To Study the Variation of Second Order Elastic Coefficient (SOEC) with Pressure for Binary Semiconductor Belonging to II-VI and III-V Groups of Semiconductors

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The variation of second order elastic coefficient (SOEC) of II-VI and III-V groups of semiconductors with pressure have been studied. On the basis of best fit data, the variation of SOEC with pressure can be well fitted by polynomial curve for C_{11} and C_{12} and linearly fitted for C_{44}. These results are in excellent agreement with the values reported by different researchers.

Key words: Second order elastic coefficient (SOEC), II-VI and III-V groups of binary semiconductors.

1. INTRODUCTION

SOEC of II-VI and III-V groups of semiconductors have been an important parameter to study these semiconductors because these semiconductors have potential applications in a variety of optoelectronic devices such as Nonlinear optics, light emitting diodes, Photovoltaic cells, photodetectors, lasers, modulators, Integrated circuits and filters [1-4]. The method enumerated in Literature [5-7] to study the variation of SOEC with pressure involve many experimentally determined parameters and tedious mathematical calculations. The dependency of SOEC on pressure for semiconductors for which experimental data [8] is available. In the present paper we have proposed new relationship of SOEC with pressure for II-VI and III-V groups of semi-conductors. This variation of SOEC with pressure can be well fitted by Polynomial curve and compared with the values reported by [9,10]. Although they have reported the variation of SOEC with pressure for few semiconductors belonging to II-VI and III-V groups of semiconductors. In this paper we will develop relationship of SOEC with pressure.

2. THEORY

The study of second order elastic coefficient (SOEC) i.e., C_{11}, C_{12} and C_{44} is quite important for understanding the nature of the interatomic forces in binary semiconductors. SOEC depends on pressure. To study the variation of SOEC (C_{11}, C_{12} and C_{44}) with pressure, we have taken ZnX (X = S, Se, Te) semiconductors for which experimental data [8] is available. We have interpolated the data i.e., plotted C_{ij} versus P in figures 1 to 3 for ZnS, ZnSe and ZnTe respectively. It is observed from these figures that the values of C_{11} and C_{12} for all ZnX semiconductors increases with the increase in pressure. These variations in C_{11} and C_{12} with pressure can be well fitted by polynomial curve. On the other hand, it is observed in case of C_{44} from Figure 1-3 that C_{44} decreases with the increase in pressure for all ZnX semiconductors. This variation of C_{44} can be well fitted by polynomial

curve, same as in case of both C_{11} and C_{12}. the variation of C_{ij} with pressure can be approximated by the following equation.

$$C_{ij}\ (C_{11},\ C_{12}) = K_{11} + K_{12}\ P + K_{13}P^2 \qquad (1)$$

where C_{ij} and P are in GPa, K_{11}, K_{12} and K_{13} are constants for a particular semiconductor of ZnX. The numerical values of K_{11}, K_{12} and K_{13} are reported in Table 1. We have calculated effect of pressure on SOEC for ZnX semiconductors by using equation (1), and the results are presented in Table 2(a), 2(b) and in 2(c) together with the experimental values. Our results are found in excellent agreement within 1% with the experimental values.To observe minutely the variation of C_{44} with pressure we have again plotted C_{44} versus P in Figures 4-6 for ZnS, ZnSe and ZnTe, respectively, A sudden fall in plots observed in all figures. For ZnS it is observed within the pressure range 16 to 18 G Pa, for ZnSe within the pressure range 12 to 15 and for ZnTe within the pressure range 8 to 10 GPa. We thought that this sudden fall in the curve is due to transition of phase from Zinc blende (B_3) to Rock salt (B_1) under pressure. We have shown this region in the figures. This prediction may be true because the experimental values [10, 11] of transition pressure are 14.5, 13 and 9, respectively for ZnS, ZnSe and ZnTe. Again, it is noted from figures (4-6) that C_{44} decreases linearly with the increase in pressure away from zero at the phase transition pressures. This feature is in accordance with the first−order. Character of the transition for all the compounds and is similar to that earlier reported in the cases of HgSe, HgTe [12,13]. Further the stable phase of a crystal is one in which the shear elastic constants C_{44}, is not zero (for mechanical stability) [14]. Also, the pressure at which C_{44} = 0, indicates the upper bound for the transition pressure. Thus, it is in inferred from figures (4-6) that the shear instability is higher than the corresponding transition pressure. This supports the high-pressure stability criterion proposed [14].To obtain the values of pressures associated with shear instability i.e., C_{44} = 0, we have again linearly fitted data points of C_{44} versus P, for ZnX in Figure 7. On the basis of these linear plots, we can write approximately.

