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Characterization of Aluminum Gallium Arsenide ($Al_xGa_{1-x}As$) Semiconductors Using MATLAB

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A semiconductor is a material that has electrical properties somewhere in the middle, between those of an insulator and a conductor. It is neither a good insulator nor a good conductor (called a semiconductor). It has very few free electrons because its atoms are closely grouped together in a crystalline pattern called a crystal lattice, however, electrons are still able to flow, but only under special conditions. One of the principal characteristics of semiconductors is that they can be doped with impurities to alter their electrical properties. The semiconductor properties are characterized by the band theory. This model states that an electron in a solid can only take on energy values within certain ranges called permitted bands, which are separated by other bands called band gaps. These materials are mainly used in electronics (diodes, transistors, etc.), microelectronics for integrated circuits, solar cells and optoelectronic devices such as light emitting diodes (LEDs). III-V semiconductors are of great interest because of their properties, they are robust, have a high thermal conductivity and a direct band gap. Devices and circuits in the III-V semiconductor group were always known by their high speed, but also by their expensive production and lower integration compared to silicon-based ones. In this paper, models for the effective density of states (N_c and N_v) in the conduction and valence bands, intrinsic carrier density n_i, temperature dependence of the energy band gap (E_g) and doping dependence of the energy band gap (E_g) of aluminum gallium arsenide ($Al_xGa_{1-x}As$) semiconductors are analyzed using MATLAB for different values of x ($0 \le x \le 1$).

Keywords: AlGaAs, GaAs, AlAs, Temperature, III-V semiconductors, Energy bands, Density of states, Intrinsic carrier density.

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1. INTRODUCTION

A semiconductor [1, 2] is a crystalline material that has electrical characteristics intermediate between those of metals and insulators. Semiconductor materials are insulators at absolute zero that conduct electricity to a limited extent at room temperature. Semiconductors are widely used in modern electronics, integrated circuits, optoelectronics, photonics, semiconductor devices, etc. [2-8]. The electrical behavior of semiconductors is generally modeled in quantum physics of solids using the energy band theory. A semiconductor material has a sufficiently small band gap so that electrons of the valence band can easily reach the conduction band. If an electric potential is applied to its terminals, a weak electric current appears, caused both by the movement of electrons and the movement of holes that they leave in the valence band.

Semiconductors are classified according to their chemical composition. There are elementary semiconductors, all belonging to group IV of the Periodic Table, such as silicon (Si) and germanium (Ge). There are also composite semiconductors, binary, ternary, quaternary or quinary, which respectively consist of two, three, four or five different chemical elements. The most common are III-V semiconductors, consisting of group III elements (aluminum, gallium, indium, etc.) and group V elements (nitrogen, phosphorus, arsenic, antimony, etc.), such as gallium arsenide, indium arsenide, gallium nitride, gallium antimonide, boron phosphide or ternary alloys such as aluminum gallium arsenide ($Al_xGa_{1-x}As$) [9-12].

This paper describes the characterization of the effective density of states (effective density of states in the valence and conduction bands), intrinsic carrier density and other important characteristics (temperature dependence of the energy band gap (E_g) and doping dependence of the energy band gap (E_g)) of $Al_xGa_{1-x}As$ semiconductors using MATLAB for different values of x ($0 < x \le 1$).

2. CHARACTERIZATION OF ALUMINUM GALLIUM ARSENIDE ($Al_xGa_{1-x}As$)

III-V semiconductors [13-16] crystallize in the zinc-blende structure. It consists of two interpenetrating subface-centered cubic lattices (FCC), one of which is formed by group III elements and the other by group V elements. These semiconductors have essentially covalent bonds with shared electrons between an element III atom and an element V atom in sp^3 hybrid orbitals.

The following expression presents the temperature dependence of the energy band gap (E_g) of semiconductors:

$$E_g = E_g(0) - \frac{\alpha T^2}{T + \beta}, \quad (1)$$

where E_g (0), α and β are material constants [17].

