# Gallium Arsenide

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**Abstract**

This review summarizes information on a few of the many physical properties of gallium arsenide. The crystal lattice and particularly the first Brillouin zone are described and related to the other properties in latter sections. Other aspects that are included are thermodynamic properties, mechanical properties and band structure.

First produced in the 1920s, gallium arsenide has had growing importance in semiconductor technology. medium grey in appearance, this substance can be cleaved most easily[1]. The two atom crystal structure is similar to a cubic Bravais lattice which affects many of its physical properties. Known as an intrinsic semiconductor with a direct band gap the conduction properties of gallium arsenide are well studied.

# 1 Lattice Structure and the Reciprocal Lattice

The crystal lattice of GaAs is a zinc blende structure. That is this structure is similar to the diamond lattice with the gallium atoms fixed on a face centered cubic (fcc) lattice and the arsenic on another fcc lattice. resulting from this structure is a translational fcc symmetry which is responsible for the structure of the first Brillouin zone. The unit cell for GaAs is shown in figure 1[1] and has a basis of one atom at (0,0,0) and the other at $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$. Four GaAs molecules fit within the unit cell, where the molecule is composed of an atom of gallium or arsenic surrounded by four atoms of the other species. The nearest neighbor bond length is $\frac{\sqrt{3}}{4}A$ ($A^3$ is the volume of the unit cell) and the seperation of the bonds is the tetrahedral bond angle[1].

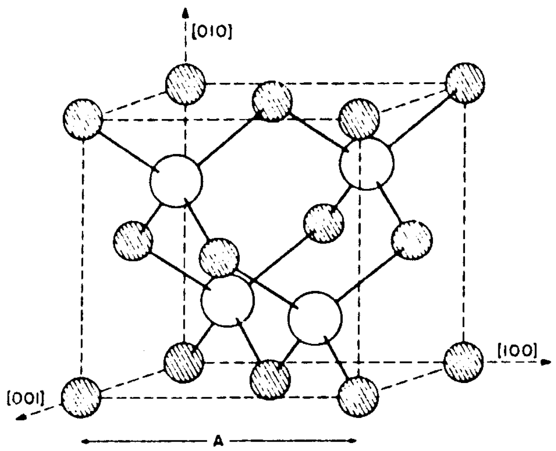


Figure 1: Crystal structure of GaAs.

Since the GaAs lattice has a translational fcc symmetry, the first Brillouin zone has the same structure as that which corresponds to a fcc crystal structure. In figure 2[1] the first Brillouin zone is represented as well as the points of high symmetry (K, L and X). Points U and K are seperated by the reciprocal lattice vector $\mathbf{G}_{1,1,\bar{1}}$ and hence are equivalent[1].The paths from the zone center ($\Gamma$) to the points of high symmetry have significance in the description of the band structure and the vibrational spectrum.

# 2 Dynamical and Thermal Properties

The elastic stiffness constants can be determined from the measurement of the speed of sound in the GaAs lattice. Then other related parameters, such as the Born ratio and

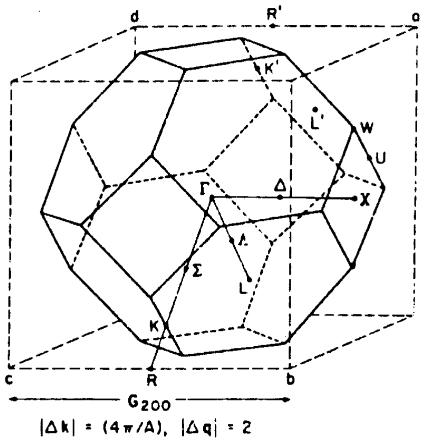


Figure 2: The first Brillouin zone.

the compressibility, can be expressed in terms of the elastic constants. Past measurments of the speeds of sound have indicated that GaAs is not isotropic in its elastic properties. This anisotropy is implied by the differing speeds of sound measured in different directions in the lattice. A perfect isotropic lattice would have a single value for the longitudinal sound speed and one value for the transverse speed of sound, irregardless of the direction of propagation. The tetrahedral bonds give rise to this anisotropy, since the bonds do not exhibit spherical symmetry[1].

The Born ratio is based on the simplest of nearest neighbor interactions. Theoretically, it is predicted to be unity. However, in GaAs (as well as other III-V semiconductors) the experimental measurement differs. This would suggest that more distant neighboring atoms have significant interactions. Also, it should be noted, that due to the simplicity of the model on which it is based, the Born ratio doesn't agree with experimental results[2].

As expected from a lattice with a two atom basis, the dispersion relation has both an acoustical and optical branch. The acoustical mode extends to $7 \times 10^{12}$ Hz and the optical to $9 \times 10^{12}$ Hz. Figure 3[1] shows the dispersion curves for GaAs at room temperature. The solid and dotted lines are two different fits of the data obtained by the inelastic scattering of slow neutrons. The dashed lines are slopes for many of the speeds of sound. As mentioned in the previous section points U and K on the boundary of the first Brillouin zone are equivalent. As a consequence of this the portion of the dispersion that represents K to R also represents the portion from U to X. In addition, the normal mode frequencies of X=(1,0,0) and R=$(1,\overline{1},0)$ are equivalent[1].

