# LINEAR AND NON-LINEAR PROPERTIES OF TERNARY CHALCOPYRITE SEMICONDUCTORS

Vijeta Jha

Patent Scientist, Samvad Partners, Chennai, India
dr_vjha@rediffmail.com

Chalcopyrite semiconductors are an important class of materials, which are having potential applications in new cutting-edge classes of electronic, photovoltaic and optoelectronic devices. The $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ groups of semiconductors crystallize in the chalcopyrite structure, which is a superlattice of the zinc blende structure obtained by doubling its unit cube along the z-axis that becomes the c-axis of the chalcopyrite structure. A considerable amount of experimental and theoretical work has been done on the synthesis and growth of $A^{I}B^{III}C_2^{VI}$ (A = Cu, Ag; B =Al, Ga, In; C = S, Se, Te) and $A^{II}B^{IV}C_2^{V}$ ($A^{II}$= Zn, Cd; $B^{IV}$= Si, Ge, Sn; $C_2^{V}$= P, As) groups of chalcopyrite semiconductors [1]. New chalcopyrite compounds of $A^{II}B^{IV}C_2^{V}$ group have been developed by replacing $A^{II}$ type atom with Be [2], Mn [3] and Mg [4] atoms. These new chalcopyrite materials are also having potential applications in the areas of magnetically controllable NLO devices and spintronics, which are less studied and only few papers are available on these materials. Recently, defect chalcopyrites of $A^{II}B_2^{III}C_4^{VI}$ family have been reported in the literature, which are obtained from their parent chalcopyrites I-III-$VI_2$ and their grandparent II-VI compounds, and having huge applications in frequency conversion and phase matching. This is because of their large birefringence, high second harmonic generation coefficients and better figure of merit. The models proposed by earlier workers for the calculation of various properties of ternary chalcopyrites are complex in nature and require experimental values of number of parameters, which are not known for some of these materials, especially the new chalcopyrites of $A^{II}B^{IV}C_2^{V}$ family and defect chalcopyrites of $A^{II}B_2^{III}C_4^{VI}$ family. In the present research work, various linear properties such as homopolar energy gap, heteropolar energy gap, average energy gap, ionicity and dielectric constant have been studied for these materials using plasma oscillation theory of solids. The refractive index and electronic polarizability have been calculated for these chalcopyrites, 13 new magnetic materials of $A^{II}B^{IV}C_2^{V}$ family, and $A^{II}B_2^{III}C_4^{VI}$ group of defect chalcopyrite semiconductors. Further, the nonlinear optical properties have been investigated for $A^{I}B^{III}C_2^{VI}$ semiconductors and second order NLO tensor coefficients ($d_{36}$) of whole family have been calculated. In almost all cases, our calculated values are in better agreement with the experimental values than the values reported by earlier workers which in turn demonstrate the soundness of the present calculations.

[1] Shay J L and Wernick J H, Ternary Chalcopyrite Semiconductors: Growth, Electronic Properties and Applications, Pergamon Press, New York, (1975).
[2] Shaposhnikov V L, Krivosheeva A V and Borisenko V E, Phys. Rev. B 85 205201(2012)
[3] Medvedkin G A and Voevodin V G, J. Opt. Soc. Am. B 22 1884(2005)
[4] Shaposhnikov V L, Krivosheeva A V, Borisenko V E, Lazzari J L, and d'Avitaya F A, Phys. Rev. B 85 205201(2012)