

## Comparison Between Silicon (Si) and Gallium Arsenide (GaAs) Using MATLAB

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The basis of operation of modern electronics components – diodes, transistors, etc. – is the ability to control the electrical conductivity of semiconductors by doping, that is, by introducing impurities into the material. Semiconductors doped differently can be brought into contact to create junctions for controlling the direction and quantity of the current flowing through the assembly. Some examples of semiconductors are silicon (Si), germanium (Ge) and gallium arsenide (GaAs). These substances are close to insulators (intrinsic semiconductors), but the addition of a small amount of dopant leads to a strong drop in electrical resistance, turning them into conductors. Depending on the kind of dopant, *n*-type or *p*-type semiconductor can be made. Silicon is a critical element for fabricating most electronic circuits. Silicon (Si) is a pure crystalline semiconductor material; it is the well-known and most used material. After silicon (Si), gallium arsenide (GaAs) is the second most common semiconductor used in laser diodes, solar cells, microwave-frequency integrated circuits and others. This paper presents a comparison between the energy band gap  $E_g$  as a function of temperature  $T$ , energy band gap  $E_g$  as a function of doping density and intrinsic carrier density  $n_i$  of silicon (Si) and gallium arsenide (GaAs) using MATLAB.

**Keywords:** Silicon (Si), Gallium arsenide (GaAs), Energy bands, Crystal structures, Semiconductor, MATLAB, Energy band gap  $E_g$ .

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### 1. INTRODUCTION

Silicon (Si) is a widely used semiconductor material [1, 2]. Their characteristics are similar to insulators (intrinsic semiconductors), but the presence of a small amount of dopant causes them to decrease electrical resistance and turns them into conductors. It is possible to make a semiconductor of *n*-type or *p*-type, depending on the type of dopant. *n*-type semiconductor is an intrinsic semiconductor doped with phosphorus (P), arsenic (As), or antimony (Sb) as an impurity. Silicon of group IV elements has four valence electrons and phosphorus of group V elements has five valence electrons. *p*-type semiconductor is an intrinsic semiconductor doped with boron (B) or indium (In). Boron of group III elements has three valence electrons. Apart from silicon, there are compound semiconductors that combine group III and V elements and group II and VI elements. For example, GaAs, InP, etc. are commonly used for high-frequency and optical devices. Semiconductor materials are used in modern electronic components: integrated circuits, optoelectronics, photonics and semiconductor devices, etc. [3-10].

Fig. 1 presents a simple energy band diagram of a semiconductor. The valence and conduction bands are indicated by the valence band edge  $E_v$  and the conduction band edge  $E_c$ , respectively; the energy band gap  $E_g$  is located between the conduction and valence bands. This paper describes a comparison between the energy bands gap (temperature dependence of the energy band gap  $E_g$  and doping density dependence of the energy band gap  $E_g$ ) and intrinsic carrier density  $n_i$  of silicon (Si) and gallium arsenide (GaAs) using MATLAB.

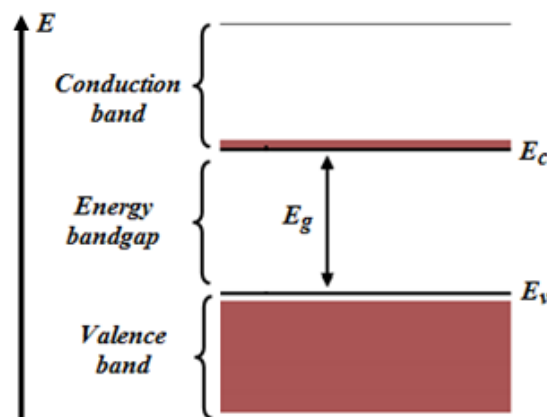


Fig. 1 – Simple energy band diagram of a semiconductor

### 2. CRYSTAL STRUCTURES AND ENERGY BANDS OF Si AND GaAs

The behavior of semiconductors, similar to that of metals and insulators [11], is described via band theory. A direct gap is when the valence band maximum and the conduction band minimum are at an adjacent value of the wavenumber  $k$  in the  $E(k)$  diagram. Conversely, an indirect gap is when the maximum of the valence band and the minimum of the conduction band are at different values of the wavenumber  $k$  in the  $E(k)$  diagram [12, 13].

The crystal structure of silicon (Si) is derived from a face-centered cubic (fcc) lattice, called the single-atom diamond crystal structure, as shown in Fig. 2a. Gallium arsenide (GaAs) has a zincblende crystal structure; the structure is similar to the diamond crystal structure, but composed of two different atomic species, as

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shown in Fig. 2b. In a periodic crystal lattice [14], the band structure is described in reciprocal space by the dispersion relations  $E(k)$ .