The doping dependence of the energy band gap (E_g) of semiconductors is given by [17]:

$$\Delta E_g(N) = -\frac{3q^2}{16\pi\varepsilon_s}\sqrt{\frac{q^2 N}{\varepsilon_s kT}}, \quad (2)$$

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where N is the doping density, q is the electron charge, ε_s is the dielectric constant of the semiconductor, k is the Boltzmann constant, T is the temperature in Kelvin (300 K).

Table 1 lists the parameters used to calculate E_g of AlAs and GaAs as a function of temperature T.

Table 1 – Parameters used to calculate E_g of AlAs and GaAs as a function of temperature T [17, 18]

	AlAs	GaAs
$E_g(0)$ (eV)	2.239	1.519
α (eV/K)	$0.6 \cdot 10^{-3}$	$0.541 \cdot 10^{-3}$
β (K)	408	204

The effective density of states in the conduction band N_c is given by:

$$N_c = 4,82 \cdot 10^{15} \left(\frac{m_e}{m_0} \right)^{3/2} \cdot T^{3/2} \text{ for } x < 0.41, \quad (3)$$

$$N_c = 4,82 \cdot 10^{15} \left(\frac{m_{cd}}{m_0} \right)^{3/2} \cdot T^{3/2} \text{ for } x > 0.41. \quad (4)$$

The effective density of states in the valence band N_v is given by:

$$N_v = 4,82 \cdot 10^{15} \left(\frac{m_h}{m_0} \right)^{3/2} \cdot T^{3/2}, \quad (5)$$

where m_0 is the free electron rest mass, m_e, m_{cd} and m_h are the effective electron mass for $x < 0.41$, effective mass of the density of states for $x > 0.41$ and effective hole mass, respectively.

The intrinsic carrier density n_i is given by:

$$n_i = \left(N_c \cdot N_v \right)^{1/2} \exp\left[-\frac{E_g}{2kT} \right]. \quad (6)$$

Aluminum gallium arsenide (AlGaAs, $Al_xGa_{1-x}As$) is a semiconductor compound of the elements gallium, arsenide and aluminum, x ($0 \le x \le 1$) is the ratio of these components in the chemical formula $Al_xGa_{1-x}As$. It is an alloy of aluminum arsenide (AlAs) and gallium arsenide (GaAs). It is a direct band gap semiconductor for $x < 0.45$ and an indirect band gap semiconductor for $x > 0.45$ with a zincblende crystal structure (Fig. 1).

The lattice parameter of such a structure depends on the nature of the chemical elements involved. The crystal lattice is much greater than the atomic number of its constituting elements. Thus, in the case of a ternary structure of $Al_xGa_{1-x}As$, indium incorporation in the crystal lattice of GaAs increases the lattice parameter (a) of the alloy. Usually for $Al_xGa_{1-x}As$, we consider this variation as quasi-linear and given by Vegard law:

$$a_{AlGaAs} = a_{GaAs} + \left(a_{AlAs} + a_{GaAs} \right) x. \quad (7)$$

Aluminum arsenide (AlAs) is a semiconductor material that has almost the same lattice constant as that of gallium arsenide (GaAs). It can form a super-lattice with gallium arsenide which results in its semiconductor properties. AlAs and GaAs find applications in the following areas:

- Optoelectronic devices,
- Solar cells,
- Quantum well devices,
- High-electron-mobility transistors.

Aluminum gallium arsenide is used as a barrier material in GaAs based heterostructure devices. The AlGaAs layer confines the electrons to a gallium arsenide region. An example of such a device is a quantum well infrared photodetector (QWIP) [19, 20].

