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Abstract.- Dutt and Spitzer have experimentally observed the localized vibrational modes related to the phospherous defect in CdTe and reported that this defect may go either to substitutional or interstitial site. In this paper we study theoretically this phospherous defect behaviour for these two possible sites by Green's function technique and we believe that phospherous goes interstitially rather than substitutionally.The localized modes paired with Ga,In andAl are also investigated and discussed in the light of the experimental results.

1.Introduction.- Dutt and Spitzer[1] measured the infrared active localized vibration modes (LVM) in CdTe when defects of phospherous paired with In,Ga or Al are introduced. Their studies on LVM could not rule out the possibilities of the P defect going to interstitial or substitutional sites. It may further go to Te or Cd sites. For interstitial configuration it may be surrounded by 4 Cd neighbours or alternatively by 4 Te neighbours.The site symmetry in all these case is T_d and the LVM falls under the F_2 representation. To throw more light on the defect configuration in the light of the experimental results ,we have made some theoretical investigations on these LVMs using lattice Green's functions and the results are presented here.

2.a) Isolated substitutional P centre.- Using the theory of Maradudin et al [2] the LVM frequencies can be obtained from the solution of the determinantal equation $\left| I - \underset{\sim}{g}(\omega)\, \underset{\sim}{\delta 1}(\omega) \right| = 0$ where $\underset{\sim}{g}$ refers to the Green's function of the host lattice entering the defect space(constituted by the defect and its 4 neighbours) and $\underset{\sim}{\delta 1}$ the corresponding matrix for the force constant changes in the same defect space.Using the symmetry coordinates these matrices can be blockdiagonalized and the blocks of interest corresopnd to a 3x3 matrix corresponding to F_2 representations. The relevant Green's functions are computed using the phonons and eigenvectors of the modified rigid ion model of Plumble et al[3]. Assuming no relaxation the force constant changes can be expressed with one parameter ΔA. If we fit the experimental LVM to this configuration we noticed an unusual increase of the force constant. When one

normally expects a force constant weakening for a lighter impurity such a large increase in the present case (About 74%) promted us to examine the interstitial situation using lattice Green's functions.

b) Interstitial case.- Here also the nearest neighbour appro i-mation with T_d symmetry gives the LVM under F_2 representation. Using the theory of Brice [4] adapted for this case gave a force constant between interstitial and the host atom first neighbour around 3.8468×10^4 dynes/cm as against 6.0×10^4 dynes/cm beteen Cd and T_e. The inclusion of the second neighbours did not alter the situation very much. This reveals that the LVM mode can be accounted in an interstitial configuration with a weaker force constant between the defect and the first neighbour. This is what one expects for a lighter impurity. In order to throw more light we have also computed the LVM modes due to the additive impurities of Ga, In and Al in both these configurations.

c) Substituted P defect paired with Ga, In and Al.- We assume P to Te site with Ga, In or Al going in any one of the 4 neighbouring Cd sites. We have now 2 LVMs associated with P centre due to the reduction of the point symmetry. Using the fitted force constants from isolated substitutional cases the LVMs are calculated for this configuration. However in these cases also one noticed Al-Te Ga-Te interactions to be larger than Cd-Te interaction.

d) Interstitial P defect paired with substitutional Ga, In and Al.- The interstitial P atom is assumed to be surrounded by 4 Cd atoms one of which is now replaced by Ga, In or Al. Now as in (c) knowing P-Cd interaction from isolated interstitial case and interaction of the type Ga-Te from isolated substituional case and Ga-P interaction from crystal data of GaP, the modified LVM frequencies are calculated.

3. Results and conclusions.- The results are summarised in Table 1. A perusal of the results indicate that for the paired case the LVMs are satisfactorily accounted for by both the configurations.

But we should bear in mind that for the substitutional cases, one encountered unusually large force constants for Cd-P, Ga-Te and Al-Te. Eventhough for these lighter impurities, due to the fact that Group III or V elements enter in CdTe, one expects some long range coulomb contributions , still such extreme force constant changes of 74% are unexpected. Taken from this angle if one looks at the interstitial results,

Table 1.

System	Calculated LVM frequencies (in cm^{-1})		Expt
	Substitutional	Interstitial	
$P\text{-}Ga_{Cd}$	318.97	318.92	301.5
	349.21	345.97	352.5
			357.5
$P\text{-}In_{Cd}$	308.99	322.4	305
	345.97	352.7	331.5
$P\text{-}Al_{Cd}$	399.98	352.72	
	430.36	420.23	-

the pair modes are fairly well explained with a weaker P-Cd interaction. Thus we feel that P may go to the interstitial site rather than to a substitutional site. A recent calculation by Vandevyer and Talwar[5] for substitutional configuration also gave a negative result. But they had not considered the case of the interstitial configuration. More data from experimental studies such as from Raman scattering would be highly desirable to throw more light on the P defect configuration in CdTe.

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