

III-V SEMICONDUCTING NITRIDES ENERGY GAP UNDER PRESSURE

P. PERLIN, I. GORCZYCA, H. TEISSEYRE, T. SUSKI, E. LITWIN-STASZEWSKA,
S. POROWSKI, I. GRZEGORY

High Pressure Research Center "Unipress", Sokołowska 29/37, 01-142 Warszawa, Poland

AND N.E. CHRISTENSEN

Institute of Physics, Aarhus University, 8000 Aarhus, Denmark

In this paper we present overview of our recent experimental and theoretical results concerning electronic band structure of III-V nitrides under pressure. It is shown here that the pressure coefficients of the direct gap for studied nitrides are surprisingly small. To describe tendency in changes of the gap with pressure we use a simple empirical relation.

PACS numbers: 71.25.Tn

1. Introduction

Nitrides of group-III metals, namely GaN, AlN, BN, InN, are characterized by very short, strong atomic bonds and relatively large ionicity. Because of that, they have many physical properties different from other III-V semiconductors. In particular, it concerns the magnitude of energy gaps and their pressure coefficients. In this paper we present the results of the pressure variation of the direct energy gap, dE_g/dp , measured for GaN and InN as well as those calculated for the four mentioned above nitrides. We find that first principle calculations reproduce experimental results very well. Comparison with other III-V compounds shows that nitrides possess much smaller dE_g/dp values and in addition it appears that neither the Phillips ionicity nor the bond length can be used as a single parameter describing the discussed behavior.

2. Experiment

Optical absorption measurements were performed with the use of diamond anvil cell on the GaN and InN crystals. The samples were grown by means of special high-pressure, high-temperature method [1]. Pressure variation of the energy gap for the bulk semiconductors was determined from the shift of the absorption edge (see Table). Details of the experimental setup are published elsewhere [2].

TABLE
Pressure coefficient of direct gaps (in meV/kbar).
Here f_i is Phillips ionicity (the data are taken from
V. Vechten [3] and Christensen [4]) and d is the bond
length (in Å).

Compound	dE_g/dp		f_i	d
	Exp.	Theor.		
GaN	4.7	4.1	0.43	1.95
AlN	—	3.6	0.50	1.89
InN	2.0	2.5	0.57	2.16
BN	—	1.2	0.38	1.56

3. Theory

The band structures of nitrides were calculated from first principles with the use of Linear Muffin Tin Orbital method, within Local Density Approximation [2]. Band structure of the four nitrides was calculated for various pressure values and thus pressure coefficients of direct gap were determined (Table).

4. Discussion

The parameters commonly used in a discussion of trends in behavior of various semiconductors are Phillips ionicity [3], and bond length (reflecting the strength of interatomic interactions). It is expected accordingly that the dE_g/dp is smaller for more ionic compounds and for those characterized by shorter bonds. Pressure coefficients of the direct gap for the four considered nitrides show very small magnitude. It is even smaller than dE_g/dp observed in II-VI semiconductors which are characterized by higher Phillips ionicity with respect to the studied nitrides. The obtained coefficients are of the order of dE_g/dp found for diamond (≈ 1 meV/kbar).

Furthermore, it can be easily seen from Table that the pressure variation of E_g 's for the considered nitrides cannot be correlated either with Phillips ionicities or bond lengths. However, if we take into account both parameters simultaneously in the form of their ratio (see Fig. 1), it becomes possible to reproduce the tendency in pressure variation of E_g for a wide class of III-V semiconductors. We believe that this empirical procedure is more useful than the one proposed recently by Adachi [5] who also anticipated a decrease in dE_g/dp with increasing ionicity in various III-V semiconductors. However, there is a need for understanding the implications of the discussed relation on the microscopic ground.

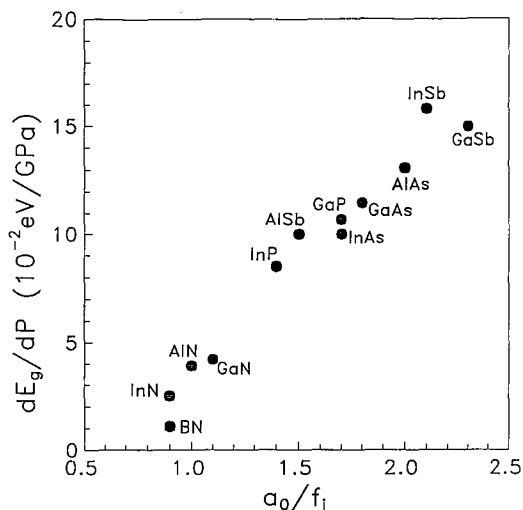


Fig. 1. Pressure coefficient of III-V nitrides in function of ratio of a_0 (lattice constant) and f_i (Phillips ionicity).

References

- [1] S. Porowski, I. Grzegory, J. Jun, in: *High Pressure Chemical Synthesis*, Elsevier, Amsterdam 1989.
- [2] P. Perlin, I. Gorczyca, N.E. Christensen, H. Teisseyre, T. Suski, *Phys. Rev. B*, to be published.
- [3] J.A. V. Vechten, *Phys. Rev.* **182**, 891 (1969).
- [4] N.E. Christensen, S. Sapathy, Z. Pawlowska, *Phys. Rev. B* **36**, 1932 (1987).
- [5] S. Adachi, *J. Appl. Phys.* **58**, R1 (1985).