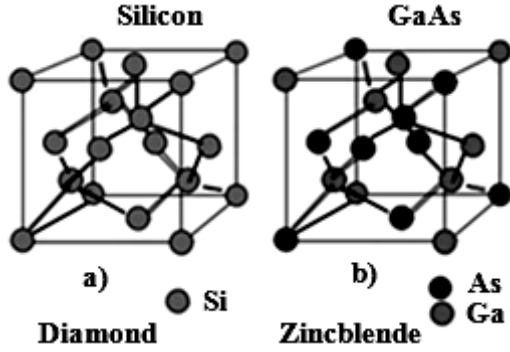


Fig. 2 – Crystal structures of Si and GaAs

In a regular semiconductor crystal,  $E_g$  is fixed owing to continuous energy states. In a quantum dot crystal,  $E_g$  is size-dependent and can be modified to produce a range of energies between the valence and conduction bands. The following expression presents the temperature dependence of the energy band gap  $E_g$  of semiconductors:

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

Equation (1) contains two parameters  $\alpha$  and  $\beta$  [15]. The first is related to the expansion of the lattice as a function of temperature changes. The second represents the interaction of electrons within the lattice. Table 1 summarizes the parameters used to calculate  $E_g$  of Si and GaAs as a function of temperature  $T$ .

Table 1 – Parameters used to calculate  $E_g$  of Si and GaAs as a function of temperature  $T$

	Si	GaAs
$E_g(0)$ (eV)	1.146	1.519
$\alpha$ (eV/K)	$0.473 \cdot 10^{-3}$	$0.541 \cdot 10^{-3}$
$\beta$ (K)	636	204

The doping density dependence of the energy band gap  $E_g$  of semiconductors is given by [16-18]:

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

where  $N$  is the doping density,  $q$  is the electron charge,  $\epsilon_s$  is the dielectric constant of a semiconductor (11.7 for Si, 12.9 for GaAs),  $k$  is the Boltzmann constant,  $T$  is the temperature in Kelvin (300 K).

In the case of an intrinsic semiconductor [19], the concentration of electrons in the conduction band is identical to the concentration of holes in the valence band. We can refer to  $n_i$  and  $p_i$  as the electron and hole concentrations, respectively, in the intrinsic semiconductor. These parameters are generally called the intrinsic electron concentration and intrinsic hole concentration. For  $n_i = p_i$ , we use the parameter  $n_i$  as the intrinsic carrier concentration or the intrinsic carrier density. The intrinsic carrier density  $n_i$  is given by [19, 20]:

$$n_i = (N_c \cdot N_v)^{1/2} \exp\left[-\frac{E_g}{2kT}\right], \quad (3)$$

where  $N_c$  is the effective density of states in the conduction band,  $N_v$  is the effective density of states in the valence band,  $E_g$  is the energy band gap,  $T$  is the absolute temperature, and  $k$  is Boltzmann constant. The effective densities of states ( $N_c$  and  $N_v$ ) in the conduction and valence bands are given by:

$$N_c(T) = N_c(300\text{ K}) \cdot \left(\frac{T}{300}\right)^{3/2}, \quad (4)$$

$$N_v(T) = N_v(300\text{ K}) \cdot \left(\frac{T}{300}\right)^{3/2}. \quad (5)$$

Table 2 summarizes the values of the effective densities of states ( $N_c$  and  $N_v$ ) in the conduction and valence bands and band gap  $E_g$  at  $T = 300$  K.

Table 2 – Values of  $N_c$ ,  $N_v$  and  $E_g$  at  $T = 300$  K

Semiconductor	$N_c$ (cm <sup>-3</sup> )	$N_v$ (cm <sup>-3</sup> )	$E_g$ (eV)
Si	$2.8 \cdot 10^{19}$	$1.07 \cdot 10^{19}$	1.1
GaAs	$4.7 \cdot 10^{17}$	$7 \cdot 10^{18}$	1.42

GaAs has electrical properties superior to those of Si; it has a higher saturation speed of electrons and a direct gap, which gives it superior optoelectronic properties. GaAs-based devices generate less noise at high frequencies than silicon-based devices, they operate at higher power. But silicon (Si) has three main advantages over GaAs; it is particularly abundant after oxygen, the existence of natural oxide (silicon dioxide SiO<sub>2</sub>), an excellent insulator, and we can make P and N transistors to form a CMOS gate with silicon. For these reasons, GaAs has not replaced Si in most applications. Fig. 3 shows the band gap structures of silicon and GaAs and the band gap  $E_g$  of semiconductors which is defined as the difference between the absolute minimum of the conduction bands and the absolute maximum of the valence bands. For gallium arsenide (GaAs), the maximum of the valence band and the minimum

