دراسة نظرية لتأثير درجة حرارة المحيط على معامل الأمتصاص

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الخلاصة

اقترحت معادلة رياضية جديدة لوصف العلاقة بين معامل الخمود او معامل الامتصاص و درجة حرارة الوسط المحيط والطول الموجي لبعض المواد المستعملة ضمن مجال الاشعة تحت الحمراء. لقد اشتقت هذه المعادلة اعتمادا على بعض المنحنيات العملية المأخوذة من مصادر خارجية مختلفة التي تصف العلاقة بين قيم النفاذية دالة للطول الموجي لقيم عديدة من درجات حرارة المحيط. ان الدراسة المكثفة و المتعمقة لطبيعة هذه المنحنيات و اسلوب تغيرها مع كلا من واعتمادا على توزيع بوز – اينشتاين الاحصائي قادت الى وضع معادلة تصف تغير الطول الموجي و درجة الحرارة معامل الخمود دالة للطول الموجي و درجة حرارة المحيط ومن ثم تغير النفاذية مع درجة حرارة المحيط ، ان الافتراض الاساسي في عملية ايجاد هذه المعادلة هو اعتبار ان التغير الرئيس في النفاذية يعود الى التغير في قيم معامل الخمود نتيجة لتغير درجة حرارة الوسط الخارجي. ان النتائج النظرية للمعادلة المقترحة اعطت تطابقا جيدا مع مجمل النتائج العملية التي تمت دراستها في هذا البحث.

Theoretical Study on the Effect of Ambient Temperature on Absorption Coefficient

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Abstract

Anew mathematical formula was proposed to describe the behavior of the extinction coefficient as a function of ambient temperature and wavelengths for some of infrared materials. This formula was derived depending on some experimental data of transmittance spectrum versus wavelengths for many ambient temperatures. The extensive study of the spectrum characteristics and depending on Bose-Einstein distribution led to derive an equation connecting the extinction coefficient or the absorption coefficient with the ambient temperature and wavelengths of the incident rays. The basic assumption in deriving process is the decreasing in transmittance value with the increasing temperature which is only due to the changing in extinction coefficient values.

Introduction

Many infrared transparent materials, especially those that are strongly absorbing materials in the visible region, have high indices of refraction in the infrared region [1]. This is especially true for semiconductors such as Ge, InAs, InSb, which are widely used in the infrared as windows, lenses, and long wavelength pass filters. Their high refractive indices cause large reflection losses so that even thin non absorbing plates of these materials transmit only 50% or less of the incident radiation. A transparent layer of another material such as SiO or ZnS to produce zero reflectance can coat these materials [1].

The design of any optical system requires the selection of materials based upon knowledge of the optical, mechanical and thermal properties available. A study of the material characteristics, particularly the absorption and dispersion processes, is therefore essential for the selection of suitable materials for use both as substrates and evaporated layer materials.

All of the observed intrinsic absorption characteristics present in the spectrum of an infrared optical material can be classified by three fundamental processes involving the interaction between the material and the incident electromagnetic radiation, namely; electronic absorption, lattice or phonon absorption and free-carrier absorption. All these processes which are affected by the ambient temperature would make the absorption or extinction coefficient and then the resulting transmittances decrease as the temperature increases.

This decrease in transmittance with the increasing temperatures is due to the changing in values of both refractive index and extinction coefficient or absorption coefficient, but since the experimental results illustrate that the change in the refractive index of both the coating and substrate materials is small comparing with the change of the extinction coefficient so it can be assumed that the transmittance decreases entirely due to an increase of absorption coefficient or extinction coefficient and not to refractive indices.

In this paper, we will propose a new mathematical formula for the relationship between the extinction coefficient of some semiconductor materials and both ambient temperature and incident wavelength.