$$C_{44} = K_{41} - K_{42}\ P \qquad (2)$$

where K_{41} (G Pa) and K_{42} (dimensionless) are constants for a particular semiconductor of ZnX. The numerical values of K_{41} = 87.378, 77.847, 54.215, and K_{42} = 1.246, 1.361, 1.430, respectively for ZnS, ZnSe and ZnTe. We have calculated the pressure associated with shear instability, by taking C_{44} = 0 in equation (2). The predicted values of pressures for which shear instability occurred are P = 69, 57 and 40 G Pa, respectively, for ZnS, ZnSe and ZnTe.

Table 1: The values of constants used in equation (1) to calculate C_{ij} (C_{11}, C_{12}) for ZnX (X = S, Se, Te).

Compound	C_{ij}	K_{11} (G Pa)	K_{12}	K_{13} (G Pa)$^{-1}$
ZnS	C_{11}	138.503	8.848	−0.151
	C_{12}	92.032	11.760	−0.175
	C_{44}	85.528	−0.759	−0.024
ZnSe	C_{11}	126.851	6.711	−0.039
	C_{12}	86.101	9.351	−0.061
	C_{44}	75.851	−0.817	−0.025
ZnS	C_{11}	96.536	7.308	−0.045
	C_{12}	69.531	9.417	−0.046
	C_{44}	57.279	−1.449	−0.001

Table 2(a): The values of SOEC (C_{11}, C_{12} and C_{44}) G Pa with pressure P (G Pa) for ZnS.

Compound	P	C_{11}		C_{12}		C_{44}	
		Exp. [9]	Cal.	Exp [9]	Cal.	Exp. [9]	Cal.
ZnS	1	150	147	105	104	85	85
	2	157	156	115	115	84	84
	3	162	164	125	126	83	83
	4	170	172	135	136	82	82
	5	175	180	144	146	81	81
	6	185	186	155	156	80	80
	7	195	193	170	166	79	79
	8	200	200	178	175	78	78
	9	205	206	182	184	77	77
	10	212	212	190	192	75	75
	11	220	218	202	200	74	74
	12	225	223	208	208	73	73
	13	228	228	212	215	71	71
	14	232	233	225	222	70	70
	15	236	237	228	229	69	69
	16	240	241	232	235	68	67
	17	248	245	242	241	67	66
	18	251	249	252	247	64	64
	19	252	252	253	252	62	62
	20	253	255	254	257	60	61

Table 2(b): The values of SOEC (C_{11}, C_{12} and C_{44}) G Pa with pressure P (G Pa) for ZnSe.

Compound	P	C_{11}		C_{12}		C_{44}	
		Exp. [9]	Cal.	Exp [9]	Cal.	Exp. [9]	Cal.
ZnSe	1	135	134	91	95	75	75
	2	140	140	105	105	74	74
	3	145	147	115	114	73	73
	4	152	153	125	123	72	72
	5	160	159	135	131	71	71
	6	165	166	140	140	70	70
	7	173	172	148	149	69	69
	8	179	178	158	157	68	68
	9	186	184	164	165	67	66
	10	189	190	172	173	65	65
	11	195	196	180	181	64	64
	12	200	202	190	189	63	62
	13	205	207	195	197	61	61
	14	215	213	205	205	59	59
	15	220	219	215	213	57	58
	16	225	224	220	220	55	56
	17	230	230	225	227	54	54
	18	237	235	237	235	53	53
	19	238	240	240	242	51	51
	20	245	245	250	249	50	49

Table 2(c): The values of SOEC (C_{11}, C_{12} and C_{44}) G Pa with pressure P (G Pa) for ZnTe.

