

Interlattice displacements and elastic constants of the A-15 compounds V_3Si , V_3Ge and Nb_3Sn

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Abstract. General expressions for the interlattice displacements of the A-15 structure compounds are obtained in terms of the strain components making use of the deformation theory. The nature of the interlattice displacements of all the 8 atoms in the unit cell is discussed. It is found that the interlattice displacements occur in such a way that the pair of atoms along any linear chain move in opposite directions with equal magnitudes. Expression for the strain energy of these compounds is developed using deformation theory and this is compared with the strain energy expression from continuum theory to obtain the elastic constants. The theoretical values of the elastic constants fairly agree with the experimental values for V_3Si , V_3Ge and Nb_3Sn .

Keywords. A-15 compounds; A_3B structure; interlattice displacements; elastic constants.

1. Introduction

In recent years the A-15 structure compounds have aroused a lot of interest because of their high temperature superconductivity and anomalous elastic properties. (Testardi 1973, Weger and Goldberg 1973). The interlattice displacements of the A-15 structure compounds have been considered by earlier workers (Viswanathan and Prabhakaran Nayar 1975, Srinivasan and Lakshmi 1976) on the basis of the de Launey model and from group theoretical internal site symmetry arguments. A study of the interlattice displacements of these compounds is cumbersome due to the large number of atoms in the unit cell and the complicated A_3B structure.

Figure 1 shows the arrangement of the different atoms in the unit cell of A_3B structure compounds. Of the eight atoms in the unit cell, six are A atoms (usually a

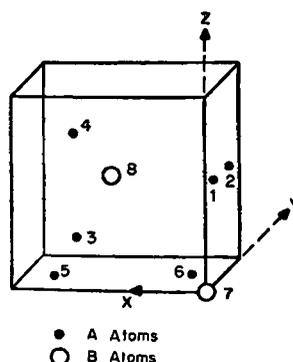


Figure 1. A_3B structure

transition metal atom like V, Nb, etc.) and two are B atoms (usually a tetravalent atom like Ge, Si, Sn, etc.). The B atoms occur on the bcc sites while the A atoms occur pairwise on each of the cube faces. They belong to the cubic space group Pm 3n. The two A atoms on a given face are separated by half the unit cell length. Each A atom has 18 nearest neighbours and each B atom has 32 nearest neighbours as can be seen from the actual structure of A_3B compounds (Testardi and Bateman 1967). We include only the nearest neighbour interactions in the present study. In this paper we derive the expressions for the interlattice displacements of the A-15 compounds in terms of the strain parameters on the basis of the deformation theory (Born and Huang 1954) and the nature of the interlattice displacements is discussed in detail. Explicit expressions for the elastic constants are also derived. The calculated elastic constants of V_3Si , V_3Ge and Nb_3Sn are reported along with the measured values for these compounds.

2. Interlattice displacements

When a lattice is homogeneously deformed, the components of the interatomic vectors are transformed as (Ramji Rao and Menon 1973)

$$\mathbf{R}'_i \left(\begin{matrix} LL' \\ \nu\nu' \end{matrix} \right) = \mathbf{R}_i \left(\begin{matrix} LL' \\ \nu\nu' \end{matrix} \right) + \sum_j \epsilon_{ij} \mathbf{R}_j \left(\begin{matrix} LL' \\ \nu\nu' \end{matrix} \right) + W_i (1 - \delta_{\nu\nu'}). \quad (1)$$

Here $\mathbf{R}_i \left(\begin{matrix} LL' \\ \nu\nu' \end{matrix} \right)$ is the vector distance between the particle ν in the cell L and the particle ν' in the cell L' in the undeformed state. $\mathbf{R}'_i \left(\begin{matrix} LL' \\ \nu\nu' \end{matrix} \right)$ refers to the vector distance in the homogeneously deformed state. i is the component index. The ϵ_{ij} are the deformation parameters related to the macroscopic Lagrangian strains η_{ij} by

$$\eta_{ij} = \frac{1}{2} (\epsilon_{ij} + \epsilon_{ji} + \sum_k \epsilon_{ik} \epsilon_{jk}) \quad (2)$$

and W_i are the components of the internal displacements of the sublattice ν relative to the sublattice ν' . The internal displacement components are replaced by

$$\overline{W}_i(\nu) = W_i(\nu) + \sum_j \epsilon_{ji} W_j(\nu). \quad (3)$$

In terms of the Lagrangian strains η_{ij} and the internal displacements $\overline{W}_i(\nu)$, the energy is invariant toward rigid rotations of the crystal. By minimizing the strain energy with respect to the internal displacements, we obtain $\overline{W}_i(\nu)$ in terms of the Lagrangian strain parameters to the first order in η_{ij} .

