

Electronic Structure and Forbidden Energy in AlAs Crystalline Alloy

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We present the energy bands and the DOS, the forbidden energy and total energy of the crystalline compound of AlAs, calculated with the LMTO orbital method within the framework of density functional theory (DFT). We solved the Schrödinger equation with a potential in the local density approximation (LDA) that uses the Barh-Hedin approximation for the term exchange and correlation. Potential calculated with a small homogeneous fraction of electron charge in the empty spheres and an electronic charge similar to that of the free atom in the atomic spheres of the crystal lattice. The structure of the energy bands presented an indirect forbidden energy gap of 0.160Ry or 2.18 eV with a minimum total energy of -18.10 Ry that fit well with the experimental results.

Keywords: energy bands, LMTO orbitals, semiconductors

INTRODUCTION

The study of the electronic properties of materials is of great importance in solid-state physics; knowing the structure of energy bands, the density of DOS states, and the forbidden energy gap allows us to determine other physical properties of semiconductor materials. In the last two decades, studies of the electronic structure of the aluminum arsenide alloy were published, the band parameters were calculated with different approaches and different methods.

In 2013 Wang, (Wang et al., 2013) published a study of the electron structure of zinc blende crystalline phase wings, reporting energy band parameters, with an indirect forbidden energy gap of 2.240 eV for AlAs calculated with first principles and using the recent semi local Tran and Blaha approximation for exchange energy in the potential (Tran & Blaha, 2009); a few years earlier in 2005, Jivani presented a study of the electronic structure parameters, total energy and other properties of AlAs, reporting an direct gap of 3.57 eV at point G calculated with a potential combining both linear and quadratic interactions using higher-order perturbation theory (Jivani et al., 2005).

The calculation of band structure for semiconductors within the framework of the theory of the generalized density function of Remediakis and Kaxiras, (Remediakis & Kaxiras, 1999) reporting the energy bands of AlAs calculated using the correction for excited states proposed by Fristche and Gu,

(Fritsche, 1991); In 2001 Vurgaftman published a study of the electronic structure of III-V semiconductor materials and their compounds (Vurgaftman et al., 2001), in which the energy band parameters of AIAs are calculated with an approximation of envelope function, called the $\vec{k} \cdot \vec{P}$ multiband method, and the theory of disturbance in the vicinity of some special point in the Brillouin zone.

The electronic structure of AIAs calculated in this work was obtained using the model reported by Cabrera for the study of the electronic system in AIP alloy calculated with the LMTO method (Cabrera, 2018), which solves the Schrödinger equation for the crystalline solid with effective potential that uses the LDA approximation (Hohenberg & Kohn, 1964) for the term of exchange and correlation reporting an electronic structure of the AIP semiconductor compound that fit well with experimental data reported in the specialty literature. Since the AIAs compound has a zinc blende crystal structure, similar to the crystal structure of AIP, this model used was very well adapted when performing the calculations of the electronic structure of the AIAs utilizing the method of linear orbitals muffin-tin LMTO (Andersen et al., 2007).

THEORETICAL FOUNDATION

Kohn's Density Functional Theory (DFT), the electronic structure of matter is based on Schrödinger's non-relativistic equation for a many-electron system with wave function Ψ and energy E , which is written in atomic units (Kohn, 1999):

$$\left\{ -\frac{1}{2} \sum_j \nabla_j^2 - \sum_{j,l} \frac{Z_l}{|\vec{r}_j - \vec{R}_l|} + \frac{1}{2} \sum_{j \neq j'} \frac{1}{|\vec{r}_j - \vec{r}_{j'}|} - E \right\} \Psi = 0 \quad (1)$$

