Kane's Two-Band Model

In versions 4.0 and 5.0 of SEMITIP, usage was made of Kane's two-band model for obtaining the decay length of the wavefunction at energies throughout the forbidden gap region (E. O. Kane, J. Phys. Chem. Solids **1**, 249 (1957)). This model describes the continuous evolution in a state from electron-character (near the conduction band edge) to hole-character (near the valence-band edge). The light-hole band is assumed to be connected in this sense to the lowest lying conduction band, whereas the heavy-hole and split-off valence bands are connected to higher lying conduction bands. See Y.-C. Chang, Phys. Rev. B **25**, 605 (1982) for a description of the relevant complex band structures. Thus, in versions 4.0 and 5.0, values for the energy gaps between the heavy-hole band and its connected conduction band and betwen the split-off band and its connected conduction band were input to the program, and these values were employed in the computation of the tunnel current. The results of the computations are generally very insensitive to these two parameters, except when observable current occurs for energies deep within the band gap. That situation might occur, e.g., when probing the current very near the onset of a band edge in the presence of large band bending, in which case the two-band solution for the decay length *can* produce an observably different current. The two-band solution for the decay length can also play a role when inversion occurs. But, additional considerations are needed to properly model that situation; when the two-band model is used and the maximal z parameter value for integration of the Schrödinger equation set in the FORT.9 input file is too large, then the inversion current will erroneously appear in *both* the computations of the VB current and the CB current. Since it might be difficult for a non-expert user to correctly set the value of this maximal z parameter, the usage of the two-band model was eliminated in versions 4.1 and 5.1, and beyond. This was accomplished e.g. in version 4 by commenting out lines 54-55 of the main program and lines 548, 556, 656, 664, 768, 783, 877, and 892 of intcurr.f. Inversion currents can still be computed, but they will occur only in the localized states of the relevant band, as is appropriate. The commented-out lines can be added back in for version 4 (or analogous lines in later versions) if one wants to evaluate the influence of the two-band effects (but again, care must be taken in setting the value of the maximal z parameter for inversion situations for inversion situations). In that case, one would also add two lines in the FORT.9 input file giving the two additional band gaps between the heavy-hole band and its connected conduction band and betwen the split-off band and its connected conduction band. For GaAs, the values are:

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4.55      heavy hole energy gap (eV)
4.71      split-off energy gap (eV)
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