General description of absorption

The electronic absorption characteristics observed towards the higher frequency end of the infrared spectrum are the result of interaction between the incident radiation and the motions of electrons or holes within the material [2]. Only electromagnetic radiation with sufficient energy to cause an electron to transfer between the valence band and conduction band (hf) will be absorbed by this mechanism. The various transitions of these electrons define the position of the short wavelength absorption edge. The resulting spectrum provides information on the width of the energy band gap of the material, and through spectral anomalies, can indicate the presence of impurities [3].

The lattice absorption characteristics observed at the lower frequency regions, in the middle to far-infrared wavelength range, define the long wavelength transparency limit of the material, and are the result of the interactive coupling between the motions of thermally induced vibrations of the constituent atoms of the substrate crystal lattice and the incident radiation.

Hence, all materials are bounded by limiting regions of absorption caused by atomic vibrations in the far-infrared (>10μm), and motions of electrons and/or holes in the short-wave visible regions. In the inter band region, the frequency of the incident radiation has insufficient energy (E=hf) to transfer electrons to the conduction band and cause absorption; here the material is essentially loss-free.

In addition to the fundamental electrons and lattice absorption process, free carrier absorption in semiconductors can be present. This involves electronic transitions between initial and final states within the same energy band. The absorption or emission of the resulting photons is accompanied with by ascattering by optical or acoustic-mode phonon vibrations or by charged impurities. This type of absorption is evident where the spectral profile of the material is highly absorbing, producing considerably lower transmission than otherwise expected.

These intrinsic absorption properties of semiconductors and insulators define the transparency of the material. To be transmitted in the region between the electronic and lattice absorption, the incident radiation must have a lower frequency than the band-gap (E_g) of the material. This is defined by the short wavelength semiconductors edge at ($\lambda = hc/eE_g$), preventing electrons transferring to the conduction band. The generalized profile of the electronic edge is known as the Urbach tail [4] where the exponentially increasing absorption coefficient follows the general relationship:

$$\frac{\partial(ln\alpha)}{\partial(hf)} = \frac{1}{k_B T} \quad \text{.......} \quad (1)$$

(k_B) is Boltzmann constant, (h) is Blank constant, (f) is the incident radiation frequency, and (T) is the temperature.

The concept of temperature and thermal equilibrium associated with crystal solids are based on individual atoms in the system possessing vibration motion. The classical theory of thermal energy by atomic vibrations, thought providing suitable explanations at elevated temperature, has proved unsatisfactory at reduced temperatures. Quantum mechanics has subsequently provided theories based upon statistical probabilities that have provided possible mechanisms to explain some of the observed phenomena. A system of vibrating atoms in a crystal is highly complicated, and beyond any realizable theoretical methods of analysis or calculations to verify spectral measurements from the total thermal energy of a crystalline substrate.

For a system of distinguishable particles, the probability statistics of the energy (E) of the system are described by Maxwell-Boltzmann general equation[5-7]:

$$f_{MB} = Ae^{-\frac{E}{k_B T}} \quad \ldots\ldots (2)$$

If particles are indistinguishable they are divided into two types:

(i) Electrons; which are subject to the Pauli Exclusion Principle[5-7] and obey Fermi-Dirac statistics

$$f_{FD} = \frac{1}{e^{\frac{E-E_f}{k_B T}}+1} \quad \ldots\ldots (3)$$

(E_f) is Fermi energy.

(ii) P Photons and phonons which are defined by Bose-Einstein statistics

$$f_{BE} = \frac{1}{e^{\frac{E-\alpha}{k_B T}}-1} \quad \ldots\ldots (4)$$

(α) is a normalizing constant, adjusted so that the total probability is equal to unity when each function is summed over all the energy states available.

For the electronic absorption edge, the effect of increasing temperature on the forbidden energy gap reduces the energy gap shifting the edge position to shorter wavelengths. This shift was fitted for various materials by the following empirical relationship[5]:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T+\beta} \quad \ldots\ldots (5)$$

Where $E_g(0)$ is the value of the energy gap at zero Kelvin and α and β are constants.

