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Research paper

Correlation trend between the bulk modulus, micro hardness and the lattice parameter of III-V semiconductors

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Abstract

This work aims to investigate the correlation between the bulk modulus as well as the microhardness and the lattice parameter of several cubic zinc-blende III-V semiconductors. Our study shows that both the bulk modulus and the microhardness correlate no-linearly with the lattice parameter of III-V binary compounds. The best fits were obtained using the Gaussian model, the coefficients of the correlation were found at around 0.993 for the bulk modulus, and 0.996 for the microhardness, respectively. Our expressions perhaps used with high accurate to predict the bulk modulus and the microhardness of other binary compounds and ternary semiconductor alloys.

Keywords: *III-V Semiconductors; Lattice Parameter; Bulk Modulus; Microhardness; No-Linear Correlation.*

1. Introduction

Group III–V semiconducting binary compounds have recently attracted great attention [1-5]. These materials have many applications in electronic and optoelectronic fields [6, 7]. At room temperature, III–V semiconductors crystallize in zincblende or wurtzite phases [8-10]. Using a microscopic empirical model based on atomic-scale parameters Xu et al. [11] have investigated the correlation between the bulk modulus of several polar covalent crystals and others parameters, especially: the bond length d, the effectively bonded valence electron (EBVE) number, n_{AB} and the coordination number product ($p = N_A N_B$). The major advantage of this microscopic empirical model is obvious for saving a lot of calculation endeavor compared with other methods using first-principles calculation.
Chen and Ravindra [12] have investigated the elastic properties of diamond and zincblende covalent crystals, and they have improved a model existing in the literature relates the average shear modulus with the bond length and Phillips ionicity.
Using the plasma oscillations theory of solids, Kumar et al [13] established a simple relationship for the calculation of bulk modulus B and microhardness H of group IV, II–VI, III–V, I–III–VI_2 and II–IV–V_2 semiconductors with tetrahedral structure.
In the present work, we investigate the correlation between the bulk modulus, the microhardness and the lattice parameter of several III-V semiconducting compounds.

2. Theory, results and discussion

Several physical quantities, such as the mass density, the elastic constants and the width of the gap in the semiconductors are strongly correlated with the lattice spacing between the atoms of crystal [1]. The experimental bulk modulus B and Knoop microhardness H of some III-V semiconducting compounds are summarized in Table 1 [14].

Table 1: Lattice Parameter a, Bulk Modulus B, and Knoop Microhardness H of Some III-V Semiconducting Compounds[14]

Materials	BN	BP	BAs	AlP	AlAs	AlSb	GaP	GaAs	GaSb	InP	InAs	InSb
a (Å)	3.615	4.538	4.777	5.463	5.661	6.136	5.451	5.653	6.096	5.869	6.058	6.479
B (GPa)	400	170	173	92.8	77.9	58.2	88.2	75.5	56.3	72.3	57.9	45.6
H (GPa)	73.0	32.0	19.0	5.5	5.0	4.0	9.4	7.5	4.7	3.9	3.8	2.9

Unlike hardness, bulk modulus B is a strictly defined thermodynamic quantity (B = VdP/dV). It can be obtained from the elastic constants [15], or by fitting the calculated total energy with Murnaghan equation of state [11]. The bulk modulus B is defined as the reciprocal of the compressibility β. A substance that is difficult to compress has a small compressibility, but a large bulk modulus [1]. The dif-

ferent data of the bulk modulus B summarized in Table 1 are plotted in Figure 1. We can observe clearly that the bulk modulus B decreases non-linearly with increase of lattice parameter a, so the results were fitted using the model of Gauss given as follow:

$$Y = Y_0 + \left(\frac{A}{w\sqrt{\pi/2}}\right)\exp\left(-2\frac{\left(x - x_c\right)^2}{w^2}\right) \quad (1)$$

Where Y_0, A, w and x_c are the model parameters. For the bulk modulus B of III-V compounds, our fitted numerical values Y_0, A, w and x_c are 32.58, 14724.09, 4.68, and - 0.98, respectively. Our model for the bulk modulus B can be expressed as follow:

$$B = 32.58 + \left(\frac{14724.09}{4.68\sqrt{\pi/2}}\right)\exp\left(-2\frac{(a + 0.98)^2}{4.68^2}\right) \quad (2)$$

where B is the bulk modulus (expressed in GPa), and a is the lattice parameter (expressed in Å). The average error of estimation on the bulk modulus B is only around 4.46%.

