CHAPTER

2

INTERLATTICE DISPLACEMENTS OF ZnS, ZnSe, ZnTe and GaAs

2.1 Introduction

The significance in the study of interlattice displacement in wide gap semiconductors is that it gives the relative displacement of various atoms in the unit cell which occur when the crystal is strained uniformly. Moreover, the pressure dependence of elastic properties in semiconducting crystals is always accompanied by relative motion of the atoms within the unit cell. The large number of atoms present in the unit cell of the crystals ZnS, ZnSe, ZnTe and GaAs make the calculation of interlattice displacements cumbersome. We have determined the interlattice displacements in these compounds by taking into account the interactions of two nearest neighbours of each atom within the unit cell of the crystal.

Fig 2.1 shows the atomic arrangement in the unit cell of ZnS. This structure is referred to as zinc blende structure (1). This structure may be viewed as two interpenetrating FCC lattices with one composed entirely of Zn atoms, the other entirely of S atoms. These FCC lattices are displaced from each other by
one-quarter of a body diagonal. The conventional cell is a cube. The co-ordinates of Zn atoms are \((0,0,0), (0,\frac{1}{2},\frac{1}{2}), (\frac{1}{2},0,\frac{1}{2}), (\frac{1}{2},\frac{1}{2},0)\) and that of S atoms are \((\frac{1}{4},\frac{1}{4},\frac{1}{4}), (\frac{3}{4},\frac{1}{4},\frac{1}{4}), (\frac{1}{4},\frac{3}{4},\frac{1}{4}), (\frac{3}{4},\frac{3}{4},\frac{1}{4})\). There are four molecules of ZnS per conventional cell. About each atom, there are four equally distant atoms of the opposite kind arranged at the corners of a regular tetrahedron \((2)\).

![Diagram of ZnS crystal structure](image)

**Figure 2.1** Arrangement of atoms in the unit cell of ZnS. There are 8 atoms per unit cell which are designated as 1, 2, 3, 4, 5, 6, 7 and 8. Their co-ordinate are \((0,0,0), (\frac{a}{2},\frac{a}{2},0), (\frac{a}{2},0,\frac{a}{2}), (0,\frac{a}{2},\frac{a}{2}), (\frac{a}{4},\frac{a}{4},\frac{a}{4}), (\frac{a}{4},\frac{3a}{4},\frac{3a}{4}), (\frac{3a}{4},\frac{a}{4},\frac{3a}{4}), (\frac{3a}{4},\frac{3a}{4},\frac{a}{4})\), respectively.
We derive here the expressions for the interlattice displacements of the atoms in the unit cell in terms of the strain parameters using the deformation theory (3). The nature of interlattice displacements of various atoms in the unit cell is also discussed.

2.2 Theory

When a crystal lattice is deformed such that the resulting structure remains a perfect lattice, the deformation is called homogeneous (3,4). When a lattice is homogeneously deformed, the components of the interatomic lattice vectors are transformed as (5)

\[
R_i' \left( \begin{array}{c} L' \\ \mu' \end{array} \right) = R_i \left( \begin{array}{c} L \\ \mu \end{array} \right) + \sum_j \varepsilon_{ij} R_i \left( \begin{array}{c} L \\ \mu' \end{array} \right) + W_i (1 - \delta_{\mu \mu'}) \quad (2.1)
\]

where \( R_i \left( \begin{array}{c} L \\ \mu \end{array} \right) \) is the vector distance between the particle \( \mu \) in cell \( L \) and particle \( \mu' \) in cell \( L' \) in the undeformed state.

