Research Letter

Correlation between the Bulk Modulus and the Metallicity in Semiconductors

Y. Al-Douri

Laboratoire CRISMAT, ENSICAEN, CNRS UMR 6508, 6 Boulevard du Maréchal Juin, F-14050 Caen Cedex, France

Correspondence should be addressed to Y. Al-Douri, yaldouri@yahoo.com

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The metallicity in semiconductors with respect to energy gap along $\Gamma \rightarrow X$ is used to calculate bulk modulus and gives reasonable results in agreement to that of experimental and Cohen results.

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1. INTRODUCTION

It has become possible [1] to compute structural, thermal, and other static properties knowing only the atomic numbers and masses of the atoms composing the materials. The transforming of a qualitative or verbal concept into a quantitative or mathematical formula represents the difficulty in defining the bulk modulus. More empirical approaches have been developed [2] with yield analytic results which can be used for exploring trends in materials properties. Because ab initio calculations are complex and consuming time, more empirical approaches have been developed [2, 3] to compute properties of materials. In many cases, the empirical methods offer the advantage of applicability to a broad class of materials and illustrate trends. These empirical approaches do not give highly accurate results for each specific material, but they are still very useful. Cohen [4] established an empirical formula for the calculation of the bulk modulus, based on the nearest-neighbor distance. His result is in agreement with experimental scale.

In this paper, we have established an empirical formula for the calculation of the bulk moduli B_0 of a specific class of materials. The theory yields a formula with three attractive features. Due to approaching their values and treating them as a common characteristic for the zinc-blende crystals, only the metallicity α_m and the energy gap along $\Gamma \rightarrow X$, respectively, are required as input, the computation of B_0 itself is trivial. This option is attractive where it allows the consideration of hypothetical structure and the simulation of exper-

imental condition that are difficult to achieve in the laboratory, for example, very high pressure.

2. RESULTS AND DISCUSSION

The goal of this study is to understand how qualitative concepts, such as bulk modulus, can be related to metallicity. This calculation is based upon metallicity α_m which has been reported previously [4–10]. An important observation for studying B_0 is the clear difference between the metallicity going from the group-IV to III-V and II-VI semiconductors as seen in Table 1. Hence, the metallicity is predominantly dependent on B_0 . A likely origin for the above result is the increase of ionicity and loss of covalency with the same chain. Because of the smaller contribution of covalency to B_0 , it is probably the increase of ionic bond charge that will reduce B_0 . Hence, the ionic contribution to B_0 is of the order 40 to 50% smaller. The differences between the metallicity and bulk moduli and the later reflects of the hardness of the materials have led to consider this model.

The basis of this model is the metallicity as seen in Table 1. The fitting of these data gives the following empirical formula:

$$B_0 = (60 - \lambda 20) \left[\frac{E_{g\Gamma X}}{\alpha_m} \right], \quad (1)$$

where α_m is the metallicity in (eV), $E_{g\Gamma X}$ is the energy gap along $\Gamma \rightarrow X$ in (eV), λ is a parameter appropriate for the group-IV ($\lambda = 0$), III-V ($\lambda = 2$), and II-VI ($\lambda = 2.65$) semiconductors, and the first term is in (GPa). The calculated bulk

TABLE 1: The calculated bulk moduli along with those of experimental and Cohen [4] values, corresponding with metallicity and energy gap E_{gTX} in (eV). ^a[4], ^b[5], ^c[6], ^d[7], ^e[8], ^f[9], ^g[10].

Compound	B_0 cal. (GPa)	B_0 exp. (GPa)	B_0 [4] (GPa)	α_m [3]	E_{gTX} (eV)
Si	100.9	98 ^a	98	0.66	1.11 ^{e,f}
GaP	74.19	87 ^a	87	0.62	2.3 ^g
InP	66.6	67 ^a	67	0.63	2.1 ^g
AlSb	58.8	58 ^a	57	0.68	2.0 ^g
GaAs	73.23	74.8 ^b	77	0.71	2.6 ^g
InAs	59.15	60 ^a	61	0.71	2.1 ^g
GaSb	56.7	57 ^a	58	0.74	2.1 ^g
InSb	45.9	47 ^a	47	0.74	1.7 ^g
ZnS	74.46	74.32 ^c	90	0.47	5.0 ^g
CdS	71.45	69 ^a	69	0.48	4.9 ^g
CdTe	45.71	47 ^a	47	0.49	3.2 ^g
ZnSe	64.7	64.7 ^d	75	0.53	4.9 ^g
ZnTe	52.8	51 ^a	59	0.53	4.0 ^g
CdSe	54.4	53 ^a	60	0.54	4.2 ^g

TABLE 2: Comparison of calculated (using (1)) and measured values of the bulk moduli of III-V and II-VI compounds. ^a[4], ^b[5], ^c[6], ^d[7].

Compound	B_0 cal. (GPa)	B_0 exp. (GPa)	(%)
GaP	74.19	87 ^a	14.7
InP	66.6	67 ^a	0.59
AlSb	58.8	58 ^a	1.3
GaAs	73.23	74.8 ^b	2
InAs	59.15	60 ^a	1.4
GaSb	56.7	57 ^a	0.5
InSb	45.9	47 ^a	2.3
ZnS	74.46	74.32 ^c	0.1
CdS	71.45	69 ^a	3.4
CdTe	45.71	47 ^a	2.7
ZnSe	64.7	64.7 ^d	0
ZnTe	52.8	51 ^a	3.4
CdSe	54.4	53 ^a	2.5

moduli values compared with those of experimental scale and Cohen [4] are given in Table 1. It may conclude that the present bulk moduli calculated in a different way than the definition of Cohen are in good agreement with the experimental values as seen in Figure 1, and exhibit the same chemical trends as those found in the values derived from the experimental scale or Cohen theory as seen in Table 1. The results of these calculations are in agreement with Cohen's [4] results and very near to results of experimental scale.

Some systematic behavior in the results of the calculated values has been noticed. For the II-VI compounds, the differences between the experimental and calculated values are less than 4% except for ZnSe where the coincidence is happened and the discrepancies are three times as larger for III-V compounds semiconductors, as shown in Table 2. The calculation estimates are larger than the measured values for the III-V compounds, and the tendency is similar for the II-VI com-

FIGURE 1: The experimental and our calculated bulk modulus scales by using formula (1) for different semiconductors.

pounds. It can be argued that the calculation-empirical differences are the same order as differences between reported measured values, and their chemical trends are real [4]. In conclusion, the empirical model obtained for the bulk modulus gives results in good agreement with the results of other scales.

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