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Determination of Structural Dislocations In Tectosilicates Compounds From The Calculation and Simulation of The Energy Bands

Rodríguez P., Omar[1], Rojas J., Germán[2] and Casas S., Javier[3]
[1.]Rodríguez P., Omar. MsC Nuclear Physics. Director of Solid State Group in Central University, Bogotá D.C.Colombia. E-mail: orodriguezp@ucentral.edu.co
[2.]Rojas J. German. Manager of COLBRAMEX. Nit. 6.765016-2. isaGerartesanias22@hotmail.com
[3.]Casas S., Javier. Msc Electronics Engineer. Central University, Bogotá D.C. Colombia. E-mail: jcasass@ucentral.edeu.co

Abstract

The behavior of the band structure of the compounds designated tectosilicates under normal pressure, temperature and density relative to the model using the Bloch periodic potentials to determine the structural dislocation of this class of materials is studied.

Keywords: Apparent density, chemical potential, electric permittivity, relative humidity, voltage

Theoretical model

The theoretical approach for the calculation of energy bands in a given structure, Bloch model [1], in the field of quantum mechanics, is a problem that requires more than analytical solutions numeric type, the number of parameters and variables involved in the model. One of the approaches proposed in this report to calculate the energy bands of tectosilicates compounds is:

$$\frac{exp(w-w_o)t}{k_o}[\mu_m\epsilon_m w^2+\mu_m\sigma_e w-k_i^2]cos(k_i x)=-e\frac{\partial V(x)}{\partial x} \tag{1}$$

Where: $k_0=\frac{2\pi}{q}$ −inverse vector lattice, q – latticeparameter; $k_i=\frac{2\pi}{\lambda_i}$ −wave number; μ_m −magneticpermeability; ϵ_m −electricpermittivity; σ_e −electricalconductivity; e – electriccharge; *V(x)* – periodicpotentialnetwork

The mathematical model shown in equation (1) is the result of the solution of the characteristic equation of vibration of a network of tetrahedral Si type compound, when the material is incident an electromagnetic wave with phase zero, as presented in [21].

Experimental Procedure

We prepare and chosea series of ten samples of stones (rocks) structure composed of silicon oxide (SiO_2: Al, K, Fe, Cu, Mn, Ni, etc.) called tectosilicates (for each group), in the laboratory COLBRAMEX company, and asked the electrical conductivity test and was determined for each bulk density DAP with an electronic device that determines in real time the DAP dielectric materials developed at the Central University by researchers ESSOPTO group, of which it has a certified patent. Parallel to the comparison and validation of the experimental data obtained, the band structure of the different compounds of silicon was simulated to determine the energy performance of each stone under normal conditions of pressure and temperature.

Analysis of The Results

The representation of the energy bands in reciprocal space or phase space, to determine: a) the possible interactions of the charge carriers in the lattice, b) the transport of energy carriers between bands, c) the properties of absorption and emission energy of the structure and its relation to the apparent density of the material and in turn to calculate the maximum of the functions that determine the behavior of the distribution of carriers in the respective bands and densities of states allowed. The simulation of the band structure in this kind of material samples most likely areas to absorb power from an external source and the behavior of the Fermi level. In crystalline terms or Bloch model, such structures are not of direct band as shown in Figures 1 and 2, making them conductive anisotropic in terms.

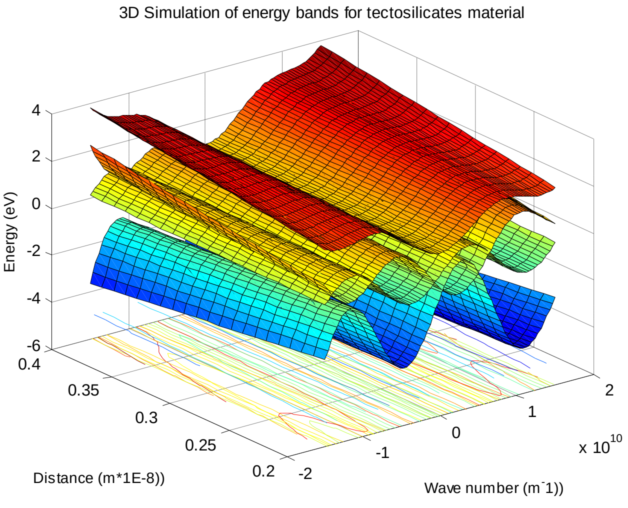

Figure 1: 3D Simulation bands structures oftectosilicate materials. The Fermi level (green curve) shows the tendency of deformation of the energy near the structural dislocations