\( R_i' \left( \begin{array}{c} L' \\ \mu' \end{array} \right) \) refers to the corresponding vector distance in homogeneously deformed state. \( i \) and \( j \) are the component indices and \( \delta_{\mu \mu'} \) is the Kronecker delta. \( \varepsilon_{ij} \) are the deformation parameters related to the macroscopic Lagrangian strains \( \eta_{ij} \) by

\[
\eta_{ij} = \frac{1}{2} \left( \varepsilon_{ij} + \overline{\varepsilon}_{ij} + \sum_k \varepsilon_{ik} \varepsilon_{jk} \right) \quad (2.2)
\]
$W_1$ are the components of the internal displacements of the sublattice $\mu$ relative to the sublattice $\mu'$. The internal displacement components are replaced by the relative internal displacements $\overline{W}_1$ by the relation

$$\overline{W}_i(\mu \mu') = W_i(\mu \mu') + \sum_j \varepsilon_{ji} W_j(\mu \mu')$$  \hspace{1cm} (2.3)

When a crystal undergoes deformation, the elastic energy between the particles is stored as potential energy of deformation of the body, and is called the strain energy. The potential energy per unit cell $\phi$ of the crystal is presumed to be an analytical function of position of the atoms due to interactions among the atoms in a given configuration and hence it can be expanded in terms of the displacements from an initial configuration. The potential energy per unit cell $\phi$ can be expanded using Taylor series involving displacement $\mathbf{u}$ of the molecules as

$$\phi = \phi_0 + \phi_1 + \phi_2 + \ldots$$  \hspace{1cm} (2.4)

where $\phi_0$ is the static potential energy of the crystal and

$$\phi_1 = \sum_{\mu} \phi_i(\mu) u_i(\mu)$$  \hspace{1cm} (2.5)

where $u_i(\mu)$ is the i-Cartesian component of $\mathbf{u}(\mu)$.

$\mathbf{u}(\mu)$ is the displacement of the $\mu$th atom in the $L$th unit cell.
Here, $\phi_1 \left( \begin{array}{c} L \\ \mu \end{array} \right) = \left[ \frac{\partial \phi}{\partial u_i \left( \begin{array}{c} L \\ \mu \end{array} \right)} \right]_0$ (2.6)

Also, $\phi_2 = \frac{1}{2} \sum_{\mu<\mu'} \phi_{ij} \left( \begin{array}{c} L \\ \mu \\ L' \end{array} \right) u_i \left( \begin{array}{c} L \\ \mu \end{array} \right) u_j \left( \begin{array}{c} L' \\ \mu' \end{array} \right)$ (2.7)

Where $u_i \left( \begin{array}{c} L \\ \mu' \end{array} \right)$ is the $i$ Cartesian component of $u \left( \begin{array}{c} L' \\ \mu' \end{array} \right)$. $u \left( \begin{array}{c} L' \\ \mu' \end{array} \right)$ is the displacement of $\mu'$ atom in the $L'$ cell.

Where $\phi_{ij} \left( \begin{array}{c} L \\ \mu \\ L' \end{array} \right) = \left[ \frac{\partial^2 \phi}{\partial u_i \left( \begin{array}{c} L \\ \mu \end{array} \right) \partial u_j \left( \begin{array}{c} L' \\ \mu' \end{array} \right)} \right]_0$ (2.8)

The subscript zero means that the derivatives have to be evaluated in the equilibrium configuration. Here $\phi$ holds both the translational symmetry of the lattice and the conditions of atomic equilibrium. $u \left( \begin{array}{c} L' \\ \mu' \end{array} \right)$ is the displacement of the $\mu'$ atom in the $L'$ cell. If we consider interactions under harmonic approximations, it can be noted that $\phi$ depends only on the square of the vector distance between atoms in the crystal. Under equilibrium condition $\phi_1$ vanishes and using harmonic approximation the contribution to the potential energy is only from the $\phi_2$ term. Therefore, the change in potential energy when the lattice is homogeneously strained can be written as
where \( k_2 = \frac{1}{2} \sum_{L' \mu'} \phi_{ij} \left[ \begin{array}{cc} L & L' \\ \mu & \mu' \end{array} \right] \)

is the second-order parameter characterising the two-body interactions between the pair of atoms \( \left( \begin{array}{c} L \\ \mu \end{array} \right) \) and \( \left( \begin{array}{c} L' \\ \mu' \end{array} \right) \).

