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RESEARCH ARTICLE

DIELECTRIC PROPERTIES: COMPUTER SIMULATION

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Abstract

In this paper we present a numerical investigation about the dielectric properties. A program based on the Lorentz model is implemented. For the understanding of some physical parameters (spectral width, specific pulsation and the number of particle), we varied these parameters to observe their influences on the real and imaginary susceptibility as well as the reflective index of the environment.

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Introduction:-

The investigation of the physical properties in the dielectric and ferroelectric materials creates a particular interest to researchers thanks to their applications in the field of the electronic and optoelectronic. Several authors have already worked in this field with diverse applications such as the energy, electronic, optic etc. We know that a material is dielectric if it does not contain electrical charges susceptible to move. Thus the environment cannot lead the electric current and by definition it's an electrical insulator [1] such as the space, the glass, the dry wood, the plastics, etc. [2]. The dielectric is not however inert electrically. Indeed, the constituents of the material can present in the atomic scale electrostatic dipoles, which interact with an applied external field. This interaction is translated by the creation of a polarization P connected with the microscopic level in this electric field, by the polarizability and in the macroscopic level by the electric susceptibility χ [2]. The dielectric materials [3-10] are classically likened to isolation materials. Insulators are materials which the resistivity is extremely raised. They are characterized by an important width of the forbidden band (4eV), the kinetic energy due to the thermal motion is consequently insufficient. Insulators are essentially materials with Ionic connections, in which the electrons of connection are strongly localized. There are several types of dielectric; however electric cables are often protected from a plastic cover to avoid the exit of the electric current.

Now a day, one puts dielectric materials [6] having a strong dielectric constant between the armatures of the condenser to increase their efficiencies. These materials belong to the ferroelectric family, in particular the products from the titanate of Barium $BaTiO_3$, which are used in the industry of the microelectronic for more than 50 years. One also notes ceramic, ancestrally used, present new applications in the domains of the technology, they play an important role in the technological challenges thrown to the industry. Most of the dielectric is also transparent in wide frequency bands, and are sometimes used to constitute an anti-reflection, for example on certain models of glasses. The dielectric [7] being difficult to ionize, the ambient air becomes a driver before them, that's why one can use them for high-voltage condensers.

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Model and Formalism:

To investigate the dielectric environment, Lorentz considered atoms as weakened oscillators bound between them by springs. By applying a variable electric field, Lorentz had noted the appearance of a polarization. By making an assessment of strengths, he defined the following strengths:

$$\vec{f}_v = -m\Gamma \frac{dr}{dt} \quad (1)$$

With \vec{f}_v : Strength of amortization bound to the losses of energies by radiation which undergoes any electrical charge in uniform movement.

$$\vec{f}_r = -m\omega_0 r \quad (2)$$

With \vec{f}_e : Strength of elastic abseiling of the electron towards the position of the studied atom.

$$\vec{f}_e = -eE \quad (3)$$

With \vec{f}_e : Electric force.

By considering the displacement “r” of an electron with regard to the core, which it is elastically connected. Such an electron obeys the equation of the movement given by the Newton’s Law [16], so we defined the radius (r) by:

$$r = \frac{-e}{m} \frac{E}{\omega_0^2 - \omega^2 - i\omega\Gamma} \quad (4)$$

The polarization is thus defined from the position r of the electrons reason why we have:

$$P = -ner = \frac{ne^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\Gamma\omega} E \quad (5)$$

One knows $P = \alpha\chi E = \frac{ne^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\Gamma\omega} E$ with $\alpha = \frac{ne^2}{m}$

χ represents the susceptibility of the dielectric environment [11].