Experimental results (Single-Layer Coating)

In this research, we depend on two types of experimental data:

(1) The transmission spectrum [1] of the semiconductor materials Ge, InAs and InSb which have refractive indices near absorption edge 4.1, 3.4 and 4.0, respectively.

In the near infrared region, the experimental and theoretical results show that SiO film is the most suitable antireflection coating for Ge, and InAs while ZnS film was found most suitable as a single layer antireflection coating for the (7-15) μm. The transmittances versus wavelength for different temperatures of one layer coatings are obtained for the following cases:

a) InAs plate (thickness 0.21 mm) with coating consists of SiO with quarter wavelength thickness (at 5.75 μm) as shown experimentally in Fig. (1-A).

b) Ge plate (thickness 2.0 mm) with coating consists of ZnS with quarter wavelength thickness (at 9.80 μm) as shown experimentally in Fig. (1-B).

c) InSb plate (thickness 0.08 mm) with coating consists of ZnS with quarter wavelength thickness (at 10.8 μm) as shown experimentally in Fig. (1-C).

All these figures show that the transmittance decreases strongly with increasing ambient temperature, while the maximum peaks of transmittance are shifted towards the high values of wavelength.

(2) The experimental studies [8-10] of some other materials like (PbS, PbSe, and PbTe) which represent the relation between the thermal energy and the photon energy at minimum absorption as shown in Fig.(2).
Both of these experimental data are used to evaluate a theoretical equation for the extinction coefficient as a function of ambient temperature and incident wavelength.

Theoretical Study

The extensive study of the experimental curves of transmittance behaviour versus wavelengths and temperature (Fig.1) gives:
(1) The extinction coefficient for the case of constant ambient temperature has the mathematical form:

$$k = a_0 e^{a_1(a_2-hf)^2} \quad \text{……} (6)$$

(a_0, a_1, a_2) are constant parameters for wavelength.

(2) The extinction coefficient for the case of constant frequency or wavelength of the incident radiation has the mathematical form:

$$k = \frac{b_0}{e^{\frac{b_1}{k_B T}}-1} e^{b_2(b_3-k_B T)^2} \quad \text{……} (7)$$

(b_0, b_1, b_2, b_3) are constant parameters for temperature depending on the incident wavelength and the material nature.

(3) The combination of both cases to find the general case of variable frequency and temperature will then has the mathematical form:

$$k = \frac{\gamma}{e^{\frac{c_1}{k_B T}}-1} e^{c_2(c_3-\Omega k_B T-hf)^2} \quad \text{……} (8)$$

(Ω) is a constant which depends on the material ,the physical meaning of the parameter Ω is the ratio between the deviations in photon energy at maximum transmittance (minimum absorption coefficient) to heat energy due to the relation:

$$\Omega = -\frac{\Delta(hf)}{\Delta(k_B T)} \quad \text{……} (9)$$

From the above equation, it is obvious that the minimum value of extinction coefficient (minimum absorption) occurs when:

$$c_3 - \Omega k_B T - hf = 0 \quad \text{……} (10)$$

This result implies that the energy of the incident light, at maximum transmittance or minimum absorption depends linearly on the heat energy. This is a real fact which can be shown via the curves in (Fig.2) for the materials (PbS, PbSe and PbTe). The parameter c_3 has a relationship with the melting temperature of the substrate (Tm), it equals to:

$$c_3 = 2k_B T_m \quad \text{……} (11)$$

By using the general form of multilayer system equation [11], one can obtain the values of the extinction coefficient that fit the experimental data of transmittance spectrum, it was found that the parameter c_1 has also a relation with melting temperature, it equals to:

$$c_1 = 2k_BT_m \quad \text{......} (12)$$

While both of parameter γ and Ω depending on the type of material. Table (1) shows these values for the chosen materials.

