Plasmon Energy and Lattice Energy of Ternary Chalcopyrite Semi-Conductors

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***Abstract*- In this paper, a simple empirical relation has been proposed to estimate the lattice energy of ternary chalcopyrite semi-conductors from their Plasmon energy. Attempts have been made to give a physical basis of the proposed co-relation.**

Index Terms- Ternary Chalcopyrite, Lattice energy, Plasmon energy

INTRODUCTION

Due to increasing scientific and technological applications, the study of various properties of ternary chalcopyrite has been renewed in recent years[1-29]. Lattice energy of these materials has, however, not been studied so much. In this study, we have tried to provide the explanation of lattice energy using Plasmon theory.

THEORY

The lattice energy (crystal energy) of a crystalline solid may be defined as the energy released when ions are combined to form a compound. It is the proportion of the cohesive forces that bind crystals. There are very few researchers who worked for the lattice energy of binary and ternary chalcopyrite.

Reddy et. al[30] suggested a linear relation between lattice energy and Plasmon energy for binary compound semiconductors. The relation is as,

$U = 381.9 + 24.3\ (\hbar w_p)$……(1)

where U represents lattice energy and $\hbar w_p$ represents Plasmon energy of compounds.

Kumar et. al[31] proposed a quadratic relation between lattice energy and Plasmon energy for binary compound semiconductors as,

$U = 421.224 + 27.940(\hbar w_p) - 0.178(\hbar w_p)^2$ (2)

where $\hbar w_p$ is Plasmon energy.

Reddy et. al[32] proposed the following relation for the calculation of lattice energy,

$U = K_1 + K_2 e^{k_3 n} - K_4 e^{k_5 n}$……(3)

where K_1, K_2,K_3 and K_4 are constants.

These results have shown that there must exist some correlation between lattice energy and Plasmon energy of materials. Lattice energy of a solid is the energy required to separate its constituent ions. In other words it is equal to binding energy of ions in the solid. Higher the value of this energy, tighter will be the binding between ions and hence higher will be the Plasmon energy. These arguments lead to a possible correlation between lattice energy and Plasmon energy. To establish such a relationship, graphs have been plotted showing the variation of U with Plasmon energy, for I-III-VI_2 semiconductors and for II-IV-V_2 semiconductor using the reported values. The plot of lattice energy vs. Plasmon energy for I-III-VI_2 is shown in fig.1 and for II-IV-V_2 is shown in fig.2.

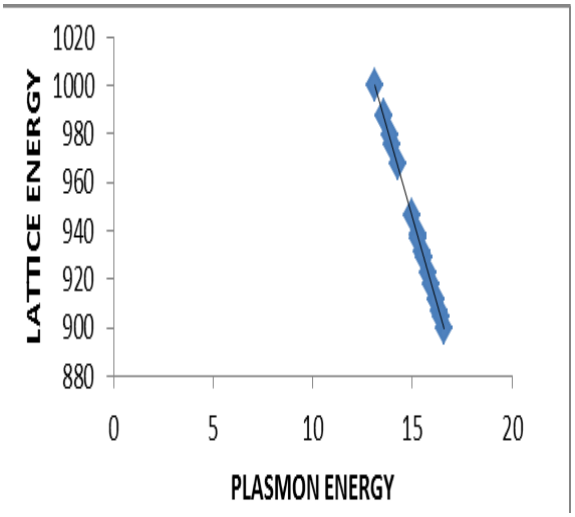

Fig.1: Plot of Lattice energy Vs Plasmon energy for I-III-VI2

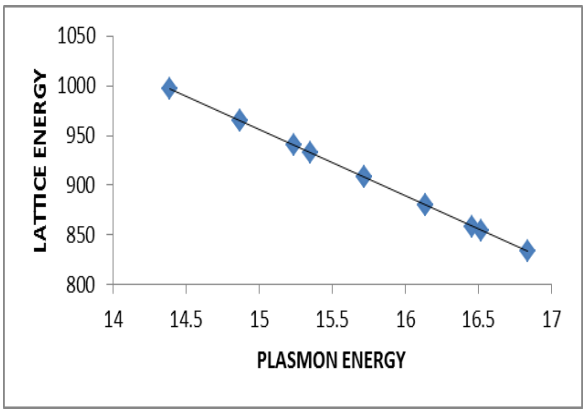

Fig.2: Plot of Lattice energy Vs Plasmon energy for II-IV-V_2.