Thus we get

$$\begin{aligned} \overline{W}_i(\nu \nu') &= \eta_{xx} \left(D_{xxx} M_{xj}^{-1} + D_{xxy} M_{yj}^{-1} + D_{xxz} M_{zj}^{-1} \right) \\ &+ \eta_{yy} \left(D_{yyx} M_{xj}^{-1} + D_{yyy} M_{yj}^{-1} + D_{yyz} M_{zj}^{-1} \right) \end{aligned}$$

$$\begin{aligned}
& + \eta_{zx} \left(D_{zzx} M_{xj}^{-1} + D_{zzy} M_{yj}^{-1} + D_{zzz} M_{zj}^{-1} \right) \\
& + 2\eta_{xy} \left(D_{xxy} M_{xj}^{-1} + D_{yyx} M_{yj}^{-1} + D_{xyy} M_{zj}^{-1} \right) \\
& + 2\eta_{xz} \left(D_{xxz} M_{xj}^{-1} + D_{xyy} M_{yj}^{-1} + D_{zzz} M_{zj}^{-1} \right) \\
& + 2\eta_{yz} \left(D_{xyy} M_{xj}^{-1} + D_{yyz} M_{yj}^{-1} + D_{yzz} M_{zj}^{-1} \right)
\end{aligned} \tag{4}$$

where the matrix $[M_{ij}^{-1}]$ is the inverse of the matrix

$$[M_{ij}] = \sum R_i \begin{pmatrix} LL' \\ \nu\nu' \end{pmatrix} R_j \begin{pmatrix} LL' \\ \nu\nu' \end{pmatrix} \tag{5}$$

and

$$[D_{ijk}] = \sum R_i \begin{pmatrix} LL' \\ \nu\nu' \end{pmatrix} R_j \begin{pmatrix} LL' \\ \nu\nu' \end{pmatrix} R_k \begin{pmatrix} LL' \\ \nu\nu' \end{pmatrix}. \tag{6}$$

Here the summations are done for all the nearest neighbours of the different atoms in the unit cell. The final expressions obtained for the interlattice displacements of the A-15 structure compounds are

$$\left. \begin{aligned}
\overline{W_x}(1) &= -\overline{W_x}(2) = \eta_{xy} (7/18) a \\
\overline{W_y}(1) &= -\overline{W_y}(2) = \eta_{xx} (1/8) a - \eta_{zz} (1/8) a \\
\overline{W_z}(1) &= -\overline{W_z}(2) = -\eta_{yz} (7/18) a
\end{aligned} \right\} \tag{7a}$$

$$\left. \begin{aligned}
\overline{W_x}(3) &= -\overline{W_x}(4) = -\eta_{xz} (7/18) a \\
\overline{W_y}(3) &= -\overline{W_y}(4) = \eta_{yz} (7/18) a \\
\overline{W_z}(3) &= -\overline{W_z}(4) = \eta_{yy} (1/8) a - \eta_{xx} (1/8) a
\end{aligned} \right\} \tag{7b}$$

$$\left. \begin{aligned}
\overline{W_x}(5) &= -\overline{W_x}(6) = \eta_{zz} (1/8) a - \eta_{yy} (1/8) a \\
\overline{W_y}(5) &= -\overline{W_y}(6) = -\eta_{xy} (7/18) a \\
\overline{W_z}(5) &= -\overline{W_z}(6) = \eta_{xz} (7/18) a
\end{aligned} \right\} \tag{7c}$$

$$\overline{W_x}(7) = \overline{W_y}(7) = \overline{W_z}(7) = \overline{W_x}(8) = \overline{W_y}(8) = \overline{W_z}(8) = 0. \tag{7d}$$

A study of eqs (7) shows that the interlattice displacements in these compounds take place in such a way that the pair of atoms along any linear chain in the lattice move in opposite directions with equal magnitudes. In other words, the displacements of the pairs of atoms 1 and 2, 3 and 4 and 5 and 6 are equal in magnitudes but opposite in directions. They could move both along the line joining them as well as perpendicular to this direction. For atoms 7 and 8 which are the B atoms, we see that there is no interlattice displacement.

If the strain components are equal, i.e. if $\eta_{xx} = \eta_{yy} = \eta_{zz}$ and $\eta_{xy} = \eta_{yz} = \eta_{zx}$,

then all the interlattice displacements vanish. So a deformation which is free of shearing strains and in which the expansion is the same in the three principal directions, will not produce any interlattice displacements. If we assume that $\eta_{xy} \neq 0$ and $\eta_{yz} = \eta_{zx} = 0$, then atoms 1 and 2 will be shifted against each other along the x-axis; 3 and 4 will be at rest, and 5 and 6 will move against each other along the y-axis.