So from the susceptibility one can define the permittivity [12-16] of the dielectric environment defines by the following relation:

$$\varepsilon(\omega) = 1 + 4\pi\chi(\omega) = 1 + \frac{4\pi ne^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\Gamma\omega} \quad (6)$$

By posing $\omega_p^2 = \frac{4\pi ne^2}{m}$: spectral Weight [17]

We obtain:

$$\varepsilon(\omega) = 1 + \frac{\omega_p^2}{\omega_0^2 - \omega^2 - i\Gamma\omega} \quad (7)$$

Results and Discussions: -

To investigate the dielectric properties in the dense environment, we choose to look at the behavior of the susceptibilities as well as the refractive index by making a variation of the spectral width, the specific pulsation (ω_0) and the number of particle (N). The spectral width allows us to understand the complex aspect of the amortization in the dielectric environment. So, in the figure 1 we observe that for values of $\omega < \omega_0$, which represent the normal dispersion, the growth of the susceptibility is a function of the increase of the spectral width Γ . For values $\omega \geq \omega_0$, the susceptibility decrease rapidly, this phenomenon corresponds to an abnormal dispersion with positive and negative values of the susceptibility. Reason why, the growth of the spectral width influences the width of the peaks

in the real susceptibility. Otherwise, more the spectral width is important more the real susceptibility increase. In the figure 2, with the imaginary susceptibility, the variation of the spectral width (Γ) influences the absorption of the dielectric environment. So for values of $\omega < 3$ and $\omega > 5$ the imaginary susceptibility is null for various values of Γ . For $3 \leq \omega \leq 5$, the imaginary susceptibility presents a peak which increases with the spectral width. Reason why, to make more absorption in materials with dense properties, the augmentation of the spectral width (Γ) on the imaginary susceptibility is better. The investigation of the reflective constant is very important in the dielectric materials because it allows the understanding of the optical behavior in the dielectric environment. Reason why, the figure3 represents the influence of the spectral width (Γ) on the reflective index. So we note that the spectral width (Γ) increases the capacity of the environment to be reflective. Moreover, certain authors [18, 19 and 20] have already used this parameter for the investigation of certain materials such as ZnO, CdS etc. Besides, the vibrational character of the materials plays an important role in the investigation of the structural properties of the physical systems, so one of the parameters responsible for this phenomenon is the specific pulsation ω_0 . The figures 4, 5 and 6 shows the influence of the pulsation ω_0 on the dielectric properties of the materials. The variation of ω_0 reveals that the susceptibilities and the reflective index decrease with the increase of the specific pulsation (ω_0). This is due to the fact that the specific pulsation is inversely proportional to the susceptibilities and the refractive index. Reason why an increase of the specific pulsation creates a change of the curves from the reflective index but decrease the maximal values of the peaks of refraction and susceptibility. In the dense dielectric material, the investigation of the statistical physic is mandatory. With the physic of particles, the large number of particle is closely linked to the strength of oscillator in the dielectric materials reason why its influence is noted in the dielectric properties. So the figures 7, 8 and 9, display the influence of the number of particle on the dielectric materials. Unlike figures 1, 2 and 3, the curves of the susceptibilities and the reflective index increase with the augmentation of the number of particle. As result, we observe an importance of the refraction as well as the absorption. The Lorentz model is a good model for investigating the dense dielectric properties but also it is very used to study the behavior of phonons and transitions inter-bands. Reason why, certain authors have already used it to investigate the reflectivity of certain materials such as YMnO_3 [21].

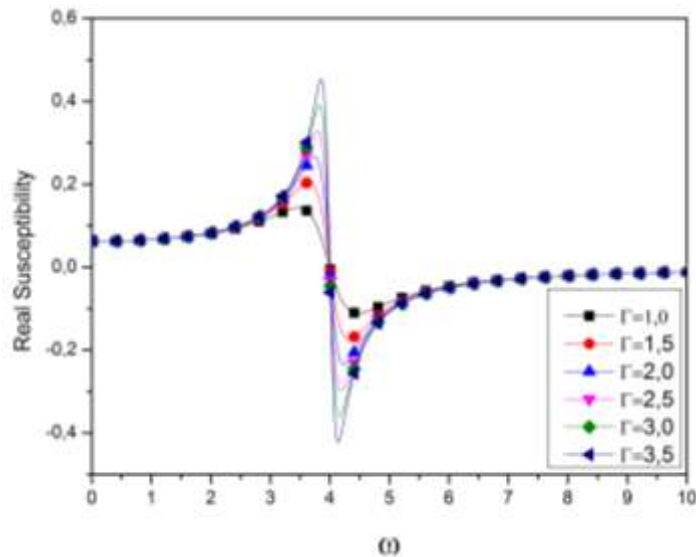


Figure 1:- Evolution of the real susceptibility according to the spectral width.