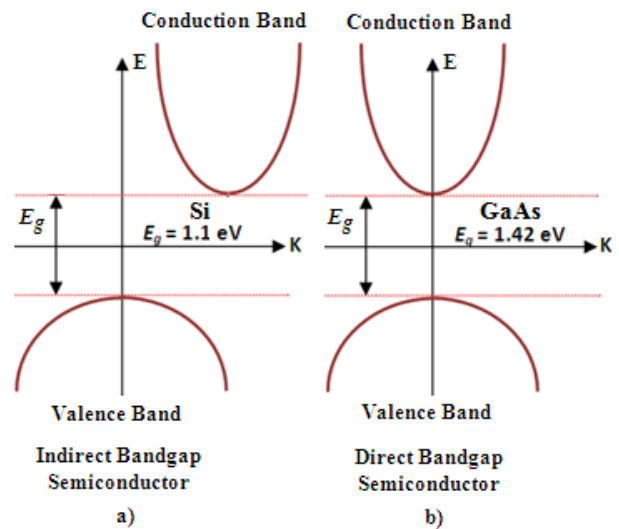


Fig. 3 – Energy band gap structure of Si and GaAs

of the conduction band are at an adjacent value of the wavenumber  $k$  in the  $E(k)$  diagram, therefore it is a direct gap semiconductor ( $E_{g, direct} = 1.42$  eV); and for silicon (Si), the maximum of the valence band and the minimum of the conduction band are at distinct values of the wavenumber  $k$  in the  $E(k)$  diagram, therefore it is an indirect gap semiconductor ( $E_{g, indirect} = 1.1$  eV).

3. RESULTS AND DISCUSSION

In this section, some important characteristics, such as the temperature dependence of the energy band gap  $E_g$  (Fig. 4), the doping density dependence of the energy band gap  $E_g$  (Fig. 5), and the intrinsic carrier density  $n_i$  (Fig. 6 and Fig. 7) of silicon (Si) and gallium arsenide (GaAs) semiconductors are examined and treated under MATLAB.

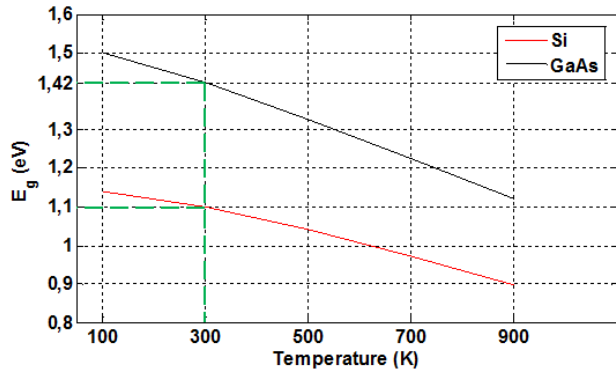


Fig. 4 – Temperature dependence of the energy band gap  $E_g$  of silicon (Si) and gallium arsenide (GaAs)

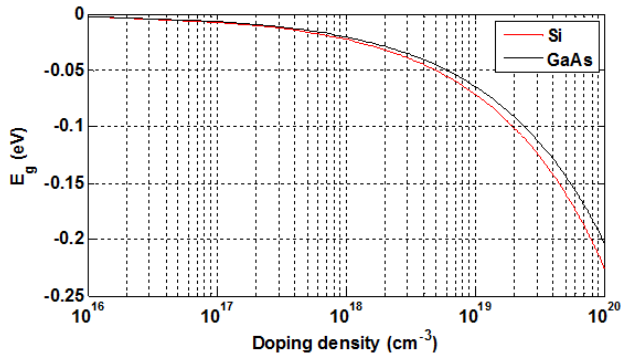


Fig. 5 – Doping density dependence of the energy band gap  $E_g$  of silicon (Si) and gallium arsenide (GaAs)

