

Dielectric Properties of Ternary Chalcopyrite Semiconductors

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The ternary chalcopyrite semiconductors with composition $A^I B^{III} C_2^{VI}$ ($A^I = \text{Cu, Ag}$; $B^{III} = \text{Al, Ga, In}$; and $C_2^{VI} = \text{S, Se, Te}$) and $A^{II} B^{IV} C_2^V$ ($A^{II} = \text{Zn, Cd}$; $B^{IV} = \text{Si, Ge}$ and $C^V = \text{P, As}$) have attracted much attention due to potential applications in nonlinear optical (NLO) devices, second harmonic generation (SHG), light emitting diodes (LED's), photo-detectors (PD's) and solar cells. Recently the author has studied the various thermal properties of these semiconductors and proposed number of models based on plasma oscillations in solids' theory for the calculation of thermal expansion coefficient and heats of formation of these semiconductors [*J. Phys. Chem. Solids* **66**, 99 (2005); *Phys. Stat. Solidi* **242**, 869 (2005)]. In this paper, we propose a simple model based on plasma frequency formalism for the calculation of dielectric constant, energy gap, and ionicity of the A-C and B-C bonds in $A^I B^{III} C_2^{VI}$ and $A^{II} B^{IV} C_2^V$ chalcopyrites. Average values of these parameters have also been calculated for these semiconductors. Special care of delocalization of noble metal d-electrons effect has been taken into account in the case of A-C bond in $A^I B^{III} C_2^{VI}$ semiconductors while calculating the values of these parameters. Calculated values are compared with the experimental values and the values reported by different workers. An excellent agreement has been obtained between the calculated and reported values.

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