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OPTICAL ABSORPTION, ELECTROLUMINESCENCE, AND THE BAND GAP OF BP†

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In hopes of extending injection electroluminescence to III-V compounds with very high band gaps, we have studied the phenomenon along with other optical properties in cubic BP which is reported to have a band gap of 6 eV.[1] Injection electroluminescence, optical absorption, and the photoelectric response of an Au-BP surface barrier, however, lead us to conclude that cubic BP has an indirect band gap of only 2 eV. Our measurements were done at room temperature on small single crystals ($0.1\times0.1\times0.01$ cm) grown by crystallization from solution in nickel phosphides.[2]

Figure 1 gives the optical transmission, T; the absorption coefficient, α, calculated for a reflectivity value of 0.31; and a typical electroluminous emittance, Φ, spectrum for a forward biased p-n junction passing a current of 500 A/cm^2. The emission peaks at 1.97 eV, with subsidiary peaks on the low-energy side spaced about 0.1 eV apart. Although no conclusive identification could be made, this appears to be the energy of the LO phonon in accordance with a 12.1μ lattice absorption band.[1] The external quantum efficiency is about 10^{-5} in agreement with that for a similar edge emission in GaP, another indirect band-gap material.[3,4]

Owing to the presence of unavoidable pinholes in the single-crystal plates, the transmittance levels off for $\alpha>180$ cm^{-1}. For lower values of α, i.e., $h\nu<2.8$ eV, the transmittance is unaffected by the pinholes. The magnitude of α (190 cm^{-1}) on the high-energy side of the absorption edge agrees with that of GaP[3,5] and SiC[6] suggesting that the edge corresponds to indirect band-to-band excitation.

The case for a fundamental edge at 2 eV and

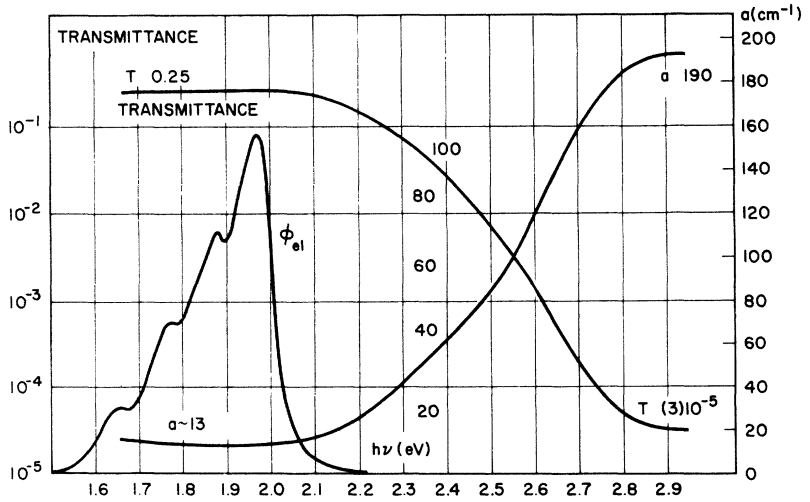

FIG. 1. Transmittance, absorption, and relative injection electroluminous emittance of BP at 300°C

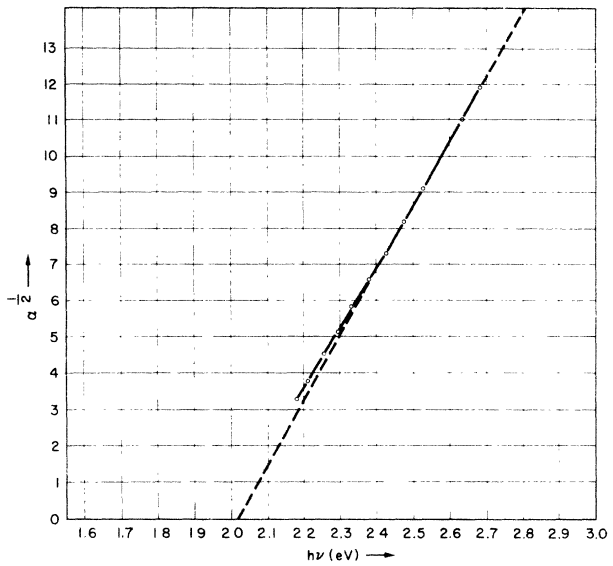

FIG. 2. Analysis of absorption data. The square root of absorption, corrected for 13 cm^{-1} background, vs photon energy.

