this figure, the x and y directions are along the diagonals of the surfaces instead of along the edges. (b) The coordinate systems before and after a 45° rotation clockwise. The unprimed and primed systems are the coordinate systems before and after the rotation

where A^T is the transpose of matrix A . The stress tensor under the [110] uniaxial stress found using both methods is

$$\tau = \frac{T}{2} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (2.16)$$

Because a stress tensor is symmetric, similar to the strain tensor case, the six coefficients, τ_{xx} , τ_{yy} , τ_{zz} , τ_{yz} , τ_{zx} , and τ_{xy} completely define the stress. Similar to a strain tensor, a second-rank stress tensor can be reduced to a 1D array form.

2.3 ELASTIC COMPLIANCE AND STIFFNESS CONSTANTS

In the linear elastic theory, Hooke's law is justified and stress is proportional to strain

$$\tau_{ij} = \sum_{\alpha\beta} C_{ij\alpha\beta} e_{\alpha\beta}, \quad i, j, \alpha, \beta = x, y, z, \quad (2.17)$$

where the coefficients $C_{ij\alpha\beta}$ are called elastic stiffness constants. Elastic stiffness constants are a fourth-rank tensor. Because of the symmetry of both the strain tensor and the stress tensor, we have

$$C_{ij\alpha\beta} = C_{ji\alpha\beta} = C_{ij\beta\alpha}, \quad (2.18)$$

so we may write both strain and stress tensor as a six-component array as

$$\mathbf{e} = (e_{xx}, e_{yy}, e_{zz}, e_{yz}, e_{zx}, e_{xy}) \quad (2.19)$$

and

$$\boldsymbol{\tau} = (\tau_{xx}, \tau_{yy}, \tau_{zz}, \tau_{yz}, \tau_{zx}, \tau_{xy}) \quad (2.20)$$

and reduce the elastic stiffness tensor to a 6×6 matrix

$$\tau_i = \sum_m C_{im} e_m. \quad (2.21)$$

This 6×6 matrix has a very simple form in cubic crystals due to the high symmetry. It has only three independent components and has the form

$$C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}. \quad (2.22)$$

This is easy to understand by inspecting (2.21) and considering the transformation of this equation under symmetry operations. First, the elastic stiffness tensor must be symmetric. Second, since for cubic crystals, the three axes are equivalent, therefore we must have $C_{11} = C_{22} = C_{33}$, and $C_{44} = C_{55} = C_{66}$. Third, a shear strain cannot cause a normal stress, so terms like $C_{14} = 0$. And a shear strain along one axis cannot induce forces causing a shear along another axis, so terms like $C_{45} = 0$. Finally in the view of a force along one axis, the other two axes are equivalent, and thus we have $C_{12} = C_{13}$, etc. These results can also be obtained by investigating the transformation of the components in (2.17) under symmetry operations using an equation similar to (2.14)

$$C'_{lk\gamma\delta} = \sum_{ij\alpha\beta} C_{ij\alpha\beta} \frac{\partial x'_l}{\partial x_i} \frac{\partial x'_k}{\partial x_j} \frac{\partial x'_\gamma}{\partial x_\alpha} \frac{\partial x'_\delta}{\partial x_\beta}. \quad (2.23)$$

For example, it is easy to verify that under a reflection and thus $x \rightarrow -x$, $C_{xyzz} = -C_{xyzz}$, so in the 6×6 matrix, $C_{63} = 0$.

In many cases it is convenient to work with the inverse of the elastic stiffness tensor, which is defined through the relation between strain and stress

$$\varepsilon_{\alpha\beta} = \sum_{ij} S_{\alpha\beta ij} \tau_{ij}. \quad (2.24)$$

The fourth-rank tensor $S_{\alpha\beta ij}$, called the compliance tensor, can also be reduced into a 6×6 matrix. Under cubic symmetry, it has the same form as the stiffness tensor

$$\begin{pmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{pmatrix}, \quad (2.25)$$

and the strain–stress relation can be written as

$$e_m = \sum_i S_{mi} \tau_i. \quad (2.26)$$

Because the elastic stiffness tensor and compliance tensor are inverse to each other, so it is easy to work out the relations between the components as

$$\begin{aligned} S_{11} &= \frac{C_{11} + C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}, \\ S_{12} &= \frac{-C_{12}}{(C_{11} - C_{12})(C_{11} + 2C_{12})}, \\ S_{44} &= \frac{1}{C_{44}}. \end{aligned} \quad (2.27)$$