That according to the Hohenberg-Kohn variational principle, E is of minimum value for a correct electron charge density $\rho(r)$ of the ground state, (Hohenberg & Kohn, 1964). Electron charge density that depends on the wave function ψ_j of an electron, defined as:

$$\rho(r) = \sum_{j=1}^n |\psi_j|^2 \quad (2)$$

The formal application of the calculus of extreme values to equation (1) and not detailed here, leads the problem of the Schrödinger equation for a system of many electrons, to a problem of solving the self-consistent Schrödinger equation of a single electron moving in a field of effective potential, which is written as:

$$\left\{ \frac{1}{2} \nabla^2 + V_{ef}(r) - \epsilon_j \right\} \psi_j = 0 \quad (3)$$

An electron interacting with an effective potential $V_{ef}(r)$ that depends on the crystalline properties and electron charge density in the crystal lattice of the solid under study. For open crystal structures such as the zincblende lattice of the AIAs, this effective potential depends additionally on the small fraction of the electronic charge residing in the empty spheres of the lattice and written in atomic units, is:

$$V_{ef}(r) = v(r) + \frac{1}{2} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' + V_{xc}(\vec{r}) \quad (4)$$

In which the last term is the $V_{xc}(r)$ exchange potential and correlation with functional dependence of the unknown electron charge density $\rho(r)$ and is usually treated with approximations. Here the exchange and correlation potential used is the approximation of a homogeneous gas of electrons of polarized Bar-Hedin spin, with the approach of McLaren, (MacLaren et al., 1991). This set of equations is known as the Kohn-Sham self-consistent equations for the calculation of electronic structure. The total energy for the ground state of the system is given by:

$$E = \sum_j \epsilon_j + E_{xc}[\rho(r)] - \int V_{xc}(r)\rho(r)dr^3 - \frac{1}{2} \int dr^3 \int \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} dr'^3 \quad (5)$$

Equation that we can calculate, because solved the Schrödinger equation, the energy eigenvalues ϵ_j and wave functions are already known. The term $E_{xc}[\rho(r)]$ is the exchange and correlation energy treated with the Barh-Hedin approximation.

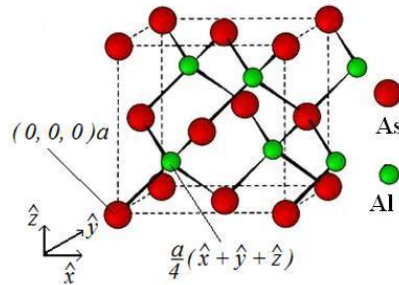
TABLE 1
LATTICE AND RADIUS CONSTANT OF THE ATOMIC AND EMPTY SPHERES OF THE ALAS LATTICE

a (Å)	R_{Al} (au)	R_{As} (au)	R_3 (au)	R_4 (au)
5.62	2.522	2.745	2.522	2.745

MATERIAL AND METHODS

The compound of AlAs its ground state adopts the cubic crystal structure type zinc blende with atoms of different class. The crystal lattice was filled with atomic spheres of different size and with empty spheres on the diagonal of the lattice, the size of the other atomic spheres, so that the radius R_{WS} were calculated preserving the symmetry and density of the Winged material. Table 1 shows the lattice parameter and the radius of the four spheres occupying the unit cell volume, necessary for the calculation of the effective potential $V_{ef}(r)$ that will be used to solve the Schrödinger equation of the crystal lattice of AlAs.

FIGURE 1
CRYSTAL STRUCTURE OF ALAS



Fountain:

The calculation of the electronic structure and the total energy of this alloy was carried out in stages. First stage: The effective potential of the arsenic atoms, aluminum and the two empty spheres that fill the unit cell of the crystal lattice was calculated. Potential with functional dependence of the electronic charge and $\rho(r)$ a small fraction of the q_R external electronic charge residing in the empty spheres of the network, model used by Cabrera Arista to calculate the electronic structure of GaP and SiC, (Cabrera, 2017). For a zinc blende crystal lattice formulated in the approximation of the atomic spheres ASA, (Skriver, 1984), this potential is the form:

$$V_{ef}(r) = -\frac{ZZ}{r} + \frac{2}{r} \int_0^r 4\pi(r')^2 \rho(r') dr' + 2 \int_r^{S_{\vec{R}}} \frac{4\pi(r')^2 \rho(r')}{r'} dr' + 2v_{xc}(r) - \sum_{\vec{R}'}^4 \sum_{\vec{T}'} \frac{2q_{\vec{R}'}}{|\vec{R}-\vec{R}'-\vec{T}'|} \quad (6)$$

