Indium Phosphide (InP)

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Abstract

In recent years there has been considerable interest in indium phosphide (InP) and related alloys because of their applications in many electronic and photonic devices. This review summarizes bonding structure, band structure, and material properties of Indium Phosphide.

1   Bonding Structure

InP crystalizes in the cubic zinc blende (sphalerite) structure with density 4.81 gcm^{-3}, which consists of two interpenetrating fcc lattices, one shifted by $a/4$ [111] (a = 5.8687Å at 291.15 K) relative to the other fcc lattice. The two fcc lattices are occupied by two different atoms, i.e., In and P. The cubic unit cell of a sphalerite structure is shown in $Figure$ 1.[2]

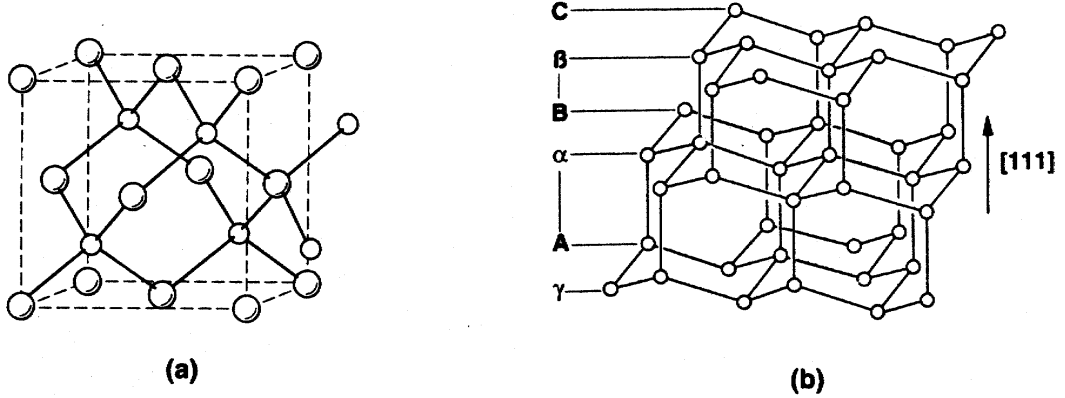(a)   (b)

Figure 1: *(a) The sphalerite structure; (b) stacking of (111) planes in the sphalerite structure. ABC... is the stacking order in one fcc lattice and $\alpha\beta\gamma$ is the stacking order in the other.[2]*

Although the bonding in the sphalerite structure consists of sp^3 hybridized orbitals, unlike in diamond cubic semiconductors, there is some charge transfer between the two types of atoms giving rise to a partial ionic character to the bonding. If f_i and f_c denote the fractions, respectively, of ionic and covalent character in the bond, then the sum $f_i + f_c$ equals unity. The f_i value of InP is 0.421.[3]

2   Band Structure

InP is a direct band gap semiconductor. The *conduction band* minimum is situated Γ. Higher conduction band minima at L and X have been detected in optical experiments. The X band minima show no camel's back structure, in contrast to most other $III - V$ compounds with zinc blende structure. The *valence band* has the structure common to all zinc blende type semiconductors.[4] The Γ point (k = 0,0,0) which is the point of highest symmetry in the Brillouin zone is the most suitable point to use as the basis for a $k \cdot p$ representation to cover the entire zone. Semiconductors with tetrahedral coordination have valence band maxima at the Γ point and many have conduction band minima also at the Γ point (e.g., $GaAs$, InP). The valence band maxima are derived from the p-like orbitals p_x, p_y, p_z, which remain degenerate under the tetrahedral group of the zinc blende lattice.[3]
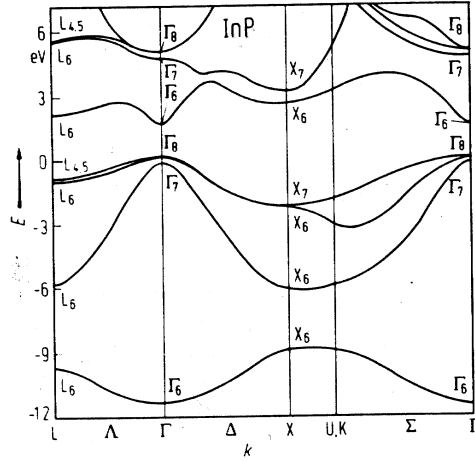
Figure 2: *Band structure obtained with a non-local pseudopotential method.[5]*

3   Material Properties

Elastic properties and sound velocity   For a cubic crystal, and so for InP, there are three independent elastic constants S_{11}, S_{12}, and S_{14}. The elastic compliance relates strain ϵ_i to stress σ_j, $\epsilon_i = \Sigma_j S_{ij}\sigma_j$. In covariant form $\sigma_i = \Sigma_j C_{ij}\epsilon_j$, where C_{ij} are the elastic stiffness constants. For a cubic crystal C_{ij} are related to S_{ij} according to

$$C_{11} = \frac{S_{11} + S_{12}}{S}, \quad C_{12} = \frac{-S_{12}}{S}, \quad C_{44} = \frac{1}{S}$$

where $S = (S_{11} - S_{12})(S_{11} + 2S_{12})$. From the point of practical utility, the elastic constants of interests are the Young's modulus E and the Poisson's ratio ν. In the cubic crystals both E and ν are anisotropic.[3]

