Spectroscopic Determination of Valence Band Parameters of InP

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We estimate the valence band parameters of InP from spectroscopy of the Zn impurity. We also discuss how impurity magnetospectroscopy may be used to obtain the valence band parameters.

1. Introduction

The semiconductor valence band may be characterised by the three dimensionless Luttinger parameters [1]: γ_1, γ_2, γ_3. Despite many investigations there is still considerable uncertainty regarding the Luttinger parameters of InP, especially for γ_2 and γ_3. This contrasts to the situation for Ge, and to a lesser extent Si and GaAs, for which the valence band parameters have received much more theoretical and experimental attention and are much better known. The data for InP has been reviewed by Hackenberg *et al*. [2] who sought to determine the Luttinger parameters by hot-electron luminescence (HEL) and discovered that many Luttinger parameter triplets were consistent with the HEL data. We investigate spectroscopic approaches to estimating valence-band parameters in InP. Calculations have been made for both the unperturbed energy levels [3,4] and the energy levels in a magnetic field [5] of acceptor impurities in semiconductors characterised by different Luttinger parameters. We compare our recent experimental data for the transitions associated with the Zn acceptor impurity in InP to determine the most appropriate set of valence-band parameters. InP is a candidate for optoelectronics, radiation detection and high-frequency electronics uses.

2. Luttinger Parameters - γ_1, $\gamma_\square$, γ_3

The general form of the Hamiltonian for an electron or hole in a cubic semiconductor has been given by Luttinger [1] and may be written using the notation of Refs. 3 and 4 as:

$$H = (\gamma_1+5/2\gamma_2)(p^2/2m) - (\gamma_2/m)(p_x^2J_x^2+p_y^2J_y^2+p_z^2J_z^2) - (2\gamma_3/m)(\{p_xp_y\}\{J_xJ_y\} + \{p_yp_z\}\{J_yJ_z\}+\{p_zp_x\}\{J_zJ_x\}) - e^2/\varepsilon_0 r.$$

3. Baldereschi/Lipari Parameters - γ_1, δ, μ

An alternative set of valence band parameters was introduced by Baldereschi and Lipari [3,4], who recognised that the Luttinger Hamiltonian could be separated into components of spherical and of cubic symmetry. Convenient parameters in this approach are γ_1, identical to the Luttinger parameter γ_1; the spherical parameter $\mu = (6\gamma_3 + 4\gamma_2)/5\gamma_1$, which gives the strength of the spherical spin-orbit interaction; and the warping parameter $\delta = (\gamma_3 - \gamma_2)/\gamma_1$, which gives the cubic contribution. The cubic term is negligible in the cases where $\gamma_3 \sim \gamma_2$.

4. Estimating the valence band parameters from the energies of acceptor transitions

The energy levels of impurity states in semiconductors depend on the valence band parameters and have been tabulated as a function of these parameters in several papers [3-5]. Here we take the inverse approach and use the experimentally determined energies of transitions between acceptor states [6] as the input data and then search the tables by bi-cubic interpolation to obtain sets of Luttinger parameters which match the experimental result within a given precision. The central-cell correction strongly affects the energy of the ground state, so we use the energy difference between the D and G lines. Results are given in Fig. 1.