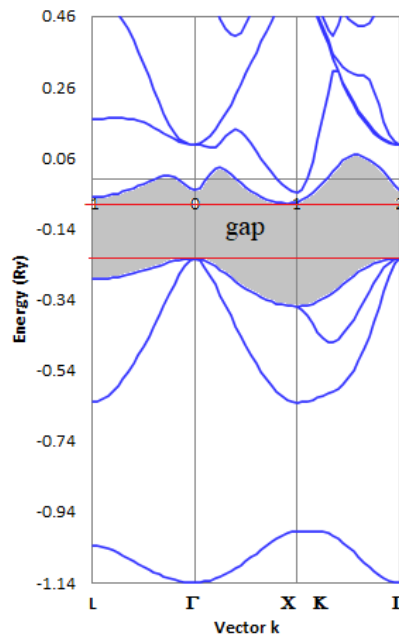
In the last term of this potential, \vec{R} it denotes the position of the empty sphere in the center of the diagonal and the position of the empty \vec{R}' sphere located 3/4 of the diagonal and the position of the \vec{T}' other

empty spheres within the crystal lattice. For the end $v_{xc}(r)$ was used the approximation the power of exchange and correlation of a homogeneous gas of electrons of polarized spin, (MacLaren, 1991). Second stage: The Schrödinger equation for the crystal lattice of this alloy of Wings is solved with this effective potential $V_{ef}(r)$ and the LMTO orbital method., which leads us to the problem of solving the calculation of the energy eigenvalues in ϵ_j reciprocal space and in the crystallographic directions of high symmetry that the wave vector takes \vec{k} . These self-values constitute the structure of the energy bands and which in turn allows to calculate the density of occupied states (DOS) of the crystalline solid. Third stage: The energy total was calculated by solving the integrals of equation (5) using the electron charge density of the crystal lattice and the energy eigenvalues already known when determining the energy bands.

RESULTS

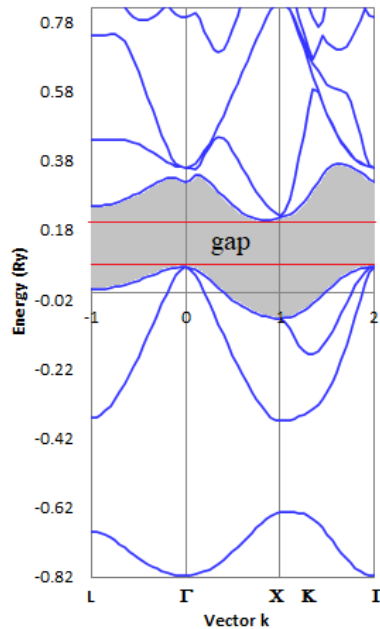
The dispersion ratio $\epsilon = \epsilon(k)$ was calculated for different values of g , which describes that small fraction of the external electronic charge returning to its atomic sphere and the rest residing in the empty spheres.

FIGURE 2
ENERGY BANDS OF ALAS OBTAINED FOR $g = 0.0$, ALL THE SMALL CHARGE Q_R
RESIDING IN THE EMPTY SPHERES OF THE NETWORK



The results calculated for the case of $g = 0.0$ presented in Figure 2, corresponds to the entire fraction of the external load q_R residing in the empty spheres of the network. The structure of the energy bands shows an indirect gap of forbidden energy, between the top of the valence band located at point G_{25} and the bottom of the conduction band located at point C_5 . The profile of the band structure is similar to that reported by Vurgaftman and Meyer (Vurgaftman et al., 2001), or Wang (Wang et al., 2013) and others.