In mechanical engineering, Young's modulus Y and Poisson ration ν are commonly used. For a homogeneous, isotropic material, strain is related to stress through

$$\begin{aligned}\varepsilon_{xx} &= \frac{1}{Y}(\tau_{xx} - \nu(\tau_{yy} + \tau_{zz})), \\ \varepsilon_{yy} &= \frac{1}{Y}(\tau_{yy} - \nu(\tau_{zz} + \tau_{xx})), \\ \varepsilon_{zz} &= \frac{1}{Y}(\tau_{zz} - \nu(\tau_{xx} + \tau_{yy})).\end{aligned}\quad (2.28)$$

In cubic systems Young's modulus and Poisson ration ν are related to the compliance constants by

$$Y = \frac{1}{S_{11}}, \quad \nu = -\frac{S_{12}}{S_{11}}. \quad (2.29)$$

2.4 EXAMPLES OF STRESS-STRAIN RELATIONS

Now we use two examples to illustrate how to determine the strain tensor from stress using the relations we have discussed earlier.

1. Biaxial stress:

A semiconductor layer pseudomorphically grown on a (001)-oriented lattice-mismatched substrate is schematically shown in Fig. 2.5. In this case, the top layer is biaxially strained, and the strain components e_{xx} and e_{yy} are

$$e_{xx} = e_{yy} = \frac{a_0 - a}{a}. \quad (2.30)$$

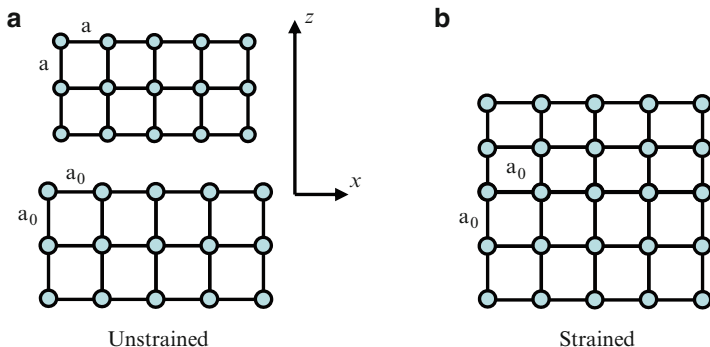


Fig. 2.5. Illustration of biaxial stress (strain). **(a)** Two different material layers have different lattice constant before growth; **(b)** After pseudomorphic film growth, the lattice constant of the top layer conforms to that of the bottom layer and is under biaxial stress (strain)

The strain is tensile in the x - y plane. To obtain the strain in the z direction, we use the strain–stress relation (2.26), i.e.,

$$\begin{bmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{zx} \\ e_{yz} \\ e_{xy} \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{bmatrix} \begin{bmatrix} \tau_{xx} \\ \tau_{yy} \\ \tau_{zz} \\ \tau_{zx} \\ \tau_{yz} \\ \tau_{xy} \end{bmatrix}. \quad (2.31)$$

In the current case, $\tau_{xx} = \tau_{yy} = T$, $\tau_{zz} = 0$, and $\tau_{zx} = \tau_{yz} = \tau_{xy} = 0$. Therefore, we have

$$\begin{aligned} e_{xx} &= e_{yy} = (S_{11} + S_{12})T, \\ e_{zz} &= 2S_{12}T. \end{aligned} \quad (2.32)$$

Thus,

$$e_{zz} = \frac{2S_{12}}{S_{11} + S_{12}} e_{xx}. \quad (2.33)$$

Strain tensor in this case is

$$e = \begin{pmatrix} e_{xx} & 0 & 0 \\ 0 & e_{xx} & 0 \\ 0 & 0 & e_{zz} \end{pmatrix}. \quad (2.34)$$

2. [110] uniaxial stress:

The x - y plane of a cubic crystal under a [110] uniaxial stress is illustrated in Fig. 2.6. The stress tensor is already obtained in Eq. (2.16), i.e., $\tau_{xx} = \tau_{yy} = \tau_{xy} = T/2$, and $\tau_{zz} = \tau_{zx} = \tau_{yz} = 0$. Substituting into (2.31), we obtain

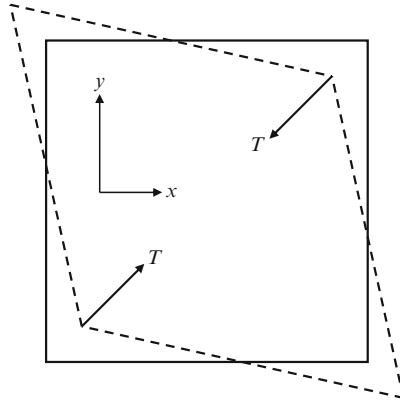


Fig. 2.6. Illustration of the [110] uniaxial compressive stress (strain)

$$\begin{aligned}
e_{xx} &= e_{yy} = \frac{S_{11} + S_{12}}{2} T, \\
e_{xy} &= \frac{S_{44}}{2} T, \\
e_{zz} &= S_{12} T.
\end{aligned} \tag{2.35}$$