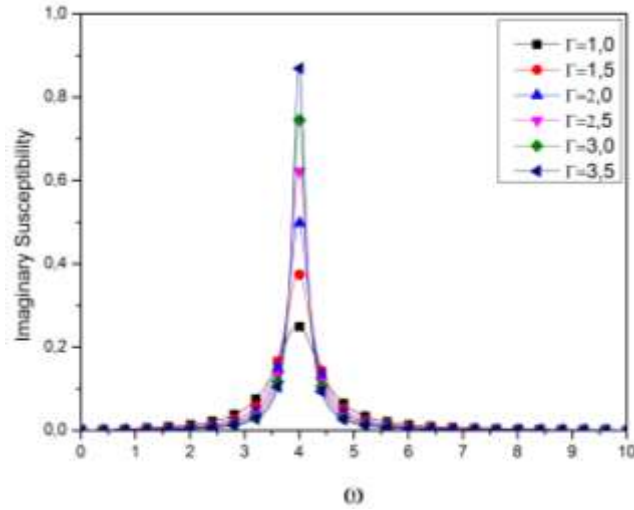


Figure 2:- Evolution of the imaginary susceptibility according to the spectral width.

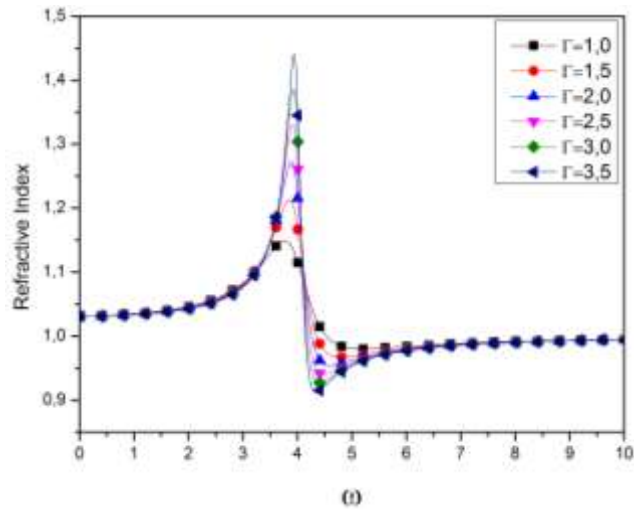


Figure 3:- Evolution of the reflective index according to the spectral width.

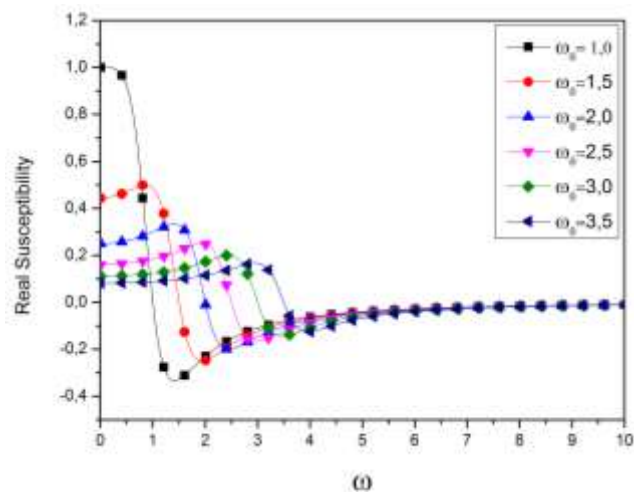


Figure 4:- Evolution of the real susceptibility according to the specific pulsation.