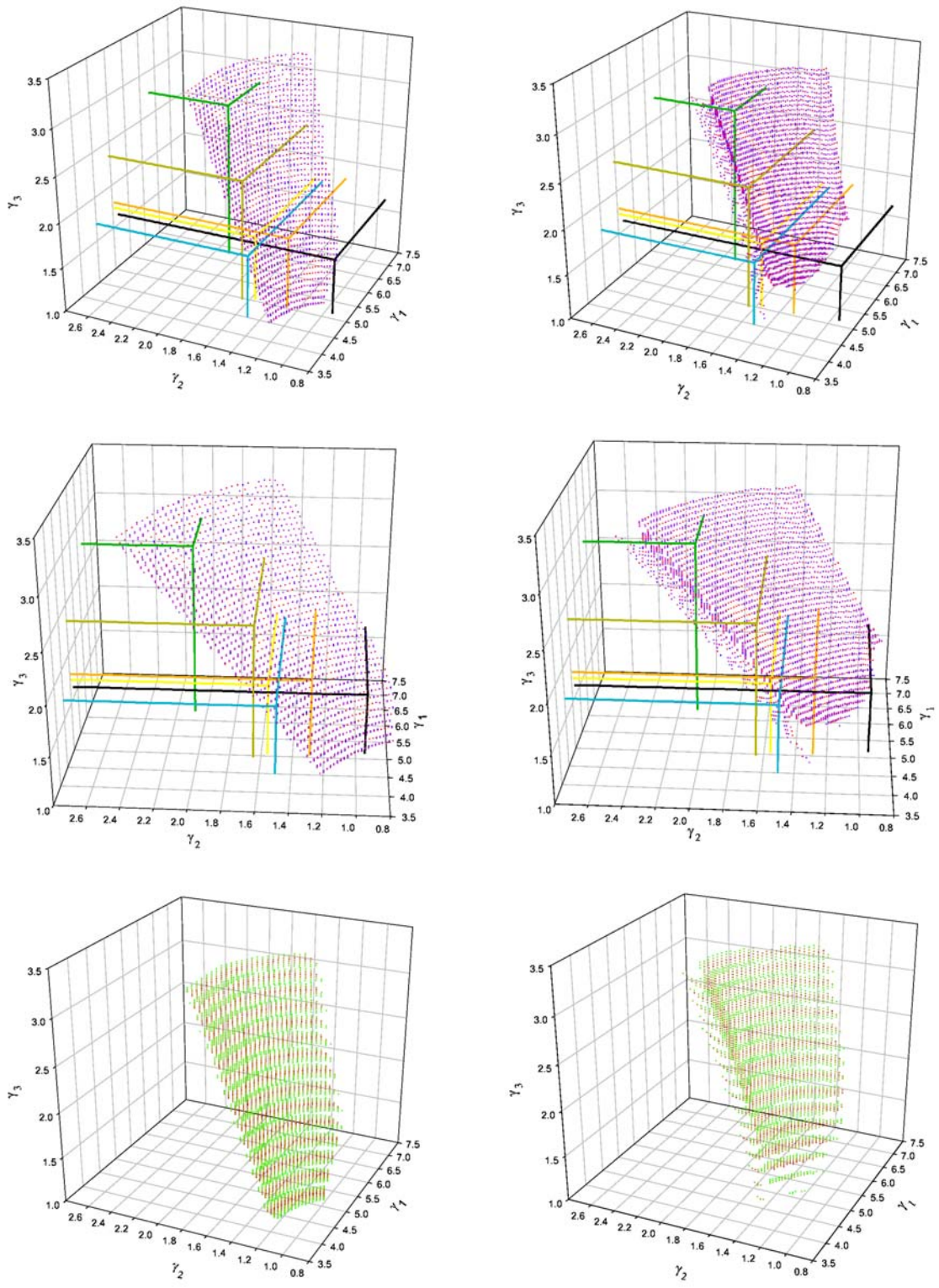

Fig. 1. Volumes in Luttinger parameter space that fit the experimental transition energies E_G = 29.94 meV and E_D = 34.84 meV of Zn in InP [6] according to the theories of Baldereschi and Lipari [3,4] (left-hand column) and Schmitt *et al.* [5] (right hand column), within 1% (top two rows; colour gradient red, 0% → blue, 1%) and within 10% (bottom row; colour gradient dark red, 0% → Green, 10%). The top two rows give different views of the same data. The straight lines in the top two rows indicate the Luttinger parameters reported by previous workers - see Table 1 for the sources and numerical values of these data.

The volumes shown in the two columns of Fig. 1 are broadly similar. The greater number of terms employed in Ref. 5 is likely to account for the differences; the origin of the "kink" is not known. It may be observed that many sets of Luttinger parameters are consistent with our experimental data, as was first pointed out by Hackenberg *et al.* [2] in analysing HEL data. Table 1 compares various sets of Luttinger parameters given in the literature with our spectroscopic data. The data of Cardona *et al*. [10] are in best agreement.

Table 1. Valence band parameters given by various authors compared to present spectroscopic data, E_D = 34.84 meV, E_G = 29.94 meV. The Luttinger parameters are given in columns 2-4 while the additional Baldereschi/Lipari parameters calculated therefrom appear in columns 5, 6. The final columns give E_D - E_G deduced from the calculations of Baldereschi and Lipari [4] and Schmitt *et al.* [5] from the valence band parameters. The %Err columns are the difference between calculated and our experimental values of E_D-E_G, divided by the latter.

							Theory [4]		Theory [5]	
First Author	γ_1	γ_2	γ_3	μ	δ	E_D-E_G (meV)	%Err	E_D-E_G (meV)	%Err
Lawaetz [7]	6.28	2.08	2.76	0.792	0.108	6.0	22	6.4	31
Bimberg [8]	4.95	1.65	2.35	0.836	0.141	10.3	110	NA	NA
Leotin [9]	5.04	1.56	1.73	0.66	0.034	4.5	9	4.5	8
Cardona [10]	5.05	1.6	1.73	0.665	0.026	5.0	1	4.7	3
Rochon[11]	5.15	0.94	1.62	0.523	0.132	2.6	47	NA	NA
Irmer [12]	5.04	1.29	1.79	0.631	0.099	3.8	22	NA	NA
Hackenberg [2]	4.5	1.5	1.7	0.72	0.044	6.3	28	6.4	30

5. Splitting of acceptor transitions in a magnetic field

The valence band parameters also play a central role in determining the *g* factors, which indicate the magnetic field splitting of the impurity transitions. To our knowledge only one calculation exists of this nature [5]. In principle, one can, by interpolation, use these tabulated data and experimental values of the *g* factors to deduce consistent sets of valence band parameters. Detailed experimental information is now available for impurity transitions of InP in strong (17.5 T) magnetic fields [6]. The work to relate this to the tabulated values of *g* factors and so determine valence band parameters by magnetospectroscopy is ongoing.

Acknowledgments

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