The Fifth International Symposium on Dielectric Materials and Applications
ISyDMA'5 : Virtual Conference 15-17 April 2020
Location: virtual

Anisotropy of conductivity and nonlinear effects in ε-GaSe crystals

M. Al-hattab[1,*], K. Rahmani[1], L. Moudou[1] , M. Khenfouch[2]

[1]*Faculty of Polydisciplinary, (ERPTM), BP 523, 23000 Beni Mellal-Morocco.*
[2] *Africa Graphene Center.*

*e-mail : med.alhattab@gmail.com

Abstract

In this paper, we have calculated the optical conductivity of the ε-GaSe layer. The calculation is based on the DFT method using the CASTEP code. This study is carried out in a field which extends energetically from 10 meV to 35eV, and they were measured for a polarization // and ⊥ with the axis c. The position of the main peaks is different for these two cases, which shows an anisotropic optical behavior of this material, because of the symmetry of a single layer, rather by the symmetry resulting from the stacking of the layers.

Keywords : *ε-GaSe*, *conductivity, Anisotropy.*

Introduction

The III-VI lamellar semiconductor binary compounds, such as Gallium Selenide (GaSe) and Indium Selenide (InSe) are of great scientific interest for their various technological applications, Gallium Selenide is a new direct band gap semiconductor. It has a lamellar structure whose basic element is a sheet. The latter consists of two Gallium planes interspersed between two planes of Selenium with a Se-Ga-Ga-Se sequence. It should be noted that within the same sheet, there are strong bonds between the atoms (ion-covalent bonds). On the other hand, all the layers constituting the 2D lamellar crystal are connected by weak Van der Walls bonds [1-3].

Theoretical framework

The conductivity of ε-GaSe are calculated using the PWPP method, using the CASTEP code [4], included in the Biovia material Studio 2017 software. This code is based on the functional density theory (DFT). The electrons are taken into account for the Ga, Se atoms are $4s^2\,4p^1$ et $4s^2\,4p^4$, respectively. The remaining electrons are kept frozen as base states. The ultrasoft pseudo-potential is selected to describe the interaction of valence electrons with nuclei.

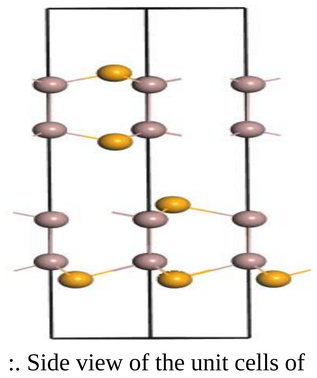

Figure 1 :. Side view of the unit cells of ε-GaSe . Orange atoms: Se, violet atoms: Ga.

Results and Discussion

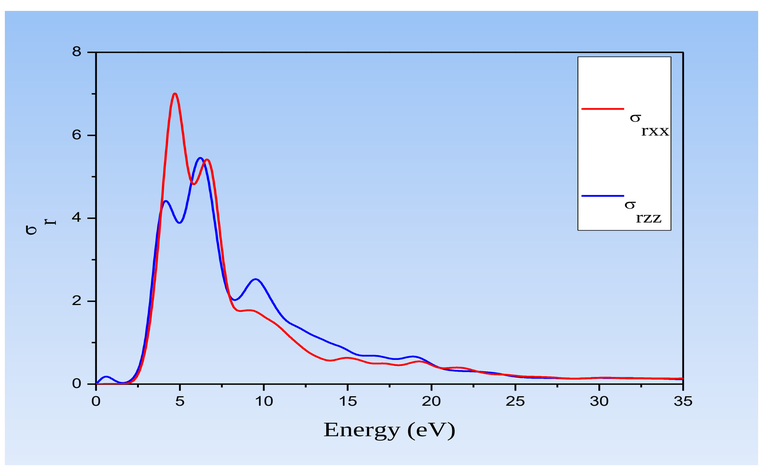

Figure 2 : The optical conductivity (real part) of the ε-GaSe polarized ⊥ and // with the c axis.