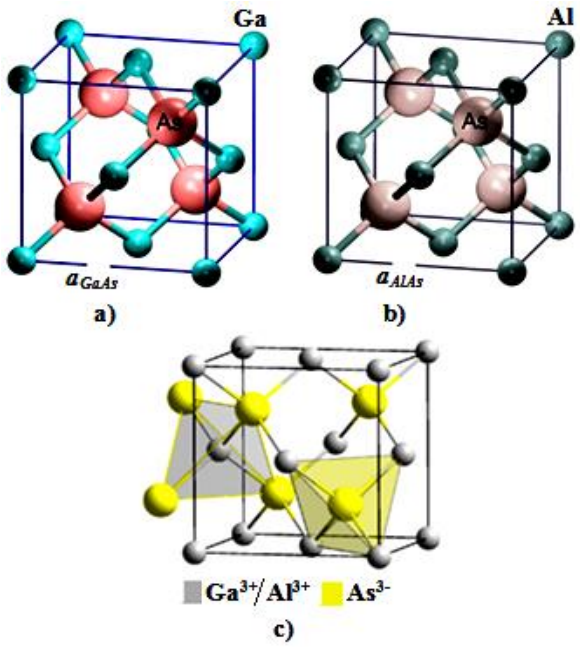

Fig. 1 – Zincblende crystal structure: a) gallium arsenide ($x = 0$), b) aluminum arsenide ($x = 1$), c) aluminum gallium arsenide ($0 < x < 1$)

3. RESULTS AND DISCUSSION

In this section, the effective density of states in the conduction and valence bands (Fig. 2 and Fig. 3), the intrinsic carrier density (Fig. 4 and Fig. 5), the temperature dependence of the energy band gap (E_g) (Fig. 6) and the doping dependence of the energy band gap (E_g) (Fig. 7) of $Al_xGa_{1-x}As$ semiconductors are treated under MATLAB for different value x ($0 \le x \le 1$).

From the results obtained (Fig. 2, Fig. 3), the effective density of states N_c in the conduction band (Fig. 2) at room temperature (300 K) for GaAs is $4.34 \cdot 10^{17}$ cm^{-3}, for AlAs is $1.5 \cdot 10^{19}$ cm^{-3}, for $Al_{0.3}Ga_{0.7}As$ is $6.97 \cdot 10^{17}$ cm^{-3} and for $Al_{0.6}Ga_{0.4}As$ is $1.68 \cdot 10^{19}$ cm^{-3}, and the effective density of states N_v in the valence band (Fig. 3) at room temperature (300 K) for GaAs is $7.56 \cdot 10^{18}$ cm^{-3}, for AlAs is $1.31 \cdot 10^{19}$ cm^{-3}, for $Al_{0.3}Ga_{0.7}As$ is $9.12 \cdot 10^{18}$ cm^{-3} and for $Al_{0.6}Ga_{0.4}As$ is $1.07 \cdot 10^{19}$ cm^{-3}.

From the results obtained (Fig. 4 and Fig. 5), the intrinsic carrier density n_i at room temperature (300 K) for GaAs is $2.15.10^6$ cm^{-3}, for AlAs is 10.2 cm^{-3}, for $Al_{0.3}Ga_{0.7}As$ is $2.01 \cdot 10^3$ cm^{-3} and for $Al_{0.6}Ga_{0.4}As$ is $1.30 \cdot 10^2$ cm^{-3}.

From the results obtained (Fig. 6, Fig. 7), the energy band gap E_g of semiconductors tends to decrease as the temperature T is increased (Fig. 6). This effect can