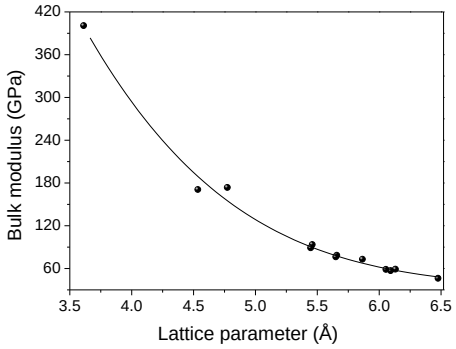

Fig. 1: Correlation Trend between the Bulk Modulus and the Lattice Parameter of Cubic Zinc-Blende III-V Functional Semiconductors.

The hardness of solid is related to crystal structure [16] and concentration of defects (vacancy, impurity, dislocations, etc) in the material [1, 17, 18]. The different data of microhardness H reported in Table 1 are plotted in Figure 2 as a function of the lattice parameter. Using the model of Gauss, our fitted numerical values concerning the Knoop microhardness H of the parameters Y_0, A, w and x_c are 3.89, 148.29, 1.65, and 3.38, respectively. So, our model for the Knoop microhardness H can be written as follow:

$$H = 3.89 + \left(\frac{148.29}{1.65\sqrt{\pi/2}}\right)\exp\left(-2\frac{(a - 3.38)^2}{1.65^2}\right) \quad (3)$$

In Eq. (3), H represents the Knoop microhardness (in GPa), while a is the lattice parameter (in Å). The average error of estimation of the Knoop microhardness H is around 15.08%.

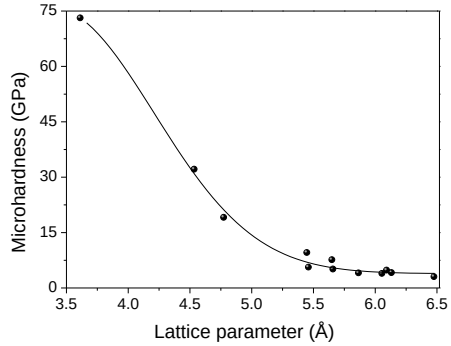

Fig. 2: Knoop Microhardness H versus Lattice Parameter in Cubic Zinc-Blende III-V Semiconductors.

For II–VI, III–V, I–III–VI_2 and II–IV–V_2 semiconductors with tetrahedral structure, Kumar et al [13] proposed a linear relationship between the bulk modulus B and the microhardness H, which is expressed by the following relation: $B = \kappa H + \gamma$, where κ and γ are the constants. The numerical values of κ and γ are, respectively, 6.18 and 35.49 GPa for III–V semiconductors [13].
The different data of microhardness H reported in Table 1 are plotted as a function the bulk modulus B in Figure 3. Using the model of Gauss, our fitted numerical values concerning H of the parameters Y_0, A, w and x_c are -1.35, 25599.93, 265.28, and 364.88, respectively.

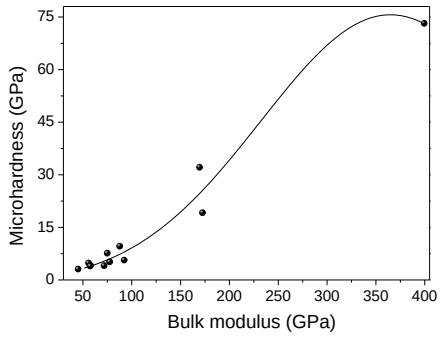

Fig. 3: Knoop Microhardness H versus Bulk Modulus B in Cubic Zinc-Blende III-V Semiconductors.

Our model for the Knoop microhardness H versus bulk modulus B in cubic zinc-blende III–V materials can be written as follow:

$$H = -5.63 + \left(\frac{59491.11}{469.99\sqrt{\pi/2}}\right)\exp\left(-2\frac{(B-566.38)^2}{469.99^2}\right) \quad (4)$$

Using our previous Gaussian model, the average error on the estimation of the Knoop microhardness H from the bulk modulus B is around 19.3%. The maximum error (46.2%) was found for AlP semiconductor, while the minimum error (0.0%) was reported for BN.

3. Conclusion

Based on some experimental data reported in the literature, we investigate the correlation between the bulk modulus, the microhardness and the lattice parameter of cubic zinc-blende III-V functional semiconductors. Both the bulk modulus and the microhardness correlate no-linearly with the lattice parameter in III-V binary compounds. The best fits were obtained using the model of Gauss. The coefficients of the correlation were found 0.993 for the bulk modulus, and 0.996 for the microhardness, respectively. The average error of estimation on the bulk modulus B is only around 4.46 %, while that on the Knoop microhardness H is around 15.08%.

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