Comments and Addenda

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Pressure dependence of the direct energy gap of GaAs

Yet-Ful Tsay* and Bernard Bendow
Solid State Sciences Division, Deputy for Electronic Technology, RADC (AFSC), Hanscom AFB, Massachusetts 01731

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By extending a pressure-dependent band-structure calculation for GaAs up to 180 kbar, we have predicted a pressure dependence of the minimum direct gap of GaAs in very good agreement with experimental data reported recently by Welber *et al.* Aside from the bulk modulus and its pressure derivative, which are needed to determine the compression of the crystal, the only other input data are the empirical pseudopotential form factors at atmospheric pressure. We find that adjustment of parameters is not required, in contrast to the calculation of Welber *et al.* in which quadratic variations of the ion core radii are assumed.

In a recent paper, Welber *et al.*[1] reported the pressure (p) dependence of the minimum direct gap E_0 of GaAs for pressures up to ~180 kbar. It was found that while the dependence of E_0 on the lattice constant is only slightly sublinear, the p dependence of the same gap shows a strong nonlinearity; in order to account for the strength of this nonlinearity, these authors introduced quadratic variations of the ion core radii of Ga and As with pressure.

The calculations reported here will be based on methods for calculating the energy-band structure of tetrahedrally bonded semiconductors at moderate p ($\lesssim$20 kbar) presented previously by the authors.[2] Salient features of the method are (a) the bulk modulus and the empirical pseudopotential form factors appropriate for describing the band structure at atmospheric p are the only input parameters; (b) the ionic pseudopotential is assumed to remain unchanged for a small variation (a few percent) of the lattice constant; (c) the p dependence of the screening effect of the valence electrons is accounted for self-consistently through a model dielectric function. The latter procedure utilizes the Penn model dielectric function as modified by Brust,[3] as well as a similar self-consistent treatment of its p dependence as presented by Brust.[4] We have applied our method to calculate the band structure of various diamond and zinc-blende-type semiconductors for pressures up to 20 kbar; the bulk modulus was assumed to remain constant throughout this pressure range. The calculated pressure coefficients of direct energy gaps for group-IV and -III-V semiconductors are generally within 25% or so of experimental data.

In this comment we extend the calculation to pressures up to ~180 kbar. The assumption of constant bulk modulus is no longer valid. There are no experimental data on the p dependence of the lattice constant at such high pressures. In order to relate the change of lattice constant with pressure, the ultrasonic data of the bulk modulus and its p derivative are employed along with the Birch's equation of state to calculate[5] the compression of GaAs for the pressure range concerned. Similar procedures were utilized by Welber *et al.*

In Fig. 1 we plot the dependence of E_0 on the change of lattice constant $\Delta a/a_0$ obtained from the present calculation. Although we obtain an essentially linear dependence, the agreement with the experimental data may be noted to be substantially better than that predicted by the nonadjusted calculations of Welber *et al.*[1] (i.e., those for which the ion core radii are taken to be constant). In our calculation we assume that the ionic pseudopotentials (and hence the core radii) are independent of small changes in lattice constant. Thus the differences between the present results and those of Welber *et al.* ought not to be attributed to the different calculational methods employed, but rather to

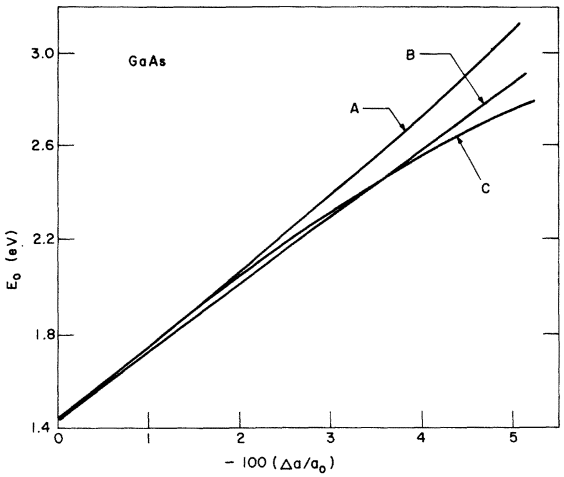

FIG. 1. E_0 vs $-(\Delta a/a_0)$. Curve A: calculation of Welber *et al.* with constant core radii; curve B: present calculation; curve C: deduced from the experimental data of E_0 vs p of Welber *et al.* using the relation between the lattice constant and pressure as described in the text.

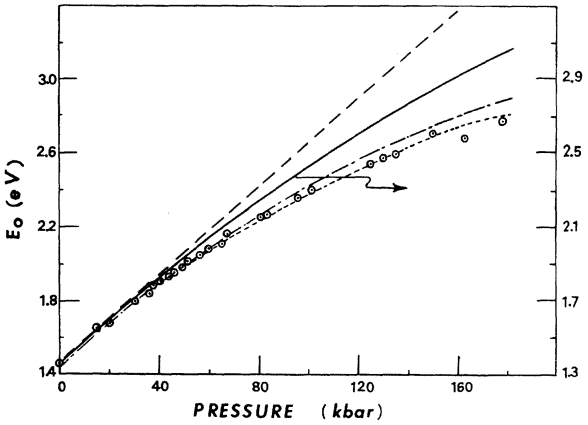

FIG. 2. E_0 vs p. Dashed curve: linear term of the experimental data of Welber *et al.*, i.e., slope equals 1.26×10^{-2} eV/kbar. Solid curve: calculation of Welber *et al.* with constant core radii, using the relation between the lattice constant and pressure as described in the text. Dot-dash curve: present calculation using the same relation between the lattice constant and pressure as that used in the solid curve. Dotted curve: same as the dot-dash curve, except the pressure derivative of the bulk modulus is increased by 20%. Circles: experimental data of Welber *et al.*

differences in physical content. In Fig. 2, we plot the results for E_0 vs p, using the compression of GaAs obtained in the fashion described above. The agreement between theory and experiment is observed to be very good. We note that even better agreement would be obtained if the p derivative of the bulk modulus were increased by about 20%, as indicated in Fig. 2. However, we are not aware of any evidence to determine the actual uncertainty in the latter quantity.

In conclusion, it appears that the strong nonlinear p dependence of E_0 in GaAs stems from the nonlinear p dependence of the lattice constant, and that our calculations (in which we do not invoke any change of core radii with lattice constant) are indeed capable of predicting a nonlinearity in good agreement with experiment.

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*National Research Council Postdoctoral Resident Research Associate.

[1]B. Welber, M. Cardona, C. K. Kim, and S. Rodriguez, Phys. Rev. B 12, 5729 (1975).
[2]Y. F. Tsay, S. S. Mitra, and B. Bendow, Phys. Rev. B 10, 1476 (1974).
[3]D. Brust, Solid State Commun. 9, 481 (1971).
[4]D. Brust, Phys. Lett. A 32, 114 (1970).
[5]H. J. McSkimin, A. Jayaraman, and J. Andreath, J. Appl. Phys. 38, 2362 (1967).