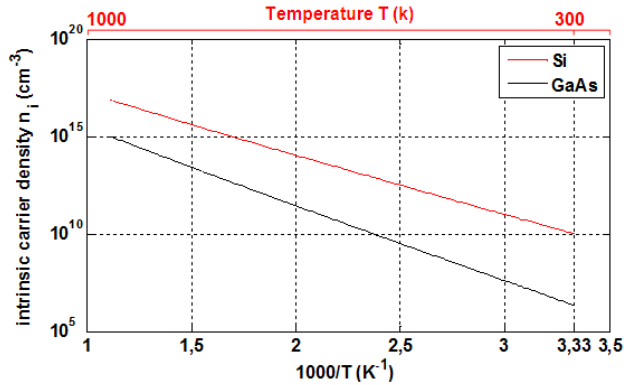


Fig. 6 – Intrinsic carrier density  $n_i$  versus  $1000/T$

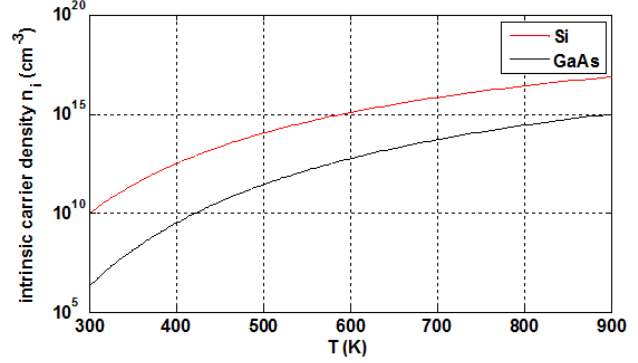


Fig. 7 – Intrinsic carrier density  $n_i$  versus temperature  $T$

The temperature dependence of the energy band gap  $E_g$  and the doping density dependence of the energy band gap  $E_g$  are some of the most fundamental properties of semiconductors and have a great influence on many different applications for many semiconductor candidates. From Fig. 4, the  $E_g$  of GaAs and Si semiconductors reduces when the temperature  $T$  rises. This effect can be understood if one considers that the amplitude of atomic vibrations rises when the interatomic spacing rises due to the raised thermal energy. The band gaps  $E_g$  of gallium arsenide (GaAs) and silicon (Si) semiconductor materials at  $T = 300$  K are 1.42 eV and 1.1 eV, respectively. From Fig. 5, a high doping density provokes a decrease in  $E_g$  of GaAs and Si semiconductors. This is evidenced by the fact that the wave functions of the electrons bound to the impurity atoms start to overlap as the density of impurities increase. This overlap obliged the energies to form an energy band rather than a discrete level.

Fig. 6 and Fig. 7 show the intrinsic carrier density  $n_i$  for silicon (Si) and gallium arsenide (GaAs) as a function of temperature.  $n_i$  is a very important function of temperature. From Fig. 6 and Fig. 7, the intrinsic carrier density  $n_i$  value for these semiconductors can vary widely by several orders of magnitude as the temperature changes over the acceptable range. The intrinsic carrier densities  $n_i$  of gallium arsenide (GaAs) and silicon (Si) semiconductor materials at  $T = 300$  K are  $2.16 \cdot 10^6 \text{ cm}^{-3}$  and  $1 \cdot 10^{10} \text{ cm}^{-3}$ , respectively.

4. CONCLUSIONS

This work presents the comparison between the temperature dependence of the energy band gap  $E_g$ , the doping density dependence of the energy band gap  $E_g$  and the intrinsic carrier density  $n_i$  of silicon (Si) and gallium arsenide (GaAs) using MATLAB. Energy band gap ( $E_g$ ) is an energy range in a solid where no electron states can exist. In graphs of the electronic band structure of solids, the term “band gap” refers to the energy difference (in eV) between the top of the valence band and the bottom of the conduction band. GaAs has a direct gap and Si has an indirect gap. Gallium arsenide has some electrical properties superior to those of silicon, but silicon has some principal advantages over gallium arsenide. For these last reasons, gallium arsenide (GaAs) has not succeeded silicon (Si) in the vast majority of applications.

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## Порівняння кремнію (Si) та арсеніду галію (GaAs) за допомогою MATLAB

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Основою роботи компонентів сучасної електроніки – діодів, транзисторів, тощо – є можливість керування електропровідністю напівпровідників шляхом легування, тобто введенням домішок у матеріал. На основі напівпровідників з різними концентраціями домішок можна сформувати контакт для керування напрямком і кількістю струму, що протікає через вузол. Ця властивість є основою роботи компонентів сучасної електроніки: діодів, транзисторів тощо. Деякими прикладами напівпровідників є кремній (Si), германій (Ge) і арсенід галію (GaAs). Ці речовини близькі до ізоляторів (власних напівпровідників), але додавання невеликої кількості легуючої домішки призводить до сильного падіння електричного опору, перетворюючи їх на провідники. Залежно від типу легуючої домішки можна виготовити напівпровідник *n*-типу або *p*-типу. Кремній є критично важливим елементом для виготовлення більшості електронних схем. Кремній (Si) є чистим кристалічним напівпровідниковим матеріалом; це добре відомий і найбільш використовуваний матеріал. Після кремнію (Si) арсенід галію (GaAs) є другим за поширеністю напівпровідником, який використовується в лазерних діодах, сонячних елементах, мікрохвильових мікросхемах та інших. У статті представлено порівняння між шириною забороненої зони  $E_g$  як функції температури  $T$ , шириною забороненої зони  $E_g$  як функції густини легування та власної густини носіїв  $n_i$  кремнію (Si) і арсеніду галію (GaAs) за допомогою MATLAB.

**Ключові слова:** Кремній (Si), Арсенід галію (GaAs), Енергетичні зони, Кристалічні структури, Напівпровідник, MATLAB, Енергетична заборонена зона  $E_g$ .