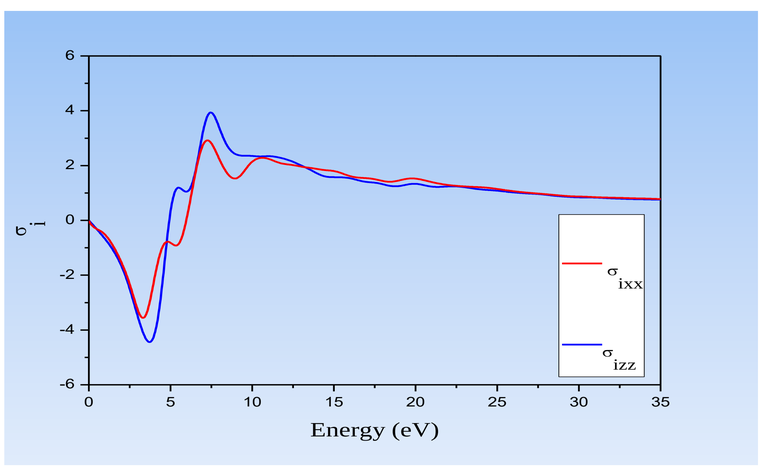

Figure 3 : The optical conductivity (imaginary part) of the ε-GaSe polarized ⊥ and // with the c axis.

Polytype	$\boldsymbol{\varepsilon - GaSe}$
$\boldsymbol{\sigma_{rxx}}$	$(E = 4{,}71eV)$ 7,00
$\boldsymbol{\sigma_{ixx}}$	$(E = 7{,}45eV)$ 3,93
$\boldsymbol{\sigma_{rzz}}$	$(E = 6{,}21eV)$ 5,45
$\boldsymbol{\sigma_{izz}}$	$(E = 7{,}26eV)$ 2,92

Table 1 : The maximum values of the optical conductivity (real and imaginary part) of the ε-GaSe polarized ⊥ and // with the c axis.

In Figure.1 and 2, we present the optical conductivity for an energy range from 10 meV to 35 eV. The conductivity begins at an energy 1,98eV in the x direction (polarization) and 1,80eV in the z direction (polarization) for, ε-GaSe. The cristale GaSe show better optical conductivity in the near UV range.

The optical conductivity will be decreases gradually (after the wavelength of the main peak) with the increase of energy . The maximum values of the real and imaginary portions of the optical conductivity are shown in Table 1.

The difference of the positions and the intensities of these maximas exhibit the anisotropic character of these lamellar material, theis anisotropic character is important for non-linear optical applications.

Conclusion

In summary, a correction of vdW interaction within the calculations of DFT is used to study the optical condictivity of GaSe monolayer. Calculations were made in both directions xx and zz (polarization). The results found both in the ultraviolet field or in the visible domain are significant and gives a strong argument for the use of these materials in various applications.

References

[1] M.Balkanski, R.F.Wallis, Semiconductor Physics and Applications, Oxford University Press, Oxford, 2000 (Chapter 1).
[2] See, e.g, F. Hulliger, Structural Chemistry of Layered-Type Phases, edited by F. Levy (Reidel, Dortrecht,1976), Chap. IV, 5b.
[3] A. Bourdon. STRUCTURE DE BANDES ELECTRONIQUE DE GaSe. Journal de Physique Colloques, 1974,35(C3), pp.C3-261-C3-267.
[4] M.D. Segall, P.J.D. Lindan, M.J. Probert, C.J. Pickard, P.J. Hasnip, S.J. Clark, M.C. Payne, First-principales simulation: ideas, illustrations and the CASTEP code, J.Phys.: Condens. Matter. 14 (2002) 2717-2744.

Acknowledgements

In conclusion, the authors sincerely thank all that contributed to this scientific work and particularly Sultan Moulay Slimane University,
Africa Graphene Center.