Compound	P	C_{11}		C_{12}		C_{44}	
		Exp. [7]	Cal.	Exp [7]	Cal.	Exp. [7]	Cal.
ZnTe	1	104	104	78	79	55	56
	2	112	111	88	88	54	54
	3	116	118	96	97	53	53
	4	126	125	108	106	52	51
	5	132	132	116	115	51	50
	6	140	139	124	124	50	49
	7	144	145	132	133	48	47
	8	152	152	144	142	46	46
	9	158	159	152	150	43	44
	10	164	165	160	159	42	44
	11	172	171	168	167	41	43
	12	180	178	176	176	39	42
	13	184	184	184	184	38	39
	14	188	190	192	192	37	37
	15	196	196	200	200	36	36
	16	204	202	204	208	36	34
	17	208	208	212	216	34	33
	18	212	213	224	224	32	32
	19	220	219	236	231	30	30
	20	224	225	240	239	28	29

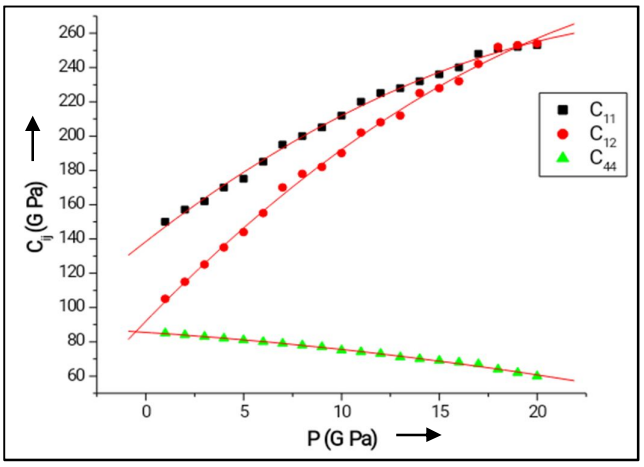

Fig. 1: Variation in SOEC C_{ij} with pressure P for ZnS.

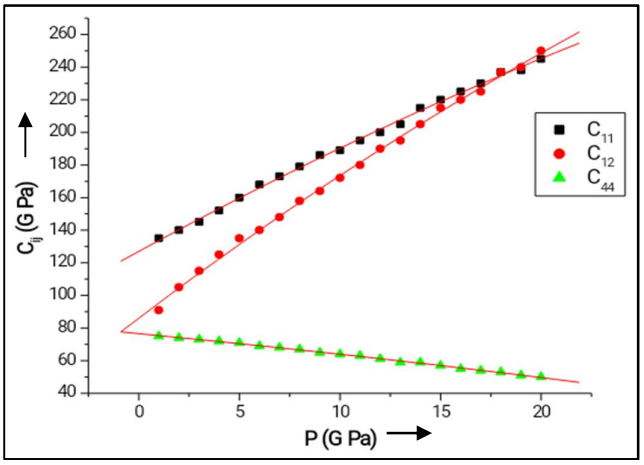

Fig. 2: Variation in SOEC C_{ij} with pressure P for ZnSe.

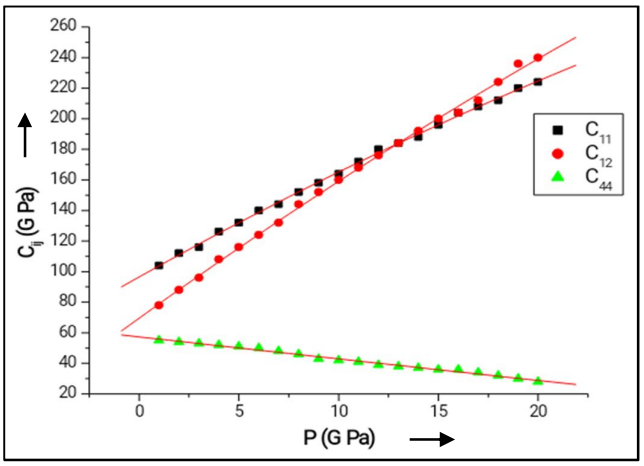

Fig. 3: Variation in SOEC C_{ij} with pressure P for ZnTe.