Also, \( \Delta R \left[ \begin{array}{cc} L \\ \mu \\ L' \\ \mu' \end{array} \right] = R' \left[ \begin{array}{cc} L \\ \mu \\ L' \\ \mu' \end{array} \right] - R \left[ \begin{array}{cc} L \\ \mu \\ L' \\ \mu' \end{array} \right] \)

(2.11)

In terms of Lagrangian strains \( \eta_{ij} \) and internal displacements \( \bar{W}_i (\mu \mu') \), the energy is invariant towards rigid rotations of the lattice. By minimising the strain energy with respect to the internal displacements, we obtain \( \bar{W}_i (\mu \mu') \) in terms of the Lagrangian strain parameters to the first order in \( \eta_{ij} \) as

\[
\bar{W}_i (\mu \mu') = -4 k_2 \sum_{jkl} \eta_{ij} D_{jkl} M_{ik}^{-1}
\]

(2.12)

where \( M_{ik}^{-1} \) is the inverse of the \( 3 \times 3 \) matrix \( M_{ik} \),

\[
M_{ik} = \begin{bmatrix}
M_{xx} & M_{xy} & M_{xz} \\
M_{yx} & M_{yy} & M_{yz} \\
M_{zx} & M_{zy} & M_{zz}
\end{bmatrix}
\]

(2.13)
\[ = 4 \kappa_2 \sum_{l \mu} \sum_{L \mu'} R_i \begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_k \begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \] (2.14)

and the matrix

\[
[D_{kl}] = \sum_{l \mu} R_j \begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_k \begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_i \begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \] (2.15)

Equation (2.12) on expansion and simplification becomes

\[
\bar{W}(\mu \mu') = -4 \kappa_2 \left[ \eta_{xx} \left( D_{xxx} M_{xi}^{-1} + D_{xyy} M_{yi}^{-1} + D_{xzz} M_{zi}^{-1} \right) \right] 
- \eta_{yy} \left( D_{yyx} M_{xi}^{-1} + D_{yy} M_{yi}^{-1} + D_{yyz} M_{zi}^{-1} \right) 
+ \eta_{zz} \left( D_{zzx} M_{xi}^{-1} + D_{zyy} M_{yi}^{-1} + D_{zzz} M_{zi}^{-1} \right) 
+ 2 \eta_{xy} \left( D_{xy} M_{yi}^{-1} + D_{xyy} M_{yi}^{-1} + D_{xyz} M_{zi}^{-1} \right) 
+ 2 \eta_{xz} \left( D_{xz} M_{yi}^{-1} + D_{zy} M_{yi}^{-1} + D_{xz} M_{zi}^{-1} \right) 
+ 2 \eta_{yz} \left( D_{yz} M_{yi}^{-1} + D_{yy} M_{yi}^{-1} + D_{yzy} M_{zi}^{-1} \right) \] (2.16)

From the above expression, the equations for \( \bar{W}_x(\mu \mu') \), \( \bar{W}_y(\mu \mu') \) and \( \bar{W}_z(\mu \mu') \) can be written as