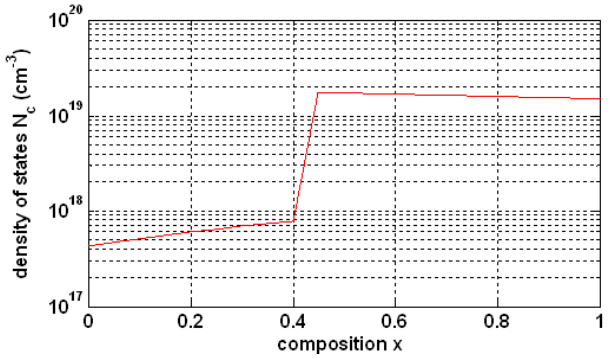

Fig. 2 – Effective density of states N_c versus composition x

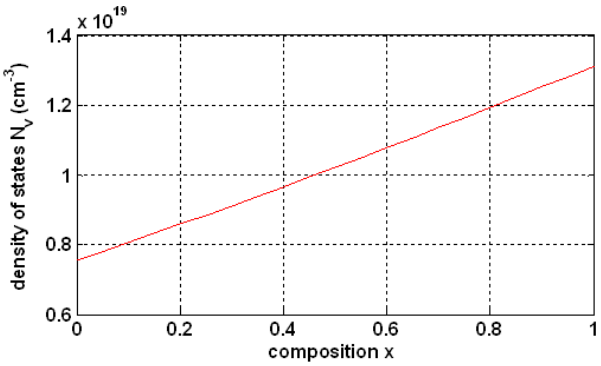

Fig. 3 – Effective density of states N_v versus composition x

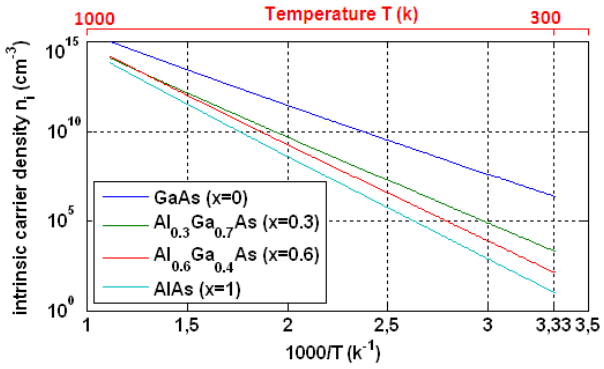

Fig. 4 – Intrinsic carrier density n_i versus $1000/T$

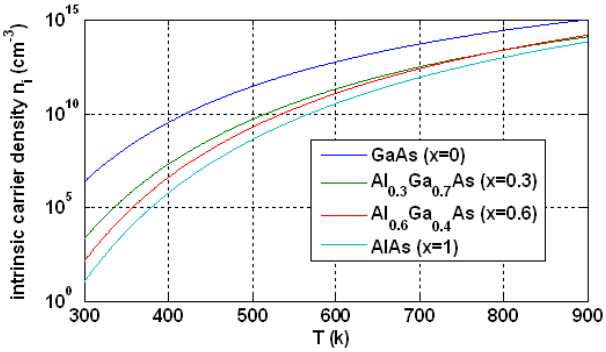

Fig. 5 – Intrinsic carrier density n_i versus temperature T

be understood if one considers that the amplitude of atomic vibrations increases when the interatomic spacing increases owing to increased thermal energy. High doping densities cause the energy band gap E_g to reduce (Fig. 7). This behavior is demonstrated by the fact that the wave functions of the electrons bound to the impurity atoms start to overlap as the impurity density increases. This overlap forces the energies to form an energy band rather than a discreet level.

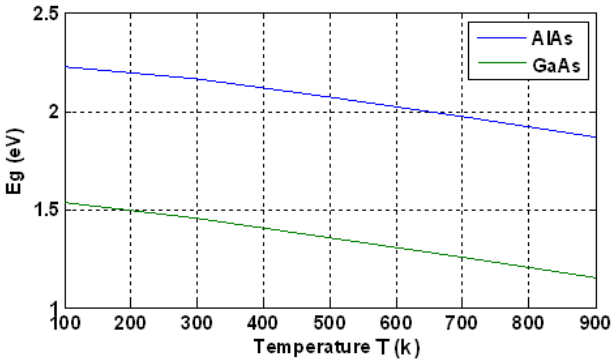

Fig. 6 – Temperature dependence of the energy band gap (E_g) of aluminum arsenide (AlAs) and gallium arsenide (GaAs)

