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A theoretical calculation of the first equilibrium pressure derivative of the bulk modulus, K_o' using the Born - Mayer theory

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ABSTRACT

Theoretical calculations of K_o' are available in the standard literature for a very large number of chalcogenides. At least, until a few years ago, experimental data were available only for four of these compounds. For these four cases, the experimental value is about 40% higher than the corresponding theoretical values. In the light of this large discrepancy, we carry out the calculations, using the Born-Mayer theory. Our values are considerably higher than the old theoretical values referred to above, except for BaO. The discrepancy between our theoretical values and the experimental values in the three cases, for which the data are available is considerably smaller than for the earlier calculation. The discrepancy for BaO is now a little more. Apart from this, in one or two other cases, there is considerable difference between our calculation and the earlier ones. Experimental measurements for these cases and a few more would help in clearing up the situation.

Key words: Derivative of bulk modulus, 'dimensionless' elastic energy $K_o V_o/E_o$, Born-Mayer theory.

INTRODUCTION

Theoretical calculations of the first equilibrium pressure derivative of the Bulk modulus, K'_o, had already been carried out for a large number of chalcogenides[1]. Experimental values are available only in four cases. The experimental value was about 40% larger than the theoretical value for all these four cases for which data are available.

We carry out the same calculations using a formula derived from the Born-Mayer theory. Our values of K'_o are higher than the older theoretical values in three cases. Only for BaO, the present value is in somewhat greater disagreement. Thus, our K'_o values are considerably better than those of the earlier calculations with regard to three of the four cases for which the data are available.

There are at least two other cases, TiO and NiO for which our theoretical value differs considerably from their older theoretical value. For TaO, the older theory predicts a negative value whereas the present calculation can not give a negative value for any case. An experimental determination of K'_o for these cases and a few more would help in deciding between the Born-Mayer theory and the one used in ref. I which also includes the dipole-dipole and dipole-quadruple interaction terms besides the main two terms and so would normally have been expected to give a better account.

RESULTS AND DISCUSSION

From our earlier paper[2], we may write down the parameter-independent formula for K'_o, obtained from the Born-Mayer theory.

Table - 1: Theoretical and experimental values of K'_o

	Compd.	$K_o V_o/E_o$ [2]	K'_o (present work)	K'_o [1]	K'_o exptl. value
1.	MgO	0.46	3.71	3.22	4.29
2.	CaO	0.53	3.92	3.37	4.85
3.	TiO	0.33	3.32	1.71	
4.	MnO	0.55	3.98	3.28	
5.	FeO	0.47	3.74	2.98	
6.	CoO	0.54	3.95	2.87	
7.	NiO	0.37	3.44	2.43	
8.	SrO	0.55	3.98	3.68	5.23
9.	CdO	0.40	3.53	2.78	
10.	BaO	0.57	4.04	4.37	5.67
11.	MgS	0.47	3.74	3.35	
12.	CaS	0.54	3.95	3.51	
13.	MnS	0.44	3.65	4.15	
14.	SrS	0.59	4.10	3.58	
15.	BaS	0.62	4.19	3.79	
16.	PbS	0.54	3.95	3.09	
17.	MgSe	0.43	3.62	3.05	
18.	CaSe	0.46	3.71	3.10	
19.	MnSe	0.44	3.65	2.77	
20.	SrSe	0.52	3.89	3.33	
21.	BaSe	0.53	3.92	3.41	
22.	CaTe	0.56	4.01	3.47	
23.	SrTe	0.36	3.41	3.70	
24.	BaTe	0.63	4.22	3.71	

$$K'_o = \left(\frac{dK}{dP}\right)_{r_o} = \left\{9\left(K_o V_o / E_o\right) + 7\right\}/3$$

Using the above formula, K'_o can be obtained for the compounds given in the table, using the values of $K_o V_o/E_o$ from our earlier work[2]. These theoretical values are given in the table which also gives the theoretical values of K'_o as obtained from the older theory. The last column gives the experimental value of K'_o. It is available only in four cases.

Only those chalcogenides have been selected here for which the experimental E_o are available and some experimental K_o are also available. The experimental values have been used in forming $K_o V_o/E_o$. Where the experimental values of K_o are not available, the theoretical values have been used.

We at once notice that our values of K'_o are considerably higher than the old theoretical values of K'_o for many cases. In three cases, our values are much closer to the experimental values than those given by the older theory.

We notice that our theoretical values for TiO and NiO differ markedly from the older theoretical values. Further, for TaO, the older theoretical values is a negative quantity whereas our value of K'_o can never be negative , as easily seen from the formula. At least, experimental measurement of K'_o should be carried out for the above three cases and possibly for a few more to resolve the marked difference between these two sets of theoretical predictions.

CONCLUSIONS

Experimental measurements of K'_o for, at least, the three compounds, TiO, NiO, and TaO and possibly a few more would greatly help in deciding what provides a better theoretical description of K'_o.

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REFERENCES

1. Jain V.K. and Shanker, J., *Phys. Stat. Sol* (b) **106**, 287 (1981).
2. Ahmad Rabia and Khan M.Z.R., Paper entitled 'Dimensionless Relationship between Bulk Modulus, Molar Volume and Cohesive Energy for some Ionic Diatomic Solids', communicated to the *Orient. J. Chem.,* Bhopal.