3. Elastic constants

We make use of the deformation theory (Born and Huang 1954) to determine the strain energy for the A-15 compounds and it is then compared with the strain energy expression from continuum theory to obtain the expressions for their elastic constants.

The potential energy per unit cell can be written as

$$\phi = \frac{1}{2} \sum_{LL'} \sum_{\nu\nu'} \phi \left(\frac{LL'}{\nu\nu'} \right). \quad (8)$$

If we consider the central interaction under harmonic approximation, $\phi \left(\frac{LL'}{\nu\nu'} \right)$ depends only on the square of the vector distance between the atoms $\left(\frac{L}{\nu} \right)$ and $\left(\frac{L'}{\nu'} \right)$.

Therefore

$$\phi = \phi_0 + \phi_1 + \phi_2 \quad (9)$$

where ϕ_0 is the static potential energy of the crystal and

$$\left. \begin{aligned} \phi_1 &= O' \phi \\ 2\phi_2 &= O'' \phi \end{aligned} \right\} \quad (10)$$

where O' is the differential operator $\left(\frac{\partial}{\partial \gamma^2} \right)$ and $O'' = (O')^2$. Under equilibrium conditions, ϕ_1 vanishes and the contribution to the change in potential energy per unit cell is only from third term. The change in potential energy with nearest neighbour central interaction is

$$\Delta \phi = \frac{1}{2} \sum_{LL'} \sum_{\nu\nu'} O'' \phi \left(\frac{LL'}{\nu\nu'} \right) \Delta R^2 \left(\frac{LL'}{\nu\nu'} \right) \quad (11)$$

where $\Delta R \left(\frac{LL'}{\nu\nu'} \right)$ is the change in the interatomic vector distance between atoms $\left(\frac{L}{\nu} \right)$ and $\left(\frac{L'}{\nu'} \right)$. Putting $k_2 = O'' \phi$, we have for the $A_3 B$ structure

$$\begin{aligned} \Delta \phi &= k_2 \sum_{LL'} \sum_{\nu\nu'} \left(4 \left[\eta_{xx}^2 R_x^4 + \eta_{yy}^2 R_y^4 + \eta_{zz}^2 R_z^4 + 2 \eta_{xx} \eta_{yy} R_x^2 R_y^2 \right. \right. \\ &\quad \left. \left. + 2 \eta_{xx} \eta_{zz} R_x^2 R_z^2 + 2 \eta_{yy} \eta_{zz} R_y^2 R_z^2 + 4 \eta_{xy}^2 R_x^2 R_y^2 + 4 \eta_{xz}^2 R_x^2 R_z^2 \right] \right) \end{aligned}$$

$$\begin{aligned}
 & + 4 \eta_{yz}^2 R_y^2 R_z^2 \Big] + 4 \Big[\overline{W}_x^2 R_x^2 + \overline{W}_y^2 R_y^2 + \overline{W}_z^2 R_z^2 + 2 \overline{W}_x \overline{W}_y R_x R_y \\
 & + 2 \overline{W}_x \overline{W}_z R_x R_z + 2 \overline{W}_y \overline{W}_z R_y R_z \Big] + 8 \left\{ \eta_{xx} \Big[\overline{W}_x R_x^3 \right. \right. \\
 & + \overline{W}_y R_x^2 R_y + \overline{W}_z R_x^2 R_z \Big] + \eta_{yy} \Big[\overline{W}_x R_x R_y^2 + \overline{W}_y R_y^3 + \overline{W}_z R_y^2 R_z \Big] \\
 & + \eta_{zz} \Big[\overline{W}_x R_x R_z^2 + \overline{W}_y R_y R_z^2 + \overline{W}_z R_z^3 \Big] \\
 & + 2 \eta_{xy} \Big[\overline{W}_x R_x^2 R_y + \overline{W}_y R_x R_y^2 + \overline{W}_z R_x R_y R_z \Big] + 2 \eta_{xz} \Big[\overline{W}_x R_x^2 R_z \\
 & + \overline{W}_y R_x R_y R_z + \overline{W}_z R_x R_z^2 \Big] + 2 \eta_{yz} \Big[\overline{W}_x R_x R_y R_z + \overline{W}_y R_y^2 R_z \\
 & + \overline{W}_z R_y R_z^2 \Big] \Big\} + 4 \left\{ \left(\overline{W}_x^2 + \overline{W}_y^2 + \overline{W}_z^2 \right) \times \left(\eta_{xx} R_x^2 + \eta_{yy} R_y^2 \right. \right. \\
 & + \eta_{zz} R_z^2 + 2 \eta_{xy} R_x R_y + 2 \eta_{xz} R_x R_z + 2 \eta_{yz} R_y R_z \Big) \Big\} \\
 & + 4 \left\{ \left(\overline{W}_x R_x + \overline{W}_y R_y + \overline{W}_z R_z \right) \times \left(\overline{W}_x^2 + \overline{W}_y^2 + \overline{W}_z^2 \right) \right\} \quad (12)
 \end{aligned}$$

where $R_i = R_i \left(\frac{LL'}{\nu\nu'} \right)$ and $\overline{W}_i = \overline{W}_i (\nu\nu')$.