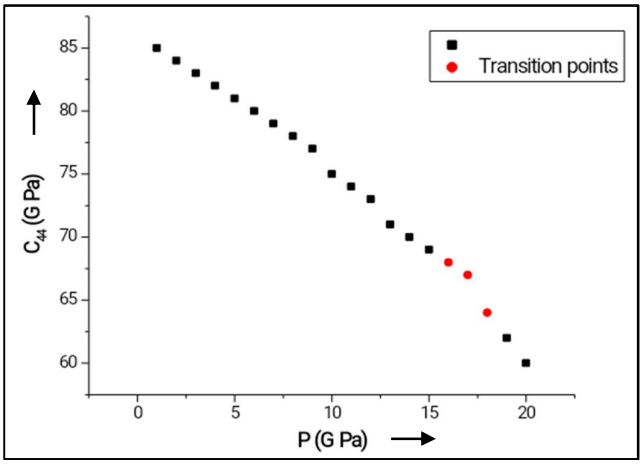

Fig. 4: Variation in SOEC C_{44} with pressure P for ZnS.

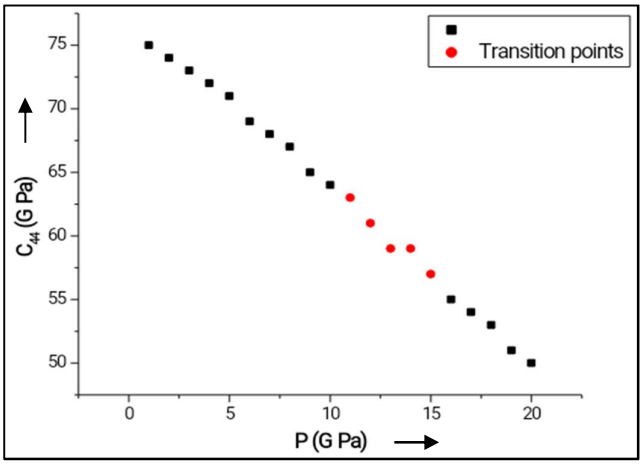

Fig. 5: Variation in SOEC C_{44} with pressure P for ZnSe.

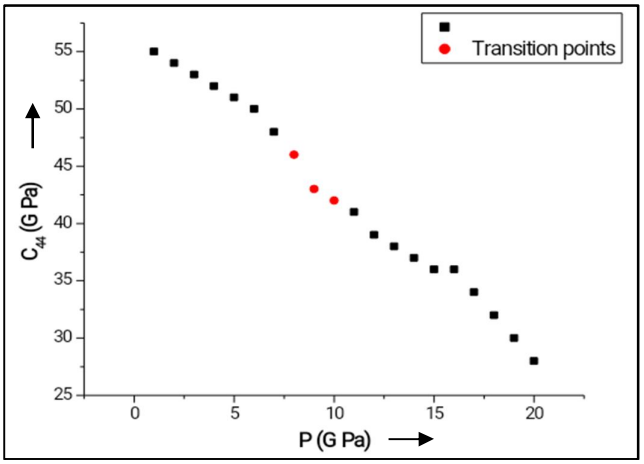

Fig. 6: Variation in SOEC C_{44} with pressure P for ZnTe.

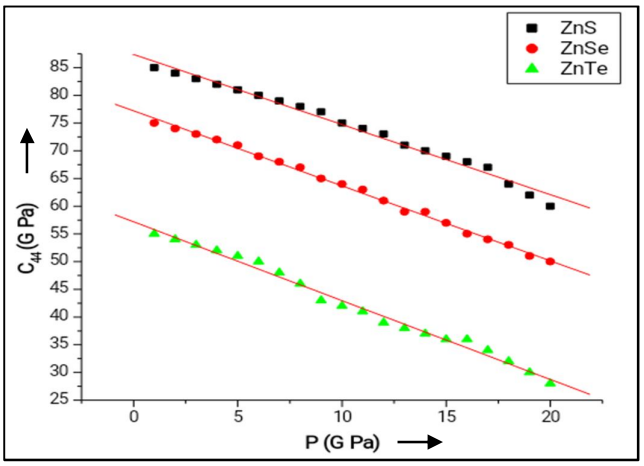

Fig. 7: Variation in SOEC C_{44} with pressure P for ZnX (X = S, Se, Te).

3. RESULT AND DISCUSSION

The present paper reports the variation of C_{ij} of SOEC for II-VI and III-V groups of semiconductors with pressure. The calculated values of SOEC are listed in Table 1 and 2 and compared with the values reported by Expt [7]. Our calculated values by using Eq. (1) and (2) listed in Table 1 and 2 and these values are reasonably in good agreement with the experimental values.

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