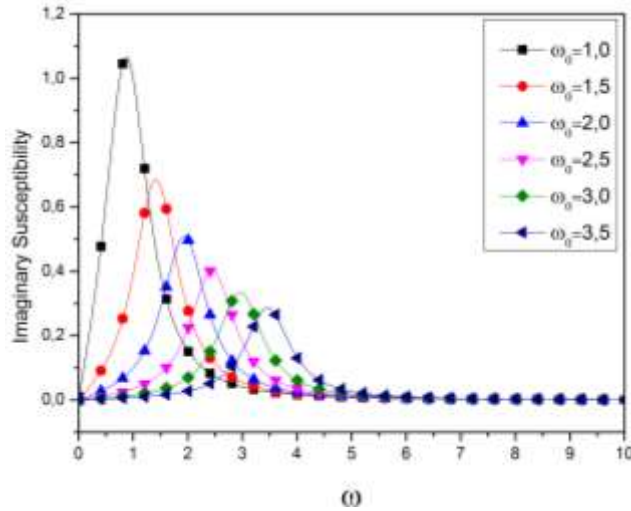


Figure 5:- Evolution of the imaginary susceptibility according to the specific pulsation.

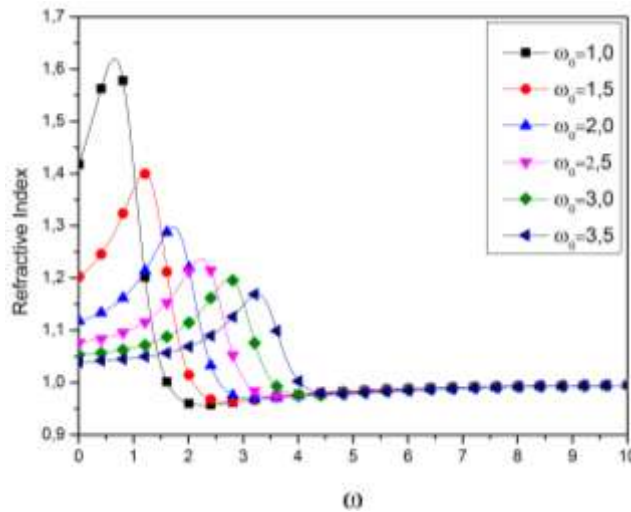


Figure 6:- Evolution of the reflective index according to the specific pulsation.

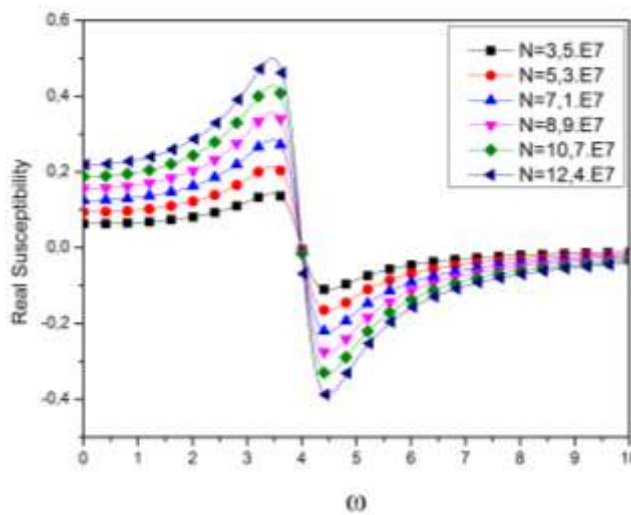


Figure 7:- Evolution of the real susceptibility according to the number of particle.