The strain tensor in this case then is

$$\varepsilon = \begin{pmatrix} e_{xx} & e_{xy}/2 & 0 \\ e_{xy}/2 & e_{xx} & 0 \\ 0 & 0 & e_{zz} \end{pmatrix}. \tag{2.36}$$

2.4.1 Hydrostatic and Shear Strain

An arbitrary strain tensor can be decomposed into three separate tensors as following:

$$\begin{aligned}
\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{pmatrix} &= \frac{1}{3} \begin{pmatrix} \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} & 0 & 0 \\ 0 & \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} & 0 \\ 0 & 0 & \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \end{pmatrix} \\
&+ \frac{1}{3} \begin{pmatrix} 2\varepsilon_{xx} - (\varepsilon_{yy} + \varepsilon_{zz}) & 0 & 0 \\ 0 & 2\varepsilon_{yy} - (\varepsilon_{zz} + \varepsilon_{xx}) & 0 \\ 0 & 0 & 2\varepsilon_{zz} - (\varepsilon_{xx} + \varepsilon_{yy}) \end{pmatrix} \\
&+ \begin{pmatrix} 0 & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & 0 & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & 0 \end{pmatrix},
\end{aligned} \tag{2.37}$$

where the first constant tensor whose diagonal element is one-third of the trace of the original strain tensor accounts for the volume change [see (2.10)], and the latter two traceless tensors account for the shape change of an infinitesimal cube. Correspondingly, the first tensor describes the effect of a hydrostatic strain, and the latter two tensors describe the effect of shear strain. Among the two shear strain tensors, the diagonal one is related to the change of lengths along the three axes and the other one with diagonal elements being zero is related to the rotation of the axes of an infinitesimal cube. For a cubic crystal, the first type of shear occurs when a uniaxial stress is applied along any of the three $\langle 100 \rangle$ axes, and the second type of shear is nonzero only when stresses are applied along $\langle 110 \rangle$ or $\langle 111 \rangle$ axes. Obviously, for a cube under the hydrostatic strain, the shape does not change, while under an arbitrary first type of shear, the shape of the cube will become orthorhombic, and under an arbitrary second type of shear, the shape of the cube will become triclinic. A cubic crystal under biaxial stress becomes tetragonal, and it becomes orthorhombic under a uniaxial stress along $\langle 110 \rangle$.

For a first look, applying a compressive uniaxial stress along [001] and a biaxial tensile stress in the x - y plane to a cubic crystal seems identical. Indeed, if for both cases the stress is T , and we decompose the resulting strain tensor into the hydrostatic and shear parts, the shear strain coincides. However, the hydrostatic strain differs in sign and a factor of 2 in magnitude.

2.5 PIEZORESISTIVITY

Piezoresistivity is an effect of stress-induced resistivity change of a material. The piezoresistance coefficients (π coefficients) that relate the piezoresistivity and stress are defined by

$$\pi = \frac{\Delta R/R}{T}, \quad (2.38)$$

where R is the original resistance that is related to semiconductor sample dimension by $R = \rho \frac{l}{wh}$, ΔR signifies the change of resistance, and T is the applied mechanical stress. The ratio of ΔR to R can be expressed in terms of relative change of the sample length $\Delta l/l$, width $\Delta w/w$, height $\Delta h/h$, and resistivity $\Delta \rho/\rho$ as

$$\frac{\Delta R}{R} = \frac{\Delta l}{l} - \frac{\Delta w}{w} - \frac{\Delta h}{h} + \frac{\Delta \rho}{\rho}, \quad (2.39)$$

where resistivity ρ is inversely proportional to the conductivity. The first three terms of the RHS of (2.39) depict the geometrical change of the sample under stress, and the last term $\Delta \rho/\rho$ is the resistivity dependence on stress. For most semiconductors, the stress-induced resistivity change is several orders of magnitude larger than the geometrical change-induced resistance change, so the resistivity change by stress is the determinant factor of the piezoresistivity.

In general conditions, resistivity $\rho = 1/\sigma$ is a second-rank tensor, and stress T is also a second-rank tensor. The resistivity change, $\Delta \rho_{ij}$, is connected to stress by a fourth-rank tensor π_{ijkl} , the piezoresistance tensor. Under arbitrary stress in linear response regime,

$$\frac{\Delta \rho_{ij}}{\rho} = -\frac{\Delta \sigma_{ij}}{\sigma} = \sum_{k,l} \pi_{ijkl} \tau_{kl}, \quad (2.40)$$

where summation is over x , y , and z .