Heat in III-V compounds is transported primarily by phonons. The thermal conductivity ($\kappa$) increases with temperature in about the same manner as the heat capacity ($C_p$). However, the thermal conductivity maximizes at a particular temperature and becomes affected by impurities present in the material. As the temperature increases beyond this point, the thermal conductivity is dependent upon phonon - phonon scattering. At very high temperatures, electrons contribute to heat transport. Three phonon scattering gives rise to a $T^{-1}$ dependence in the thermal conductivity, yet the data suggests a $T^{\frac{-5}{4}}$ dependence. Four phonon scattering may account for this, but three phonon scattering including optical and acoustical phonons seems to be more accepted. Two types of three phonon processes contribute to thermal resistance. Normal phonon processes conserve momentum and change low momentum phonons into high momentum phonons. However, these processes could not account for the thermal

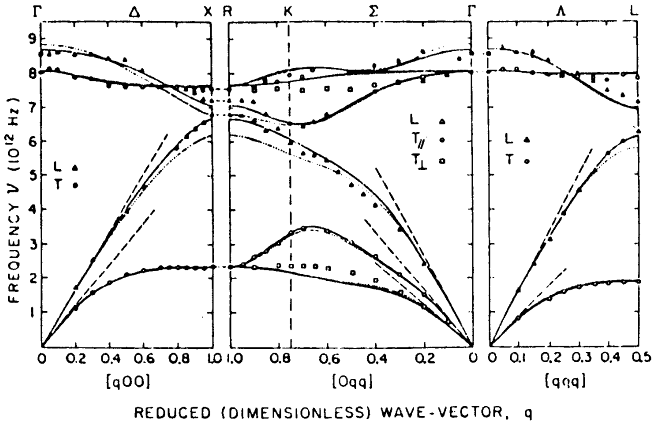


Figure 3: Dispersion curves.

resistance alone. The Umklapp processes are the other contribution and decrease quickly as temperature decreases[2].

The thermal conductivity also has a dependence on the heat capacity. The thermodynamic heat capacity (classical result) is $C_v$=3NK. This is not the quantity measured for a solid. The heat capacity that is measured is the heat capacity at constant pressure. Then it becomes necessary to measure $C_p - C_v$ which is given by $A{C_p}^2T$, where $A$ is a constant. Around the Debye temperature $C_p$ approximates the classical result[2].

# 3 Band Stucture

In the III-V coumpounds, bonding is mixed ionic and covalant. In the atomic basis on the unit cell, the 4s (As) and 4p (Ga) subshells provide the electrons for bonding[3]. The covalent bond has the structure $Ga^-As^+$ and the ionic $Ga^{+3}As^{-3}$. The actual bond can be considered a superposition of both ionic and covalent bonding. This structure has the form $Ga^{+x}As^{-x}$ where $x \simeq 0.4$. In order to preserve the tetrahedral bond structure, the bonding must be dominated by the covalant bond. This mixture of bonding creates a bond that is stronger than a purely covalent bond[1].

The band structure of GaAs is shown in figure 4[5]. GaAs has what is known as a direct band gap, that is the minima of the conduction band coincides with the maxima of the valance band at $\Gamma$[4]. The energy gap lies btween $\Gamma_8$ and $\Gamma_6$.

GaAs is also an intrinsic semiconductor. The thermal excitation of an electron to the conduction band results in a hole in the valance band. Both holes and electrons are fermions, so the density of states (g($\epsilon$)) for both the valance and conduction bands becomes important. The density is zero between $g_c(\epsilon)$ (conduction) and $g_v(\epsilon)$ (valance)[3]. This is a manifestation of the energy gap in the band structure. The density of states also depends upon the effective mass ($m^*$) of the electrons and holes. The effective mass is a consequence of the charge carriers moving in a lattice as opposed to a vacuum. Also diamagnetic or paramagnetic behavior of the charge carriers is related to the effective mass[4].

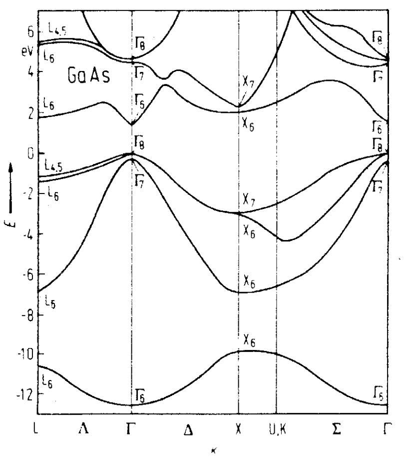


Figure 4: Band structure.

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|---|---|---|
| Lattice constant (300K)[6] | $A$ | 5.65325 Å |
| Volume of unit cell (300K)[1] | $A^3$ | $1.80674 \times 10^{-22} \AA^3$ |
| Nearest neighbor distance (300K)[6] | $\frac{\sqrt{3}}{4}A$ | 2.44793 Å |
| Bond angle[1] | $\phi$ | $109.47^o$ |
| Elastic stiffness constants[6] | $C_{11}$ | $1.174 \times 10^{11} NM^{-1}$ |
| | $C_{12}$ | $0.526 \times 10^{11} NM^{-1}$ |
| | $C_{44}$ | $0.597 \times 10^{11} NM^{-1}$ |
| Born ratio (298K)[7] | $\frac{4C_{11}(C_{11}-C_{44})}{(C_{11}+C_{12})^2}$ | 0.948 |
| Thermal conductivity (300K)[6] | $\kappa$ | $0.54 Wcm^{-1}$ |
| Molar heat capacity[6] | $C_p$ | $47.026 Jmol^{-1}K^{-1}$ |
| Energy gap[8] | $E_g$ | $1.424 ev$ |

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