The summations are done using the position co-ordinates of the atoms of the neighbours of the eight atoms with the help of the interlattice displacements from eqs (7). Thus we have

$$\begin{aligned}
 \Delta\phi = k_2 \Big[& \eta_{xx}^2 (325/8) a^4 + \eta_{yy}^2 (325/8) a^4 + \eta_{zz}^2 (325/8) a^4 \\
 & + \eta_{xx}\eta_{yy} (239/8) a^4 + \eta_{xx}\eta_{zz} (239/8) a^4 + \eta_{yy}\eta_{zz} (239/8) a^4 \\
 & + \eta_{xy}^2 (122/3) a^4 + \eta_{xz}^2 (122/3) a^4 + \eta_{yz}^2 (122/3) a^4 \Big]. \quad (13)
 \end{aligned}$$

Comparing this with the energy density expression from continuum theory, we get the following expressions for the elastic constants of A-15 compounds,

$$\left. \begin{aligned}
 C_{11} &= (325/4) \frac{a^4}{V_2} k_2 \\
 C_{12} &= (239/8) \frac{a^4}{V_a} k_a \\
 C_{44} &= (61/3) \frac{a^4}{V_a} k_2
 \end{aligned} \right\} \quad (14)$$

where V_a is the volume of the unit cell and a is the nearest neighbour distance.

Table 1. Calculated values of the elastic constants, shear modulus, elastic anisotropy and bulk modulus of V_3Si , V_3Ge and Nb_3Sn .

Compound	$C_{11} \times 10^{12}$ dynes/cm ²		$C_{44} \times 10^{12}$ dynes/cm ²		Shear modulus $(C_{11} - C_{12})/2$ $\times 10^{12}$ dynes/cm ²		Elastic anisotropy $2C_{44}/(C_{11} - C_{12})$		Bulk modulus $(C_{11} + 2C_{12})/3$ $\times 10^{12}$ dynes/cm ²	
	Theory	Expt	Theory	Expt	Theory	Expt*	Theory	Expt*	Theory	Expt*
V_3Si	1.06	1.20 ^a	0.72	0.81 ^a	0.91	0.82	0.79	0.96	1.66	1.76
V_3Ge	1.09	1.04 ^b	0.74	0.70 ^b	0.94	0.96	0.79	0.63	1.71	1.68
Nb_3Sn	0.90	1.09 ^c	0.61	0.41 ^c	0.77	0.68	0.79	0.60	1.42	1.54

(a) Testardi *et al* (1965); (b) Rosen *et al* (1969); (c) Rehwald *et al* (1972); *Testardi (1973)

Here, we have considered the lattice contribution to the elastic constants. The A-15 compounds have a very narrow electronic *d*-band structure (Clogston and Jaccarino 1961) and the physical properties of the compounds can be explained in terms of this property. It has been suggested (Weger 1964) that their electronic properties are due to an extremely anisotropic band structure, which is a consequence of the particular crystallography emphasizing the one-dimensional chains of atoms in the β -tungsten structure. The electronic contribution to the elastic constants of A-15 compounds is significant and it can be calculated by expanding the internal energy as a power series in the strain components, and retaining the second-order terms. A theoretical model has been presented (Rosen *et al* 1969) which gives an estimate of the contribution of electronic states to the elastic constants, if the effect of strain on the shifting of the bands (the deformation potential) is known.

The elastic constants of V_3Si have been measured by Testardi *et al* (1965). The elastic constants of V_3Ge have been reported by Rosen *et al* (1969). Rehwald *et al* (1972) have measured the elastic constants of Nb_3Sn . Making use of these experimental values of C_{11} , we determine the interatomic potential parameter k_2 . Then this value of k_2 has been made use of to obtain the elastic constants for V_3Si , V_3Ge and Nb_3Sn . Table 1 gives the calculated values of the elastic constants of V_3Si , V_3Ge and Nb_3Sn together with the measured values. In the table we also report the calculated values of the shear modulus, elastic anisotropy and bulk modulus of V_3Si , V_3Ge and Nb_3Sn along with experimental values. The agreement between theoretical and experimental values is good. The discrepancy between theoretically calculated and experimental values of the elastic constants can be attributed as due to the negligence of the electronic contribution to the elastic constants of A-15 compounds.

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