The graphs have been plotted using least square fitting method. From the graphs it is clear that Lattice energy shows a linear relation with Plasmon energy for both types of ternary chalcopyrite crystals.

Using the nature of graphs, we have predicted a relation between Lattice energy and Plasmon energy for ternary chalcopyrites which is as,

$$U = \alpha(\hbar w_p) + \beta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

where α = -29.31 and β = 1385.5 for I-II-VI_2 and α = -66.887 and β = 1959.7 for II-IV-V_2 respectively.

RESULTS AND DISCUSSION

The Lattice energy of $A^{I}B^{III}C_2^{VI}$ & $A^{II}B^{IV}C_2^{V}$ type chalcopyrite structure solids are estimated using equation (IV). In table 1, the estimated values of U for $A^{I}B^{III}C_2^{VI}$ and in table 2 the estimated values of U for $A^{II}B^{IV}C_2^{V}$ are listed along with the results of earlier researchers. It is observed that the calculated values are in better agreement with the other results.

Table-1 : Lattice energy of I-III-VI_2 type chalcopyrite semiconductors-

Compounds	From equation(4)	Ref.[33]
$CuAlS_2$	899.54	899.51
$CuAlSe_2$	922.98	922.96
$CuAlTe_2$	967.53	967.51
$CuGaS_2$	904.22	904.20
$CuGaSe_2$	928.85	928.82
$CuGaTe_2$	975.74	975.72
$CuInS_2$	911.26	911.24
$CuInSe_2$	938.22	938.20
$CuInTe_2$	987.47	987.44
$AgAlS_2$	906.57	906.55
$AgAlSe_2$	931.19	931.17
$AgAlTe_2$	979.26	979.24
$AgGaS_2$	911.26	911.24
$AgGaSe_2$	937.05	937.03
$AgGaTe_2$	987.47	987.44
$AgInS_2$	918.29	918.27
$AgInSe_2$	946.43	946.41
$AgInTe_2$	1000.36	1000.34

Table-2: Lattice energy of II-IV-V2 type chalcopyrite semiconductors-

Compounds	From equation(4)	Ref.[33]
$ZnSiP_2$	833.32	833.64
$ZnGeP_2$	854.72	854.97
$ZnSnP_2$	880.14	879.86
$ZnSiAs_2$	908.23	908.30
$ZnGeAs_2$	932.98	933.18
$ZnSnAs_2$	965.09	965.18
$CdSiP_2$	858.73	858.53
$CdGeP_2$	880.14	879.86
$CdSnP_2$	908.23	908.30
$CdSiAs_2$	940.34	940.29
$CdGeAs_2$	965.09	965.18
$CdSnAs_2$	997.19	997.17

CONCLUSION

We have proposed an empirical relation to estimate lattice energy using Plasmon energy. The physical basis of the correlation has been discussed. The proposed model is simple and accurate. It is important to note that the constants appearing in the proposed relation are characteristics of the crystal structures. For a given crystal structure their values remain the same. The results obtained are in excellent agreement with the reported values and support the basis of the proposed model. From the above results it is clear that just by knowing Plasmon energy one can easily determine the values of Lattice energy. The proposed relation yield not only satisfactory results but also a comparison with the standard data provides a direct and precise check of the validity. In the approach, the calculation is simple, fast and more accurate. The only information needed is Lattice energy and no other experimental values are required. It is natural to say that present approach can easily be extended to the other more complex crystals.

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