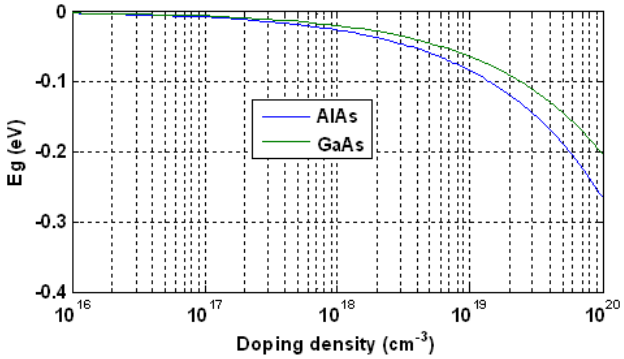

Fig. 7 – Doping dependence of the energy band gap (E_g) of aluminum arsenide (AlAs) and gallium arsenide (GaAs)

4. CONCLUSIONS

In the course of the development of advanced semiconductor devices using multi-material semiconductors, III-V materials therefore offer many possibilities for fast microelectronics, optoelectronics, photonics, etc. The transitions between the valence and conduction bands will then usually radiative. This characteristic gives them remarkable optical properties (photon emission by recombination "band to band" excess carriers allowing their use for the manufacture of lasers or light emitting diodes, good electron-photon conversion efficiency can be used in photodetection). Among them is a ternary compound of group III-V materials, named aluminum gallium arsenide $Al_xGa_{1-x}As$.

In this work, the effective density of states (n_c and n_v) in the conduction and valence bands, respectively, intrinsic carrier density n_i (AlAs, GaAs, $Al_{0.3}Ga_{0.7}As$ and $Al_{0.6}Ga_{0.4}As$ for $x = 1$, 0, 0.3 and 0.6, respectively) and some other important characteristics, such as the temperature dependence of the energy band gap (E_g) (AlAs and GaAs for $x = 1$ and 0, respectively) and the doping dependence of the energy band gap (E_g) (AlAs and GaAs for $x = 1$ and 0, respectively) of $Al_xGa_{1-x}As$ semiconductors have been treaded and analyzed using MATLAB for different values of x ($0 \le x \le 1$).