\[
\bar{W}_x(\mu \mu') = 4 \kappa_2 \left[ \eta_{xx} \left( D_{xxx} M_{xi}^{-1} + D_{xyy} M_{yi}^{-1} + D_{xzz} M_{zi}^{-1} \right) \right] 
+ \eta_{yy} \left( D_{yyx} M_{xi}^{-1} + D_{yy} M_{yi}^{-1} + D_{yyz} M_{zi}^{-1} \right) 
+ \eta_{zz} \left( D_{zzx} M_{xi}^{-1} + D_{zyy} M_{yi}^{-1} + D_{zzz} M_{zi}^{-1} \right) 
+ 2 \eta_{xy} \left( D_{xy} M_{yi}^{-1} + D_{xyy} M_{yi}^{-1} + D_{xyz} M_{zi}^{-1} \right) 
+ 2 \eta_{xz} \left( D_{xz} M_{yi}^{-1} + D_{zy} M_{yi}^{-1} + D_{xz} M_{zi}^{-1} \right) 
+ 2 \eta_{yz} \left( D_{yz} M_{yi}^{-1} + D_{yy} M_{yi}^{-1} + D_{yzy} M_{zi}^{-1} \right) \]
\[
\bar{W}_s (\mu \mu') = -4k_2 \left[ \eta_{xx} \left( D_{xx, M}^{-1} + D_{xy, M}^{-1} + D_{xz, M}^{-1} \right) \right. \\
+ \eta_{yy} \left( D_{yy, M}^{-1} + D_{yx, M}^{-1} + D_{yz, M}^{-1} \right) \\
\left. + \eta_{zz} \left( D_{zz, M}^{-1} + D_{zx, M}^{-1} + D_{zy, M}^{-1} \right) \right] \quad (2.17)
\]

\[
\bar{W}_z (\mu \mu') = -4k_2 \left[ \eta_{xx} \left( D_{xx, M}^{-1} + D_{xy, M}^{-1} + D_{xz, M}^{-1} \right) \right. \\
+ \eta_{yy} \left( D_{yy, M}^{-1} + D_{yx, M}^{-1} + D_{yz, M}^{-1} \right) \\
\left. + \eta_{zz} \left( D_{zz, M}^{-1} + D_{zx, M}^{-1} + D_{zy, M}^{-1} \right) \right] \quad (2.18)
\]
The co-ordinates of all the two nearest neighbours of eight atoms in the unit cell of ZnS are given in the Appendix I. The atoms are numbered as shown in Figure 2.1. The evaluation has been done for all the nearest neighbours of the eight atoms to obtain \( \bar{W}_x (\mu \mu') \), \( \bar{W}_y (\mu \mu') \) and \( \bar{W}_z (\mu \mu') \). The results so obtained for the components of interlattice displacements are given below.

\[
\begin{align*}
\bar{W}_x (2) &= -0.5a_1
, \\
\bar{W}_y (2) &= -0.5a_1
, \\
\bar{W}_z (2) &= -0.5a_1
, \\
\bar{W}_x (3) &= -0.5a_1
, \\
\bar{W}_y (3) &= -0.5a_1
, \\
\bar{W}_z (3) &= -0.5a_1
, \\
\bar{W}_x (4) &= -0.5a_1
, \\
\bar{W}_y (4) &= -0.5a_1
, \\
\bar{W}_z (4) &= -0.5a_1
, \\
\bar{W}_x (5) &= 0.5a_1
, \\
\bar{W}_y (5) &= 0.5a_1
, \\
\bar{W}_z (5) &= 0.5a_1
, \\
\bar{W}_x (6) &= 0.5a_1
, \\
\bar{W}_y (6) &= 0.5a_1
, \\
\bar{W}_z (6) &= 0.5a_1
, \\
\bar{W}_x (7) &= 0.5a_1
.
\end{align*}
\]
Here the number in the parentheses is the label assigned to the atoms in the unit cell as in Figure 2.1. a is the lattice parameter.