The parameter c_2 was found to depend on the thickness of coating layer and gap energy of the substrate layer, it has the form:

$$c_2 = \frac{4\pi\lambda}{ndE_g{}^2} \quad \text{......} (13)$$

(n and d) are the refractive index and the thickness of the coating layer, (E_g) is the energy gap of the substrate. Then the new formula of the extinction coefficient has the form:

$$k = \frac{\gamma}{e^{\frac{E_m}{k_BT}}-1} e^H \quad \text{......} (14)$$

$$H = 4\pi \frac{\lambda}{nd} (\frac{E_m - \Omega k_BT - hf}{E_g})^2 \quad \text{......} (15)$$

Results and Discussion

(1) The theoretical study for the behaviours of the experimental transmittance spectrum of the substrate materials Ge, InAs and InSb gives a value of 1.0 for the parameter Ω which means that the heat energy equals to (k_BT), while it's positive value means that the maximum peak of transmittance (λ_m) increases with the increase of the temperature.

The theoretical studies of the materials (PbS, PbSe, and PbTe) give a value (-3.5) for the parameter Ω, which means that the heat energy equals to ($\frac{7}{2}k_BT$), while the minus value means that the maximum peak of transmittance decreases with the increase of the temperature which is a different behaviour comparing with the semiconductor materials.

The maximum transmittance occurs at the minimum value of the extinction or absorption coefficient, the wavelength λ_m at which minimum extinction coefficient can be obtained by letting the derivative of k in equation [13] with respect to λ for constant temperature equals to zero, that will give the result:

$$hf_m = 2k_BT_m - \Omega k_BT \quad \text{......} (16)$$

From the above equation, the maximum transmittance wavelength can be obtained:

$$\lambda_m = \frac{hc}{k_B(2T_m - \Omega T)} \quad \text{......} (17)$$

Equation (17) has important conclusion states that the increasing of temperature led to increase the value of λ_m when Ω has positive values and decrease the value of λ_m when Ω has negative values. Since the values of temperature are bounded between zero and T_m that means the values of λ_m are bounded between two values:

$$\lambda_m(max) = \frac{hc}{k_BT_m(2-\Omega)} \quad \text{......} (18)$$

$$\lambda_m(min) = \frac{hc}{2k_B T_m} \quad \ldots\ldots (19)$$

(2) Equation (13) is a new semi-empirical equation evaluated from the experimental values of the transmittance versus wavelength for different values of temperatures. By using the general equation of multilayer system, and introducing the value of refractive index, as a constant and extinction coefficient according to equation (13), one can obtain the theoretical transmittance. The results of theoretical transmittance are nearest to the experimental values within an average error less than 10.0% as shown in the case of the semiconductor substrate materials discussed above. The theoretical and experimental results are shown in figures (3). The agreement between the theoretical and experimental results are good for InSb, but there is a shift in the maximum values of transmittance for InAs, while for Ge substrate, the agreements are good except for the temperature 398 K in which the theoretical transmittances are lower within less 10% comparing with the experimental values.
(3) The melting temperatures (T_m) for lead compound (PbS, PbSe, and PbTe) are (1387, 1338, and 1190) K, and the thicknesses of the samples are (1.25, 0.68 and 0.35) mm, respectively. Figures (2) represent the theoretical and experimental values of minimum absorption wavelength at different temperatures. The agreements are good for PbS and PbTe, but for PbSe there is a shift between the theoretical and experimental curves due to the value of E_m which is related to melting temperature

Conclusions

The final semi-empirical formula for the extinction coefficient was derived depending on transmittance spectrum of some semiconductor materials. The resulting formula has a good accuracy comparing with the experimental results of the transmittance spectrum for the materials InAs (coated with SiO), Ge (coated with ZnS) and InSb (coated with ZnS), also the agreement is good for the experimental results of incident photon energy versus heat energy at minimum absorption coefficient for the materials PbS, PbSe and PbTe. The use of the mathematical model depends on Bose-Einstein statistics and on behaviour study of the experimental curves through using fitting theory. The need is still up to study more materials to reach an exact equation for the extinction coefficient as a function of wavelength and ambient temperature.