REFERENCES

1. S.A. Holgate, *Understanding Solid State Physics, 2nd Edition* (Boca Raton: CRC Press, Taylor & Francis Group: 2021).
2. S.M. Sze, Y. Li, K.K. Ng, *Physics of Semiconductor Devices, 4th Edition* (New Jersey: John Wiley & Sons: 2021).
3. J.A. Hernández-Cordero, M. Hautefeuille, *Field Guide to Optoelectronics and Photonics* (Washington: Spie Press-Book: 2021).
4. V. Dugaev, V. Litvinov, *Modern Semiconductor Physics and Device Applications, 1st Edition* (Boca Raton: CRC Press, Taylor & Francis Group: 2021).
5. D. Nirmal, J. Ajayan, P. Fay, *Semiconductor Devices and Technologies for Future Ultra Low Power Electronics, 1st Edition* (Boca Raton: CRC Press, Taylor & Francis Group: 2021).
6. Y-C. Kao, H-M. Chou, S-C. Hsu, A. Lin, C-C. Lin, Z-H. Shih, C-L. Chang, H-F. Hong, R-H. Horng, *Sci. Rep.* **9** No 1, 4308 (2019).
7. S. Mokkapati, C. Jagadish, *Mater. Today* **12** No 4, 22 (2009).
8. H.J. Joyce, Q. Gao, H.H. Tan, C. Jagadish, Y. Kim, J. Zou, L.M. Smith, H.E. Jackson, J.M. Yarrison-Rice, P. Parkinson, M.B. Johnston, *Prog. Quantum Electron.* **35** No 2-3, 23 (2011).
9. F. Janiak, M. Dyksik, M. Motyka, K. Ryczko, J. Misiewicz, K. Kosiel, M. Bugajski, *Opt. Quantum Electron.* **47** No 4, 945 (2015).
10. G.E. Cirlin, R.R. Reznik, I.V. Shtrom, A.I. Khrebtov, I.P. Soshnikov, S.A. Kukushkin, L. Leandro, T. Kasama, N. Akopian, *J. Phys. D: Appl. Phys.* **50** No 48, 484003 (2017).
11. X. Dai, S. Zhang, Z. Wang, G. Adamo, H. Liu, Y. Huang, C. Couteau, C. Soci, *Nano Lett.* **14** No 5, 2688 (2014).
12. L. Nádvorník, P. Němec, T. Janda, K. Olejník, V. Novák, V. Skoromets, H. Němec, P. Kužel, F. Trojánek, T. Jungwirth, J. Wunderlich, *Sci. Rep.* **6**, 22901 (2016).
13. R.J. Malik, *III-V Semiconductor Materials and Devices* (Amsterdam: North Holland: 2012).
14. S. Adachi, *Properties of Semiconductor Alloys: Group – IV, III-V and II-VI Semiconductors* (Chichester: John Wiley & Sons Ltd: 2009).
15. K.W. Böer, U. Pohl, *Semiconductor Physics, 1st Edition* (Cham: Springer International Publishing AG: 2018).
16. D.W. Palmer, *The semiconductors-information WEB-SITE: Properties of the III-V compound semiconductors* (2006).
17. B. Van Zeghbroeck, *Principles of Semiconductor Devices* (Colorado: Boulder. Dept. of Electrical and Computer Engineering, University of Colorado: 2011).
18. V. Palankovski, *Simulation of Heterojunction Bipolar Transistors, PhD Theses* (Faculty of Electrical Engineering and Information Technology, Vienna University of Technology: Vienna, Austria: 2000).
19. S.D. Gunapala, S.V. Bandara, J.K. Liu, J.M. Mumolo, S.B. Rafol, D.Z. Ting, A. Soibel, C. Hill, *IEEE. J. Sel. Top. Quantum Electron.* **20** No 6, 154 (2014).
20. A. Rogalski, *Opto-Electron. Rev.* **20** No 3, 279 (2012).

Характеристики напівпровідників алюмінізованого арсеніду галію ($Al_xGa_{1-x}As$) за допомогою MATLAB

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Однією з основних характеристик напівпровідників є те, що вони можуть бути леговані домішками для зміни їх електричних властивостей. Властивості напівпровідників характеризуються зонною теорією. Ця модель стверджує, що електрон у твердому тілі може приймати значення енергії лише в певних діапазонах, які називаються дозволеними зонами, що розділені іншими зонами, які називаються забороненими зонами. Ці матеріали в основному використовуються в електроніці (діоди, транзистори тощо), мікроелектроніці для інтегральних схем, в сонячних елементах та оптоелектронних пристроях, таких як світлодіоди. Напівпровідники III-V представляють значний інтерес через свої властивості, вони міцні, мають високу теплопровідність і пряму заборонену зону. Пристрої та схеми в групі напівпровідників III-V завжди були відомі своєю високою швидкістю, а також дорогим виробництвом та меншою інтеграцією порівняно з кремнієвими. У цій роботі моделі ефективної густини станів (N_c і N_v) у зоні провідності та валентній зоні, власної густини носіїв n_i, температурної залежності енергетичної забороненої зони (E_g) та залежності від легування ширини забороненої зони (E_g) напівпровідників алюмінізованого арсеніду галію ($Al_xGa_{1-x}As$) аналізуються за допомогою MATLAB для різних значень x ($0 \le x \le 1$).

Ключові слова: AlGaAs, GaAs, AlAs, Температура, Напівпровідники III-V, Енергетичні зони, Густина станів, Власна густина носіїв.