FIGURE 3
ENERGY BANDS OF ALAS OBTAINED FOR $g = 1.0$, ALL THE SMALL CHARGE q_R
RESIDING IN OWN ATOMIC SPHERES OF THE NETWORK



The structure of energy bands obtained for $g = 1.0$, which corresponds to the case of empty spheres without any fraction of the charge, q_R is shown in Figure 3. Here the profile of the band structure also presents an indirect gap of forbidden energy, but of smaller magnitude. Next, we present the energy values of the main directions of high symmetry of the crystal lattice. Energies obtained from the band structure calculated for $g = 0.0$, which is associated with the minimum total energy calculated here.

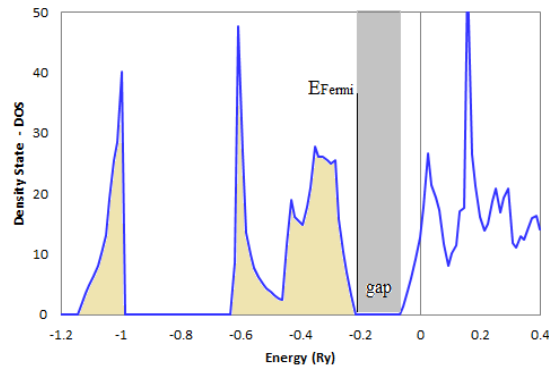
TABLE 2
ENERGY GAP E_G OF THE POINTS OF SYMMETRY G, C AND L WITH RESPECT TO POINT
G, OBTAINED HERE. E_A OBTAINED BY WANG (WANG ET AL., 2013),
 E_B EXPERIMENTAL VALUE VURGAFTMAN

<i>PS</i>	E_g (Ry)	E_g (eV)	E_a (eV)	E_b (eV)
G	0.194	2.64	3.087	3.099
C	0.160	2.18	2.24	2.24
L	0.174	2.36	2.8	2.46

Vurgaftman et al., 2001

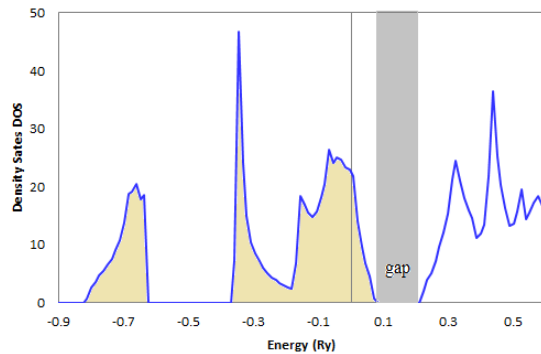
The DOS was calculated for all those values of g used in the calculation of the energy bands of Wings. Figure 4 shows the DOS obtained with $\square = 0.0$, these results confirm the indirect gap of prohibited energy already obtained in the structure of the energy bands, as can be seen in the top of the states of Valencia (yellow region) and the background of the conduction states (region without color).

FIGURE 4
THE DENSITY OF STATES CALCULATED WITH $G = 0.0$, ALL THE SMALL CHARGE q_R
RESIDING IN THE EMPTY SPHERES OF THE NETWORK



The DOS calculated for the other values of g present a slight shift of energy from the valence states and an appreciable decrease in the energy gap, which is observed up to the DOS calculated with $g = 0.8$. This shift is modified in the DOS calculated with $g = 1.0$, with all that small fraction of electronic charge of external valence, residing in its own atomic sphere of the crystal lattice.