2.3 Interlattice Displacements of Zinc Sulphide (ZnS)

Figure 2.1 gives the zinc blende structure. In this interpenetrating FCC lattices, one composed entirely of Zn atoms and the other entirely of S atoms. The co-ordinates of Zn atoms are \((0,0,0), (0,\%\%,\%), (\%,0,\%), (\%,\%,0)\) and that of S atoms are \((\%,\%,\%), (\%,\%,\%), (\%,\%,\%), (\%,\%,\%)\) (1). For ZnS, the lattice parameter \(a = 0.541\) nm (6). Using the value of lattice parameter \(a\), we get the following expressions for interlattice displacements of ZnS from equation (2.20) as

\[
\begin{align*}
\vec{W}_x (2) &= -0.271 \eta_{yz} \\
\vec{W}_y (2) &= -0.271 \eta_{xz} \\
\vec{W}_z (2) &= -0.271 \eta_{xy} \\
\vec{W}_x (3) &= -0.271 \eta_{yz} \\
\vec{W}_y (3) &= -0.271 \eta_{xz} \\
\vec{W}_z (3) &= -0.271 \eta_{xy}
\end{align*}
\]
\[ \dot{W}_x (4) = -0.271 \eta_{yz} \]
\[ \dot{W}_x (4) = -0.271 \eta_{xz} \]
\[ \dot{W}_x (5) = 0.271 \eta_{yz} \]
\[ \dot{W}_x (5) = 0.271 \eta_{xz} \]
\[ \dot{W}_x (5) = 0.271 \eta_{xy} \]
\[ \dot{W}_x (6) = 0.271 \eta_{yz} \]
\[ \dot{W}_x (6) = 0.271 \eta_{xz} \]
\[ \dot{W}_x (6) = 0.271 \eta_{xy} \]
\[ \dot{W}_x (7) = 0.271 \eta_{yz} \]
\[ \dot{W}_x (7) = 0.271 \eta_{xz} \]
\[ \dot{W}_x (7) = 0.271 \eta_{xy} \]
\[ \dot{W}_x (8) = 0.271 \eta_{yz} \]
\[ \dot{W}_x (8) = 0.271 \eta_{xz} \]
\[ \dot{W}_x (8) = 0.271 \eta_{xy} \] (2.21)

2.4 Results and Discussion

Equations (2.20) and (2.21) show that the x component of interlattice displacements for ZnS is:

\[ -\dot{W}_x (2) = -\dot{W}_x (3) = -\dot{W}_x (4) = \dot{W}_x (5) = \dot{W}_x (6) = \dot{W}_x (7) = \dot{W}_x (8) = 0.5 \eta_{yz} \]

Similarly for y component of interlattice displacements.
and the $z$ component of interlattice displacements,

\[- W_z(2) = - W_z(3) = - W_z(4) = W_z(5) = W_z(6) = W_z(7) = W_z(8) = 0.5a \eta_{xy}\]

This shows that the zinc atoms 2,3,4 move with equal amplitude but opposite in direction to that of sulphur atoms 5,6,7 and 8. Thus the sublattice of all zinc atoms move with equal amplitude but opposite in direction relative to the sublattice of sulphur atoms when the crystal is deformed (7). The three components of interlattice displacements of all second neighbour atoms are zero.

### 2.5 Interlattice Displacements of Zinc Selenide (ZnSe)

ZnSe crystallises in zinc blende form as shown in Figure 2.1. In this structure two FCC lattices are displaced from each other by one quarter of a body diagonal. The conventional cell is a cube, which contains eight atoms. The interlattice displacement components of different atoms in ZnSe is evaluated from equations (2.20) by substituting the values of lattice parameter, $a = 0.567$ nm (6). The components of $\overline{W}_i$ in terms of Lagrangian strain $\eta_{ij}$ for various atoms thus obtained are given below.