Within the group of samples tested, three of them (pink opal, serpentine and structure commonly called jet, which is not owned by tectosilicate group was a good comparison sample), the behavior of theI vs V (current vs voltage), shown in Figure 3, provides an approximation to the band structure of these materials. Indeed when comparing the curves obtained in the simulation of bands with Mathlab program were found: a) the red curves in both Figures 2 and 3 have the same trend, b) the blue curves in the two figures also retain the same tendency as the curves of green color. Well we should clarify that part of the graph of the I - V, as the data were obtained only up to 3500 volts.

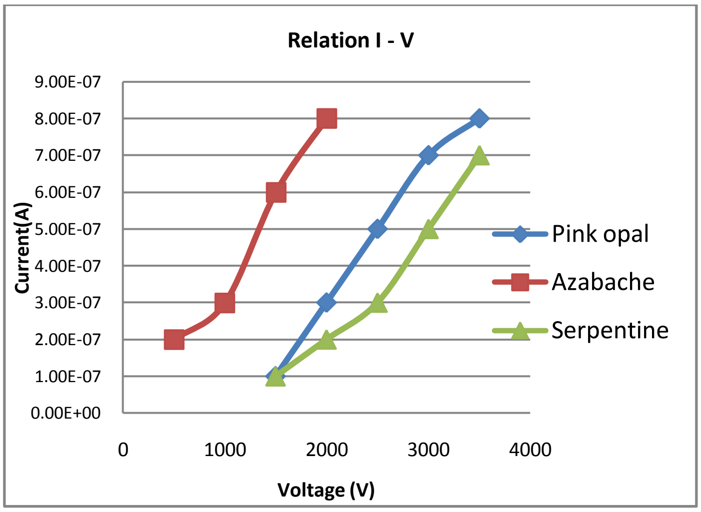

Figure 2: Behavior I - V structure samples (SiO_{2-x}: X), where the change in curvature of the graph can be seen due to structural failure of the material, that is, dislocation defects

Other but not least a result of this report was the creation of two-dimensional behavior of the bulk density of this class of materials, shown in Figure 4 The shades of colors (from light blue to dark gray) correspond to bulk density values in the range (2.2 to 3.7) typical values of compounds of (SiO_2, Al, Fe, Mn, Mg, K.) the data of apparent density is made with an electronic device patented by the Central University and the first author, using a capacitive registration system, in which the sample acts as a dielectric between the plates of the capacitor. The voltage values generated by the samples are translated into data density.

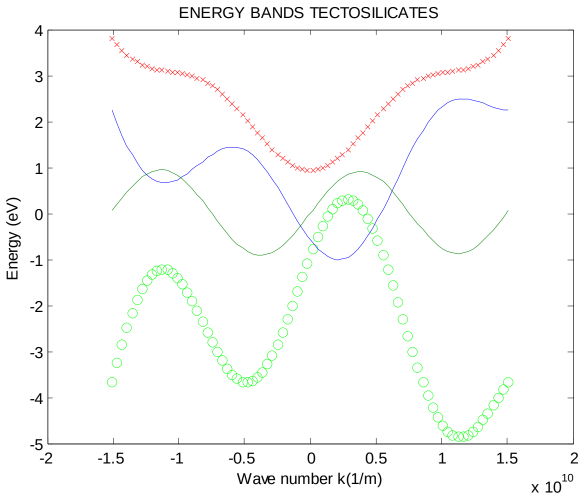

Figure 3: Determination of dislocations of a material simulation tectosilicate energy bands. The Fermi level (green curve) shows the tendency of deformation of the energy near the structural dislocations

Conclusions

The data obtained in this research show the possibility of using these materials to generate sensors coherent radiation but lateral absorption, that is, radiation produced dislocations in tectosilicates structures to divert perpendicular radiation generated by the source external. This would lead to improved efficiency of absorption of radiation sensors. The 3D simulation of the band structure for this class of materials (Figure 1), (Amethyst) shows the possibility of its use of lateral radiation sensors.

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