FIGURE 5
THE DENSITY OF STATES CALCULATED WITH $G = 1.0$, ALL THE SMALL CHARGE q_R
RESIDING IN OWN ATOMIC SPHERES OF THE NETWORK

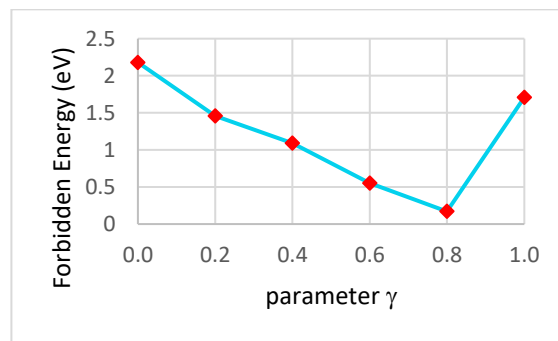


The forbidden energy, gap between the minimum point of the conduction band and the top point of the valence band, was obtained indirectly from the structure of the energy bands calculated for each value of g , the results shown in Table 3.

TABLE 3
FORBIDDEN ENERGY GAP E_g , FERMI ENERGY E_F AND TOTAL ENERGY E_T OF ALAS,
CALCULATED FOR FRACTIONS OF THE SMALL ELECTRONIC CHARGE q_R RESIDING
IN ITS OWN ATOMIC SPHERE AND IN THE EMPTY SPHERES OF THE LATTICE

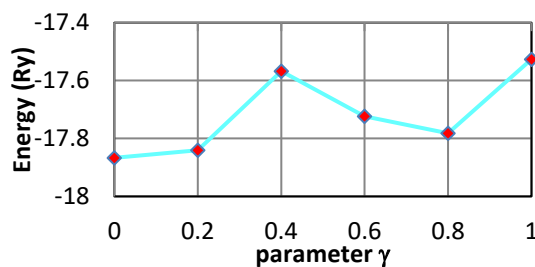
g	E_g (eV)	E_F (Ry)	E_T (Ry)
0.0	2.18	-0.218	-18.1
0.2	1.46	-0.165	-18.04
0.4	1.09	-0.118	-17.76
0.6	0.55	-0.065	-17.81
0.8	0.17	-0.004	-17.86
1.0	1.71	0.084	-17.54

FIGURE 5
FORBIDDEN ENERGY GAP OF ALAS IN EV, CALCULATED FOR FRACTIONS OF THE
SMALL ELECTRONIC CHARGE RESIDING IN ITS OWN ATOMIC SPHERE AND IN
THE EMPTY SPHERES OF THE RED



The total energy calculated for different fractions of the small electronic charge q_R residing in its own sphere and in the empty spheres on the diagonal of the lattice, are also presented in Table 3. The results show a minimum total energy for $g = 0.0$.

FIGURE 6
THE TOTAL ENERGY, IN RY UNIT, OBTAINED FOR EACH OF THE ENERGY BANDS



CONCLUSIONS

For this alloy of AlAs, the best calculated electronic structure is that obtained for the case of the entire small fraction of the external electronic charge q_R residing in the empty spheres of the crystal lattice. The

structure of energy bands with an indirect forbidden energy gap of 2.18 eV, Confirmed by the profile of the density of states both calculated for $g = 0.0$ fit very well to the values obtained with other methods such as: that of 2.18 eV reported by Johnson and Ashcroft (Johnson & Ashcroft, 1998); with a difference of 2.17% of the value 2.24 eV reported by Vurgaftman and Meyer (Vurgaftman (Vurgaftman et al., 2001)with a difference of 15.3% of the value 2.573 eV reported by Remediakis and Kaxiras (Remediakis & Kaxiras, 1999).

The results show that the total energy of the alloy of Wings is minimized to $g = 0.0$, Case in which the entire small fraction of the external electronic charge q_R is residing in the empty spheres of the crystal lattice. With a minimum energy of -18.10 Ry obtained with $g = 0.0$, which implies greater stability of the system. This allows us to conclude that the LMTO method and the density functional theory (DFT) are good for a theoretical study of the electronic structure of materials and alloys.

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