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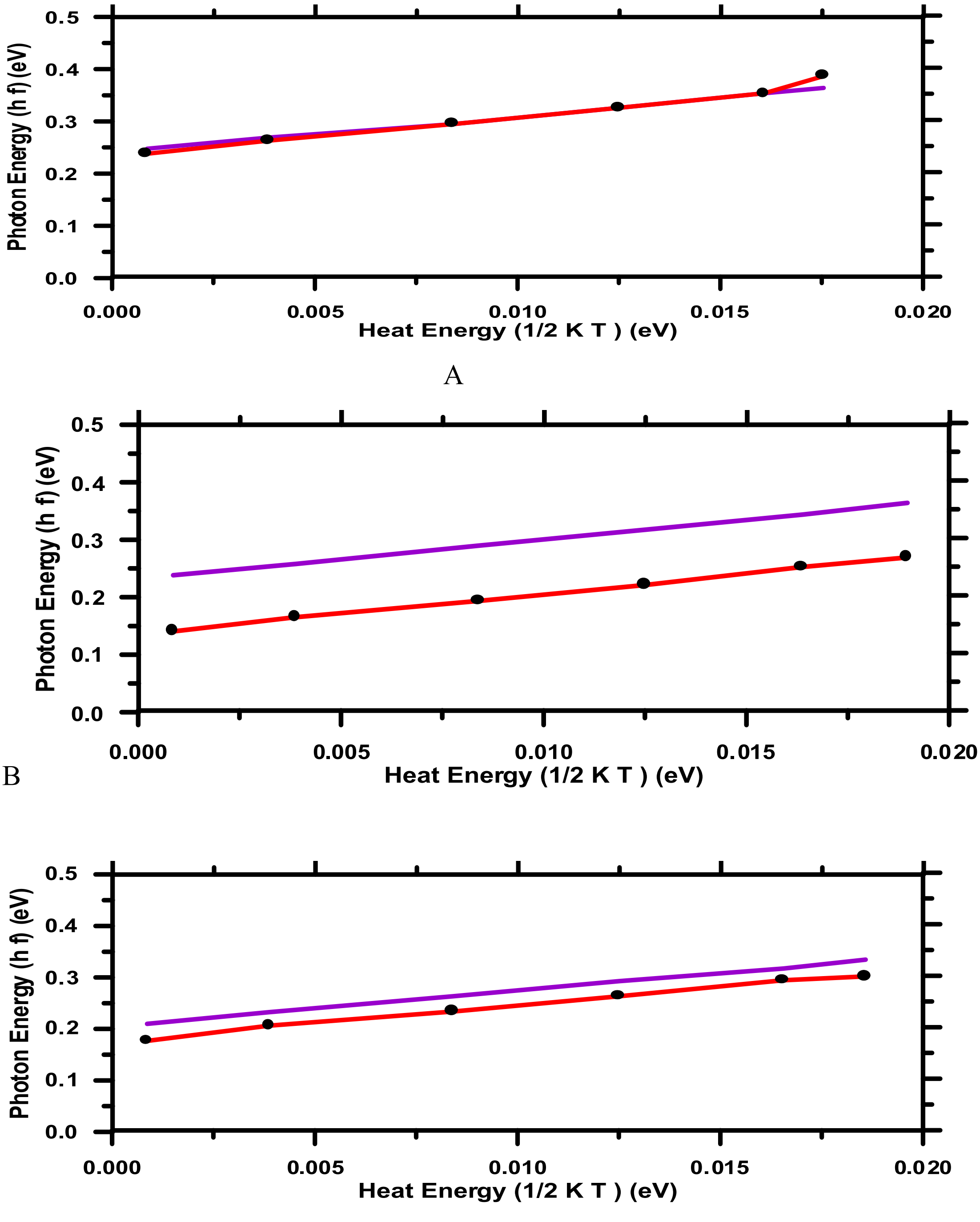

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Fig. (2): Comparison between the present work and experimental results of incident photon energy versus heat energy at minimum absorption coefficient for:
The smooth line represents the theoretical results.
The dotted line represents the experimental data.