\[
\begin{align*}
\overline{W}_x(2) &= -0.284 \eta_{yz} \\
\overline{W}_y(2) &= -0.284 \eta_{xz} \\
\overline{W}_z(2) &= -0.284 \eta_{xy} \\
\overline{W}_x(3) &= -0.284 \eta_{yz} \\
\end{align*}
\]
\[ \tilde{W}_x(3) = -0.284 \eta_{xy} \]
\[ \tilde{W}_x(3) = -0.284 \eta_{xy} \]
\[ \tilde{W}_x(4) = -0.284 \eta_{yz} \]
\[ \tilde{W}_x(4) = -0.284 \eta_{xz} \]
\[ \tilde{W}_x(5) = 0.284 \eta_{yz} \]
\[ \tilde{W}_x(5) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(5) = 0.284 \eta_{xy} \]
\[ \tilde{W}_x(6) = 0.284 \eta_{yz} \]
\[ \tilde{W}_x(6) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(6) = 0.284 \eta_{xy} \]
\[ \tilde{W}_x(7) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(7) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(7) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(8) = 0.284 \eta_{xz} \]
\[ \tilde{W}_x(8) = 0.284 \eta_{xz} \]

\[ \tilde{W}_x(8) = 0.284 \eta_{xz} \]

(2.22)

2.6 Results and Discussion

From equations (2.20) and (2.22) the x component of interlattice displacements for ZnSe is

\[ -\tilde{W}_x(2) \cdot -\tilde{W}_x(3) \cdot -\tilde{W}_x(4) = \tilde{W}_x(5) = \tilde{W}_x(6) = \tilde{W}_x(7) = \tilde{W}_x(8) = 0.5a \eta_{xz} \]
the $y$ component of interlattice displacements,

\[- \bar{W}_y (2) = - \bar{W}_y (3) = - \bar{W}_y (4) = \bar{W}_y (5) = \bar{W}_y (6) = \bar{W}_y (7) = \bar{W}_y (8) = 0.5 \alpha \eta_{xx}\]

and the $z$ component of interlattice displacements,

\[- \bar{W}_z (2) = - \bar{W}_z (3) = - \bar{W}_z (4) = \bar{W}_z (5) = \bar{W}_z (6) = \bar{W}_z (7) = \bar{W}_z (8) = 0.5 \alpha \eta_{xy}\]

This shows that the zinc atoms 2, 3, 4 move with equal amplitude but in opposite direction to that of selenium atoms 5, 6, 7, and 8. Thus as in ZnS, the sublattice of all zinc atoms move with equal amplitude but opposite in direction relative to the sublattice of selenium atoms while the crystal is deformed (8). The three components of interlattice displacements of all second neighbour atoms are zero.

### 2.7 Interlattice Displacements of Zinc Telluride (ZnTe)

ZnTe crystallizes in zinc blende form as shown in Figure 2.1. There are eight atoms per unit cell. About each atom, there are four equally distant atoms of the opposite kind arranged at the corners of a regular tetrahedron. The interlattice displacements of ZnTe have also been worked in a similar way as that of ZnS and ZnSe using the deformation theory. The lattice parameter of ZnTe is $a = 0.61$ nm (6). The components of the interlattice displacements for different atoms in ZnTe systems are obtained as
\[ \bar{W}_x(2) = -0.305 \eta_{yz} \]
\[ \bar{W}_x(2) = -0.305 \eta_{xz} \]
\[ \bar{W}_x(2) = -0.305 \eta_{xy} \]
\[ \bar{W}_x(3) = -0.305 \eta_{yz} \]
\[ \bar{W}_x(3) = -0.305 \eta_{xz} \]
\[ \bar{W}_x(3) = -0.305 \eta_{xy} \]
\[ \bar{W}_x(4) = -0.305 \eta_{yz} \]
\[ \bar{W}_x(4) = -0.305 \eta_{xz} \]
\[ \bar{W}_x(4) = -0.305 \eta_{xy} \]
\[ \bar{W}_x(5) = 0.305 \eta_{xz} \]
\[ \bar{W}_x(5) = 0.305 \eta_{xz} \]
\[ \bar{W}_x(5) = 0.305 \eta_{xy} \]
\[ \bar{W}_x(6) = 0.305 \eta_{yz} \]
\[ \bar{W}_x(6) = 0.305 \eta_{xz} \]
\[ \bar{W}_x(6) = 0.305 \eta_{xy} \]
\[ \bar{W}_x(7) = 0.305 \eta_{yz} \]
\[ \bar{W}_x(7) = 0.305 \eta_{xz} \]
\[ \bar{W}_x(7) = 0.305 \eta_{xy} \]
\[ \bar{W}_x(8) = 0.305 \eta_{yz} \]
\[ \bar{W}_x(8) = 0.305 \eta_{xz} \]
\[ \bar{W}_x(8) = 0.305 \eta_{xy} \]