Following the same discussion for compliance and stiffness tensor, and writing $\Delta \rho_{ij}$ to a vector form $\Delta \rho_i$, where $i = 1, 2, \dots, 6$, as we did for stress and strain, we can rewrite (2.40) as

$$\frac{\Delta \rho_i}{\rho} = \sum_{k=1}^6 \pi_{ik} \tau_k, \quad (2.41)$$

where π_{ik} is a 6×6 matrix. For cubic structures, it has only three independent elements due to the cubic symmetry,

$$\pi_{ik} = \begin{pmatrix} \pi_{11} & \pi_{12} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{12} & 0 & 0 & 0 \\ \pi_{12} & \pi_{12} & \pi_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{44} \end{pmatrix}. \quad (2.42)$$

Among the three independent π -coefficients, π_{11} depicts the piezoresistive effect along one principal crystal axis for stress along this principal crystal axis (longitudinal piezoresistive effect), π_{12} depicts the piezoresistive effect along one principal crystal axis for stress directed along one perpendicular crystal axis (transverse piezoresistive effect), and π_{44} describes the piezoresistive effect on an out-of-plane electric field by the change of the in-plane current induced by in-plane shear stress.

The detailed discussion of semiconductor piezoresistivity will be covered in Chap. 5.

2.6 PIEZOELECTRICITY

Different from the piezoresistive effect, the piezoelectric effect arises from stress-induced charge polarization in a crystal that lacks a center of inversion. Thus, the piezoelectric effect does not exist in Si, Ge, etc. elementary semiconductors. The zinc-blende semiconductors are the simplest crystals with this property. The polarization is related to stress through the piezoelectric tensor \bar{e} ,

$$\mathbf{P} = [e] \mathbf{e}_{\text{strain}}, \quad (2.43)$$

where \mathbf{P} is the polarization vector and $\mathbf{e}_{\text{strain}}$ is the strain written as a six-component vector. Thus the piezoelectric tensor is a 3×6 matrix. For zinc-blende semiconductors, the piezoelectric tensor only has one nonvanishing tensor element, e_{14} , and the polarization induced by strain is then given by

$$\begin{pmatrix} P_x \\ P_y \\ P_z \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & e_{14} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{14} & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{14} \end{pmatrix} \begin{pmatrix} e_{xx} \\ e_{yy} \\ e_{zz} \\ e_{yz} \\ e_{zx} \\ e_{xy} \end{pmatrix}. \quad (2.44)$$

Because of the special form of the piezoelectric tensor, only the shear strain generates the piezoelectricity. For zinc-blende semiconductors such as GaAs grown on (001) direction, the biaxial strain does not generate piezoelectricity.

The piezoelectric effect is largest along the $\langle 111 \rangle$ axes, since the anions and cations are stacked in the (111) planes, thus strain creates relative displacement between them.

The piezoelectric constants of GaAs were measured and theoretically calculated ([Adachi, 1994](#)). The commonly adopted value is

$$e_{14} = -0.16 \text{ C/m}^2. \quad (2.45)$$

On the other hand, the applied electric field across the piezoelectric material can generate strain. The piezoelectric strain tensor \bar{d} has the same form as the piezoelectric tensor and also has only one nonvanishing component, d_{14} , for zinc-blende semiconductors. It is related to e_{14} by

$$d_{14} = S_{44}e_{14}. \quad (2.46)$$

The commonly adopted value for d_{14} for GaAs is $-2.7 \times 10^{-12} \text{ m/V}$.

The sign of e_{14} or d_{14} is negative for III–V semiconductors. If the crystal is expanded along the $\langle 111 \rangle$ direction, the A-faces (cation faces) becomes negatively charged. This is different from the II–V semiconductors, where e_{14} is positive.

For the other semiconductors lacking inversion symmetry, the piezoelectric tensor may have more than one nonvanishing component. In wurtzite semiconductors such as GaN, there are three nonvanishing components, e_{13} , e_{33} , and e_{15} . Piezoelectric effect may play an important role in semiconductor transport. In an AlGaIn/GaN heterostructure, the spontaneous polarization and the piezoelectric effect can induce large density of electrons even when there is no doping ([Bernardini and Fiorentini, 1997](#); [Jogai, 1998](#); [Sacconi et al, 2001](#)). In GaAs/InGaAs superlattices grown in the $\langle 111 \rangle$ direction, piezoelectricity induced band bending can greatly change the potential profile, and thus alter the charge distribution and transport properties ([Smith and Mailhot, 1988](#); [Kim, 2001](#)).

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