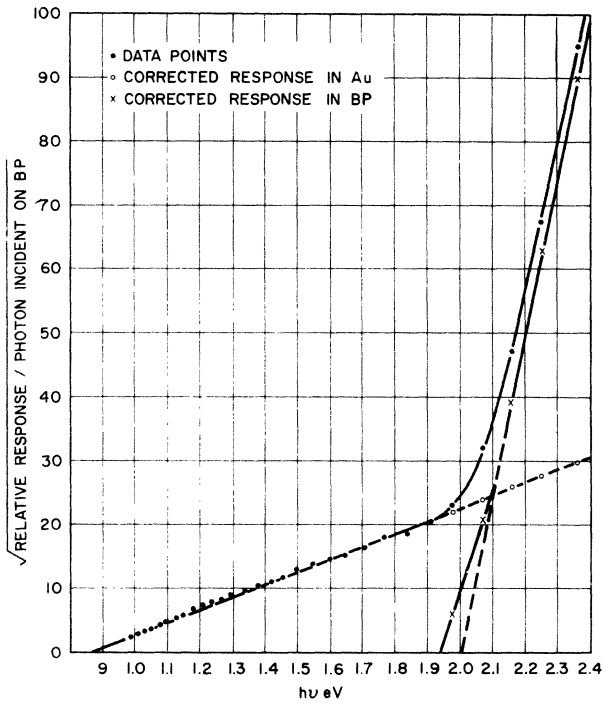

FIG. 3. Photoelectric response of an Au–p-type BP contact at 300°C.

phonon-assisted optical transitions is further bolstered by the linearity of $\sqrt{\alpha}$ vs $h\nu$ plotted in Fig. 2 after subtracting the background absorption of 13 cm^{-1}. An upper limit for the value of the BP band gap is obtained from the extrapolated intercept of the upper linear region which corresponds to the phonon emission branch[7] [$\alpha \propto (h\nu - E_g - E_{phonon})^2$] in analogy to similar curves for Ge,[8] Si,[8] Si-Ge,[9] GaP,[3,5] and SiC.[6] The departure at lower energies is ascribed to the phonon absorption branch. However, due to the above-mentioned background correction, its extrapolation is not considered sufficiently accurate to establish its intercept.

Further corroboration for our interpretation of the optical absorption data comes from measurements of the photoelectric yield[10] of an Au–p-type BP contact. Since the yield is proportional to α, as long as the penetration depth of the light is larger than the space-charge width plus the carrier diffusion length, the plot of the square root of the response vs $h\nu$ should duplicate the intercept of Fig. 2. Data for an Au barrier on p-type BP are shown in Fig. 3. Excellent agreement between intercepts is obtained; the value in Fig. 3 is also 2.02 eV. Spitzer and Mead[11,12] have shown that these kinds of photoresponse data give intercepts in good agreement with the established band gaps of GaAs, GaP, AlSb, and AlAs.

A lower limit for E_g is the maximum of the electroluminous emission band at 1.97 eV. With our interpretation of the $\alpha^{1/2}$ vs $h\nu$ intercept, the room-temperature band gap of BP is thus bracketed within a 50-meV interval.

Stone and Hill[1] deduced a 6-eV band gap from a large, abrupt decrease in the transmittance of vapor-deposited BP films at that energy. Because of the above-mentioned pinholes, we are unable to corroborate this finding. They also noted the 2-eV absorption edge, which is responsible for the red color of cubic BP, but suggested that it is contributed by an un-ionized impurity level. In our experience, both p- and n-type cubic BP crystals have the same red color.