\[(2.23)\]
2.8 Results and Discussion

Above equations (2.20) and (2.23) show that the atoms 2,3,4 move with equal amplitude but opposite in direction to that of atoms 5,6,7 and 8. Thus the sublattice of all zinc atoms move with equal amplitude but opposite in direction relative to the sublattice of tellurium atoms while the crystal is deformed (8). Here also, the three components of interlattice displacements of all second neighbour atoms are zero.

2.9 Interlattice Displacements of Gallium Arsenide (GaAs)

GaAs exists in zinc blende (9) form as shown in Figure 2.1. Infact, it is identical to the diamond structure except that the two interpenetrating FCC sublattices are of different atoms - one composed entirely of Ga atoms, the other entirely of As atoms. This is a true face centred cubic structure with a basis of two different atoms. The four nearest neighbours to a particular atom in this case are of opposite kind but disposed tetrahedrally. This structure is loosely packed and does not possess a center of inversion symmetry at the midpoint of a line connecting nearest neighbour atoms. The interlattice displacement components of different atoms in GaAs is evaluated from equation (2.20) by substituting the value of lattice parameter $a = 0.565 \text{ nm}$ (6). The components of the interlattice displacements for different atoms in the GaAs system are obtained as
\[\bar{W}_1(2) = -0.283\eta_{yz}\]
\[\bar{W}_2(2) = -0.283\eta_{xz}\]
\[\bar{W}_3(2) = -0.283\eta_{xy}\]
\[\bar{W}_1(3) = -0.283\eta_{yz}\]
\[\bar{W}_2(3) = -0.283\eta_{xz}\]
\[\bar{W}_3(3) = -0.283\eta_{xy}\]
\[\bar{W}_4(4) = -0.283\eta_{yz}\]
\[\bar{W}_5(4) = -0.283\eta_{xz}\]
\[\bar{W}_6(4) = -0.283\eta_{xy}\]
\[\bar{W}_1(5) = 0.283\eta_{yz}\]
\[\bar{W}_2(5) = 0.283\eta_{xz}\]
\[\bar{W}_3(5) = 0.283\eta_{xy}\]
\[\bar{W}_4(6) = 0.283\eta_{yz}\]
\[\bar{W}_5(6) = 0.283\eta_{xz}\]
\[\bar{W}_6(6) = 0.283\eta_{xy}\]
\[\bar{W}_1(7) = 0.283\eta_{yz}\]
\[\bar{W}_2(7) = 0.283\eta_{xz}\]
\[\bar{W}_3(7) = 0.284\eta_{xy}\]
\[\bar{W}_4(8) = 0.283\eta_{yz}\]
\[\bar{W}_5(8) = 0.283\eta_{xz}\]
\[\bar{W}_6(8) = 0.283\eta_{xy}\]
2.10 Results and Discussion

As in the previous cases, equations (2.20) and (2.24) show that the sublattice of all gallium atoms move with equal amplitude but opposite in direction relative to the sublattice of arsenic atoms while the crystal is deformed. The contributions to the interlattice displacement from second neighbouring atoms are zero. Thus, the study of interlattice displacement provides us with a physical picture of the relative displacements of the different atoms in the crystal lattice when the lattice is strained.

The interlattice displacements obtained in this chapter used to evaluate the second- and third-order elastic constants of the compounds ZnS, ZnSe, ZnTe and GaAs in chapter III and chapter IV respectively.
References