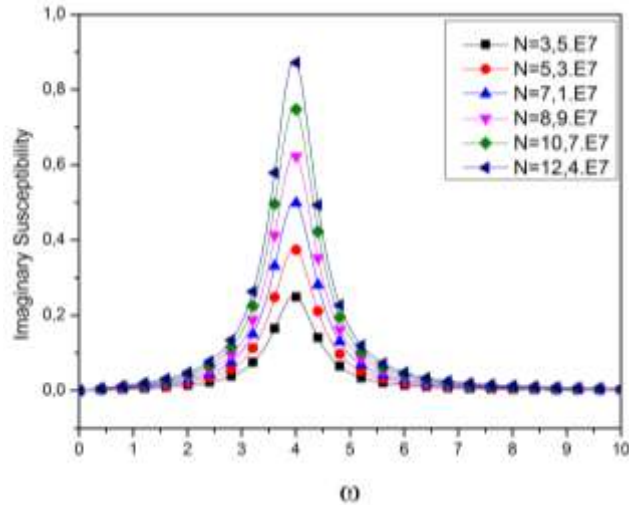


Figure 8:- Evolution of the imaginary susceptibility according to the number of particle.

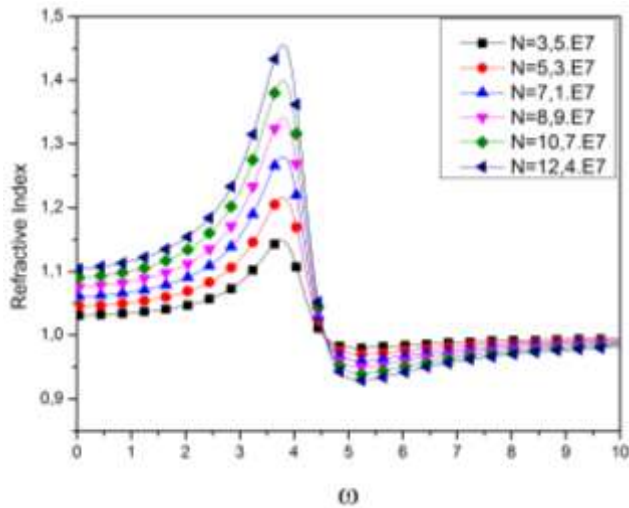


Figure 9:- Evolution of the reflective index according to the number of particle.

Conclusion:-

The present paper was dedicated to model and investigate the physical dielectric properties of the dense dielectric environment. The work led during this study brought numerous answers on the influences of the number of particle, the spectral width and the pulsation in the dielectric properties. However, several studies deserve to be pursued. In particular, the study of the dielectric properties in the artificial fibers and also the importance of its applications the industry and new technology. Several investigators have already implanted a model to investigate the properties of materials according to their membership [22-23]. But in our case one of the perspectives is to implement a model which allows to investigate any type of materials.

Computer Simulation:

```

!*****
! Program_Dielectric_Simulation
!*****
implicit double precision (a-h,o-z)
parameter(alpha=3.5,a=5,e=1.6,cmass=0.91 ,Om0=4)
parameter(eps=1 , tau=1 )
realbN1,bN2, D, fKRe, fKIm
!*****
    
```

```

open(Unit=1 , File=' Real Susceptibility Dense ')
open(Unit=2 , File=' Imaginary Susceptibility Dense ')
open(Unit=3 , File=' Permittivity')
open(Unit=5 , File=' Reflective Index')
!*****
do Om=0.01,40,0.01
!*****
!In A Dense Environment
!*****
      bN1=(Om0**2 - Om**2)
      bN2=(Om)/tau
      D=((Om0**2) - (Om**2))**2 + (Om/tau)**2
!*****
!Real Susceptibility
!*****
      fKRe=alpha*bN1/D
!*****
!Imaginary Susceptibility
!*****
      fKIm=alpha*bN2/D
!*****
! Permittivity
!*****
      epsR= 1+(fKRe + fKIm)
!*****
! Reflective Index
!*****
      Refr=sqrt(epsR)
!*****
! Display& Record
!*****
      write(1,4)Om,fKRe
      write(2,4)Om,fKIm
      write(3,4)Om,epsR
      write(5,4)Om,Refr
      format(2f7.3)
      enddo
      End
!*****

```

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