A: PbS, B: PbSe, C: PbTe.

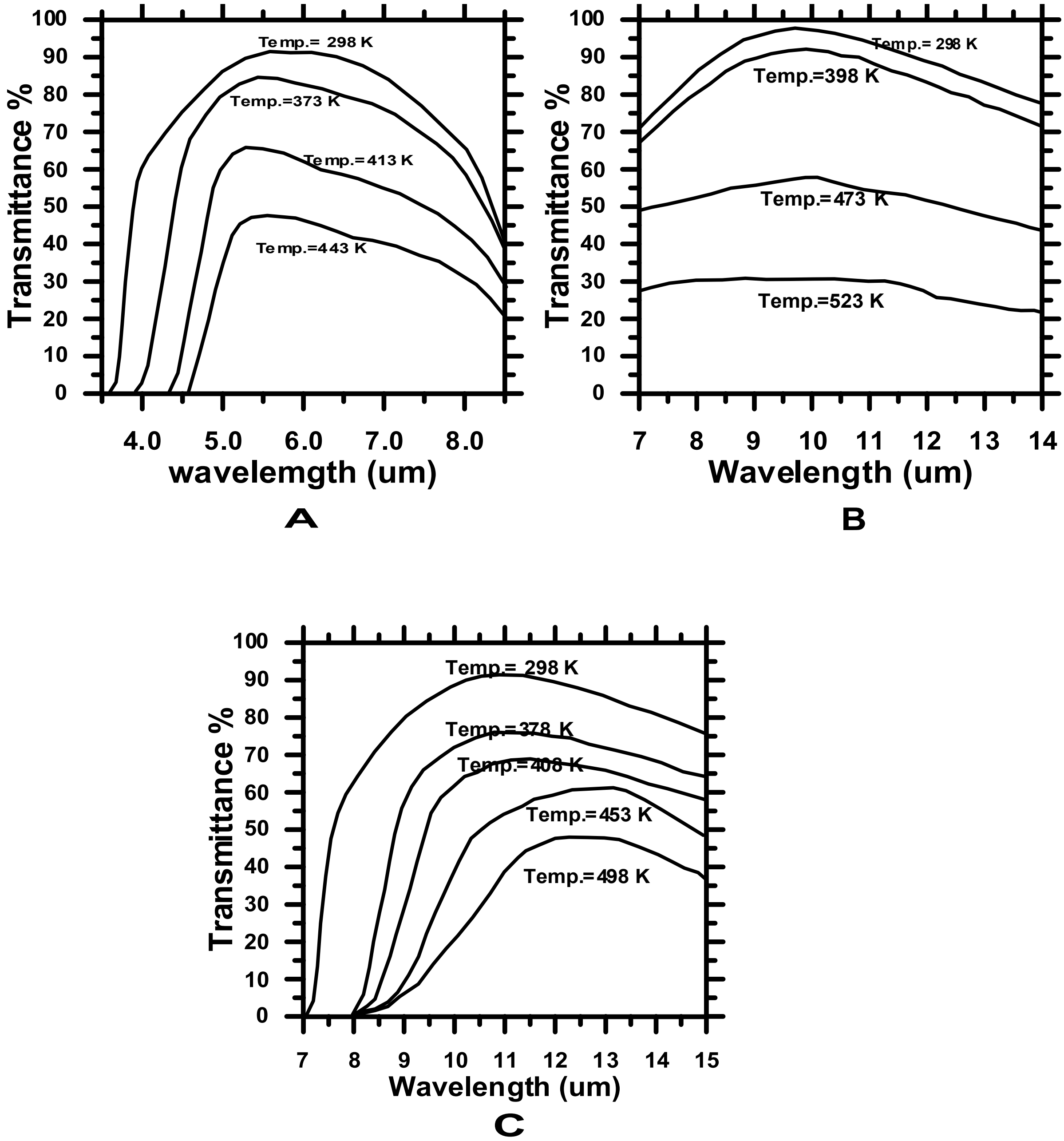
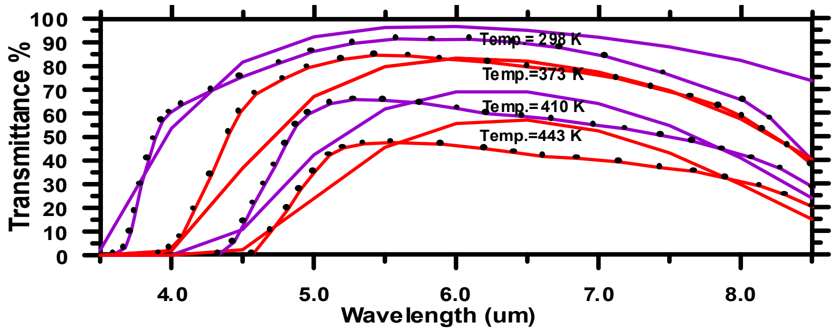