So far, there has been no theoretical determination of the energy band gap of cubic BP. It should be pointed out that, in disagreement with our results, Sclar's empirical formula[13] leads to a value of 6.2 eV for the band gap of BP.

We want to thank L. E. Sobon of our laboratory for the synthesis of the BP crystals.

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SPIN WAVE–SPIN WAVE SCATTERING IN A HEISENBERG FERROMAGNET*

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We have obtained an exact expression for the scattering cross section of two spin waves in a simple cubic Heisenberg ferromagnet by solving the Lippmann-Schwinger equation by methods discussed in detail elsewhere.[1] In the long-wavelength limit the cross section agrees with that given by Dyson.[2] Moreover, the scattering amplitude contains denominators which vanish at the energies of two-spin-deviation bound states found by Wortis[3] and Hanus,[4] and which may provide scattering resonances elsewhere.

For background information on spin waves and the type of spin-wave interaction problem considered here, see the Article by Dyson[2] and the references contained therein. Our calculation (like Dyson's) is based strictly on the Heisenberg exchange Hamiltonian.

The lattice parameter and exchange integral J are natural units of distance and energy, respectively.

The number n of spin deviations from the totally aligned ferromagnetic ground state is conserved. We restrict ourselves to the case $n=2$ and omit the index n hereafter. It is conventional to start from normalized basis vectors for which the lattice sites $\vec{R}_j, \vec{R}_k$ of the two spin deviations are specified. Then Fourier summation on these two indices yields basis vectors identified by spin-wave vectors $\vec{\tau}, \vec{\tau}'$.

The interaction between two spin waves conserves total wave vector (up to a reciprocal lattice vector). It is convenient to make a transformation of coordinates so that we need consider only states with a given total wave vector. The appropriate lattice variables to use are the center $\vec{C} = \frac{1}{2}(\vec{R}_j + \vec{R}_k)$ and the radius $\vec{R} = \vec{R}_j - \vec{R}_k$. The appropriate spin-wave variables are the total wave vector $\vec{K} = \vec{\tau} + \vec{\tau}'$ and the relative wave vector $\vec{\lambda} = \frac{1}{2}(\vec{\tau} - \vec{\tau}')$. On Fourier summing over the index $\vec{C}$ we obtain a set of states specified by the total wave vector $\vec{K}$ and the radius $\vec{R}$. Since the Hamiltonian H is diagonal in the total wave vector, we omit it as an index hereafter.

In terms of this basis for the subspace of states of fixed total wave vector, an orthogonal set of two-spin-wave states normalized to unit volume is given by

$$u_{\vec{\lambda}}(\vec{R}) = 2^{1/2}\{[1+\delta(\lambda)][1+\delta(R)]\}^{-1/2}\cos\vec{\lambda}\cdot\vec{R}.$$

These are eigenfunctions of a Hamiltonian H_0 which is nearly equal to H and is chosen to yield energy eigenvalues

$$E_{\vec{\lambda}} = -8S\sum_{\alpha}\cos\tfrac{1}{2}K\alpha\cos\lambda_{\alpha}.$$

Here S is the spin and K_α, λ_α are rectangular components of the vectors $\vec{K}, \vec{\lambda}$.

The wave functions are real since $\vec{R}$ and $-\vec{R}$ specify the same state. They further differ from simple exponentials by multiplicative factors which are necessary to insure orthogonality.

Let $V = H - H_0$ be the interaction Hamiltonian. Its matrix elements with respect to the basis given above are

$$V(\vec{R},\vec{R}) = -2,$$

$$V(0,\vec{R}) = V(\vec{R},0) = 4\sqrt{2}S\{1-[(2S-1)/2S]^{1/2}\}\cos(\vec{K}\cdot\vec{R}/2)$$