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Warping of the bulk dispersion of InSb

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Abstract. We calculate the warping of the bulk dispersion of InSb in the **k**-space using different models for the bulk band structure near the Γ point. It is shown that the dispersion of the conduction band Γ_6 is well described by the simplified six-band model, while the fourteen-band model is more accurate for the valence bands.

Keywords. Warping; bulk dispersion; InSb.

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1. Introduction

Understanding the details of the band-structure of zinc-blende semiconductors like InSb near the fundamental gap at the Γ-point is important because they govern the motion of carriers in external fields. This knowledge is becoming more and more essential for the design of semiconductor devices, the operation of which depends on peculiar characteristics of the band structure. Examples of such devices are infrared detectors, MIS-structures of compound semiconductors, tunnel diodes, etc.

To study the form of the energy dispersion near a band edge in semiconductors the so called **k**·**p**-approximation is appropriate because for these materials one generally has to consider only carriers within a narrow range of energies above the energy at the band extremum. The **k**·**p**-approximation, used to calculate the possible forms of the dispersion $E_n(\mathbf{k})$ in the vicinity of the band edge, results from a combination of the group theory and the perturbation treatment. Many theoretical calculations, from the classic paper of Kane (1957), till the recent work of Cardona *et al* (1986), have been devoted to this problem. In these calculations more attention is usually paid to describe the dispersion of the conduction band Γ_6 along the main symmetry directions. This band is non-parabolic due to the proximity of the valence band Γ_8 (the band-mixing effect), and for directions other than $\langle 100 \rangle$ and $\langle 111 \rangle$ it is spin-orbit split and warped due to the influence of remote bands.

In this paper we calculate the warping, i.e. the angular dependence in **k**-space, of the dispersion of the conduction and valence bands of InSb using three different band-models developed by Rössler (1984), which are based on Kane's **k**·**p**-method (Kane 1957). The calculation of the warping is more time-consuming because many directions in the **k**-space have to be considered, but the results obtained are informative and can serve to test the capabilities of different band-models to describe the band structure of InSb near the Γ-point.

2. Results and discussion

The three **k·p**-models, compared in the present paper, were developed by Rössler (1984), who also applied them to GaAs. More information about these band-models is given by Trebin *et al* (1979) and Ranvaud *et al* (1979). The spin and the spin-orbit coupling are taken into account in the three models, and the dispersion $E_n(\mathbf{k})$ is calculated from the equation

$$[H_n(\mathbf{k}; \text{b.p.}) - I_n E] = 0, \tag{1}$$

where the subscript ($n = 6, 8, 14$) denotes the number of the bands considered in the model, i.e. n is the size of the Hamiltonian matrix H_n, which describes the band-mixing, I_n is the unit matrix, $\mathbf{k}$ is the wave vector, E is the energy, and b.p. means all band-parameters, which participate in the model. Their values are given by Ranvaud *et al* (1979) for InSb and Ge, and by Rössler (1984) for GaAs.

The three band-models, compared here, are the following

Band model	Sub-space
Six-band-model (SBM, $n = 6$)	$(\Gamma_{6c}, \Gamma_{8v})$
Eight-band-model (EBM, $n = 8$)	$(\Gamma_{6c}, \Gamma_{8v}, \Gamma_{7s})$
Fourteen-band-model (FBM, $n = 14$)	$(\Gamma_{8c}, \Gamma_{7c}, \Gamma_{6c}, \Gamma_{8v}, \Gamma_{7s})$,

(2)

where the bands Γ_6 and Γ_7 are two-fold degenerate at $\mathbf{k} = 0$, while the bands Γ_8 are four-fold degenerate at this point. The subscripts c, v, s denote the conduction, valence and the split-off valence bands respectively. In the present calculations we consider all band terms in the Hamiltonian matrix, as derived by Rössler (1984).

The warping of the dispersion $E_n(\mathbf{k})$ of InSb in the plane (k_x, k_y), calculated with the three models (2), is shown in figure 1 for $k_z = 5{\cdot}10^8\ \text{m}^{-1}$. There are two loops on every plot because of the spin-splitting of the bands. The superscript l.h. denotes the light-holes band and h.h. the heavy-holes band. They both belong to the valence band Γ_{8v}.

Common for all the figures is the inner loop which always passes through the point $(k_x, k_y, k_z) = (k_0, 0, k_0)$ or $(0, k_0, k_0)$, where $k_0 = 5{\cdot}10^8\ \text{m}^{-1}$, i.e. through the $\langle 110 \rangle$ direction. This way we can compare the warping of the different bands, or the warping of the same bands ($\Gamma_{6c}, \Gamma_{8v}^{\text{lh}}, \Gamma_{8v}^{\text{hh}}, \Gamma_{7s}$) but obtained by the different models as in (2) using suitable values for the energy E in equation (1). On the corresponding plot then, E is kept constant for the other directions because all curves, which we plot on figure 1, are actually contours of constant energy.

Comparing the results presented in figure 1, one can see how the different models describe the warping and the spin-splitting of the bands. For example, the light-holes band Γ_{8v}^{lh} is very dependent on the choice of the model. On the other hand, the conduction band Γ_{6c}, which is important for the transport and optical properties of the semiconductor, is well described by the simplified SBM compared to the more accurate, but more elaborate FBM. This agrees with the treatment of Marques and Sham (1982), who used a six-band model to describe the surface sub-band structure of InSb, although in their calculations the influence of the remote bands was not considered.

The electron density n_c, given by

$$n_c(E) = \frac{1}{4\pi^3} \int_A \mathrm{d}^3 k, \tag{3}$$

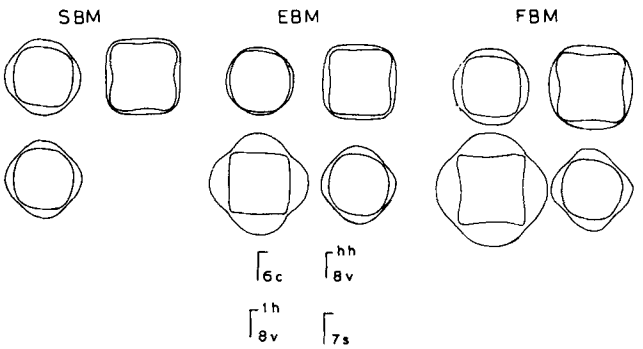

Figure 1. Warping of the conduction and valence bands of InSb calculated by the three models in equation (2). All curves are in the plane (k_x, k_y) and $k_z = 5{\cdot}10^8$ $(1/m)$.

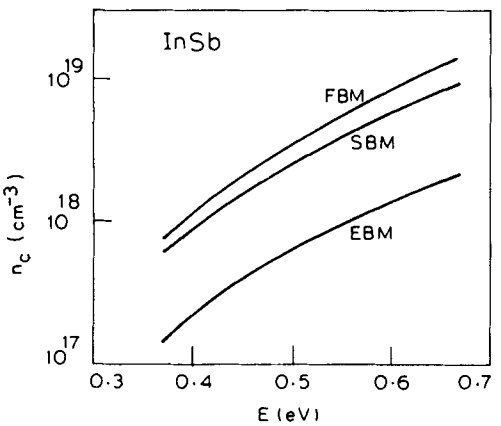

Figure 2. Electron density $n_c(E)$ calculated by the three band-models in equation (2).

where A is the volume of **k**-space for given energy E, is shown on figure 2. It is calculated with the three models given in (2). One can see that again the SBM gives results close to that obtained with the FBM, and this is in agreement with the conclusion drawn from figure 1.

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