Fig.(1): Experimental transmittance versus wavelength for different temperatures.
A: for InAs substrate coated with SiO.
B: for Ge substrate coated with ZnS.
C: for InSb substrate coated with ZnS.

Table (1): The important parameters values of some materials

Material	E_g eV	T_m K	γ	Ω
Germanium (Ge)	0.69	1210	0.15	1.0
Indium Arsenide (InAs)	0.39	1216	0.64	1.0
Indium Antimonide (InSb)	0.23	808	0.20	1.0



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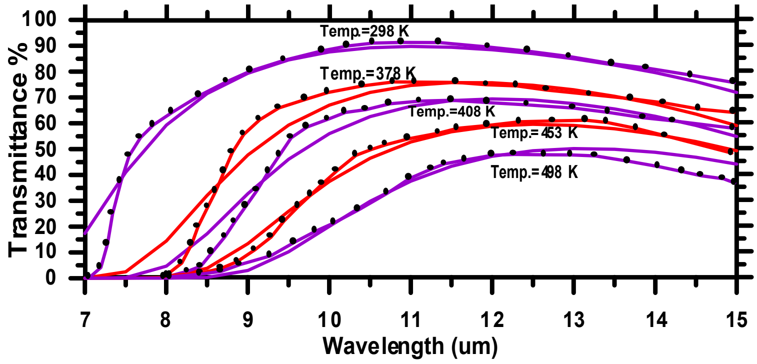

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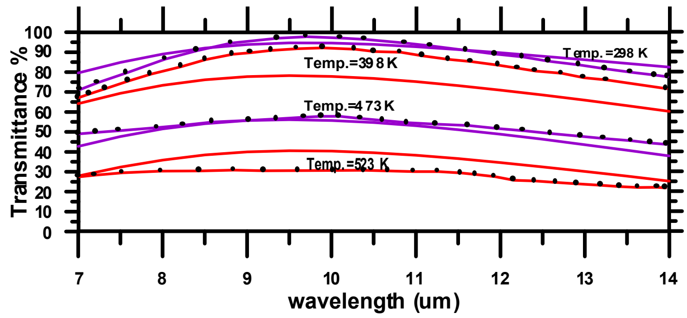

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Fig. (3): Comparison between the present work and the experimental transmittance versus wavelength for different temperatures.
A: InAs substrate, B: InSb substrate, C: Ge Substrate
The smooth line represents the theoretical results.
The dotted line represents the experimental results