Sound velocity of InP is strongly dependent on the propagation directions. The bulk sound velocity v (long-wave length, nondispersive) can be calculated by the equation,

$$v = \sqrt{\frac{C_{ij}}{g}}$$

where g is the crystal density.[1]

Optical Properties $In_{1-x}Ga_xAs_yP_{1-y}/InP$ hetrostructures become increasingly interesting as light sources and detectors for optical fiber communication systems in the $1.4 \sim 1.7$ μm wavelength region. Knowledge of optical properties is very important in the design and analysis of such optoelectronic devices.[1] The optical absorption of solids can be described either by the complex index of refraction $n + ik$ or by the comlpex dielectric function $\epsilon_1 + i\epsilon_2$, where n, k, ϵ_1, and ϵ_2 are all real functions of the frequency ω. The functions $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ are connected by the Kramers-Kroenig relations,

$$\epsilon_1 = n^2 - k^2, \quad \epsilon_2 = 2nk$$

The absorption coefficient α is related to k by $\alpha = 2\omega k/c$, where k is the imaginary part of the refractive index and c is the extinction coefficient. For InP, refractive index $n = 3.41$ near

the band gap energy E_g, dielectric constants $\epsilon(0) = 12.61$ and $\epsilon(\infty) = 9.61$, and temperature dependence $\frac{1}{n}\frac{dn}{dT} \simeq 2.7 \times 10^{-5} K^{-1}$.[2]

Thermal Properties   The measured C_p for InP is nearly the same as C_v at temperatures below 70 K, but exceeds C_v above 70 K as a result of thermal expansion of the crystal lattice.[1] Thermal resistivity of semiconductors is an important parameter in the design of power-dissipating devices such as semiconductor lasers. It is also important in calculating the figure of merit of thermoelectric devices. For InP near room temperature, coefficient of thermal expansion is 4.75×10^{-6} $/^\circ C$ and thermal conductivity 0.68 $W cm^{-1} K^{-1}$.[2]

Dispersion Curves   Research on the crystal dynamics of perfect lattices has aroused considerable interest in compounds having a zinc blende structure. This development is the outcome of many experimental results, particularly inelastic neutron scattering data for phonon dispersion curves.
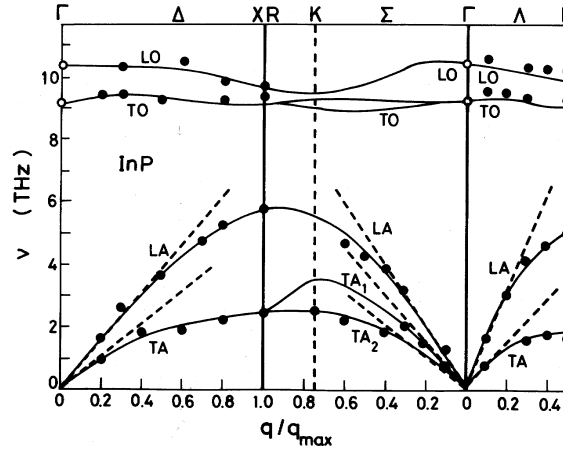

Figure 3: *Phonon dispersion curve of InP.[1]*

In *Figure* 3 the phonon frequency (ν) versus reduced wave vector (q) results for **q** along the principal symmetry directions [100], [110], and [111] of InP at room temperature, as obtained from these studies. The solid circles are the neutron scattering data, and the solid lines are calculated results. The open circles show the values of zone-center LO and TO phonon frequencies obtained from Raman scattering data. The dashed lines near **q** $\to$ 0, $\nu \to$ 0 represent the initial slopes of the acoustic modes as calculated from the sound velocities. It is recognized that the dispersion curves of InP exhibit major features similar to those of other zinc blende crystals, such as $GaAs$, GaP, $InSb$, $GaSb$, $CdTe$, $ZnTe$, and $ZnSe$.[1]

Transport Properties   The transport in n-type samples is determined up to 800 K by the electrons in the Γ_{6c}-minimum. Only at very high temperatures L_{6c}-electrons contribute to the conductivity. In high purity samples polar scattering dominates at room temperature. Mobility values for single crystal and poly crystalline samples are mostly lower. Best values at 300 K are around 4000 cm^2/Vs. At 77 K values up to 130,000 cm^2/Vs have been reported in [6].

Impurities and Defects   Discrimination of donor chemical species is made difficult because of the small electron effective mass ($m_c^* < 0.1 m_0$) and large dielectric constant ($\epsilon_s \simeq 12$).

This leads to small values of electron binding energy at donor states. The effective mass donor Rydberg for InP is 7.31 meV. Zinc and Carbon are often common residual acceptors in InP. The Group IV elements, except for C and Ge do not substitute for P, and so show no amphoteric behavior.[4]

References

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