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Lattice-matched heterostructure envelope functions and band-to-band transmission through broken-gap heterostructures BART SOREE, MAARTEN VAN DE PUT, WIM MAGNUS, imec, WILLIAM VANDENBERGHE, University of Texas at Dallas, Richardson, Texas — We developed an envelope function formalism capable of describing the electronic structure in lattice matched heterostructures. The formalism takes into account the different nature of the materials involved by using matrix elements in the basis formed by the solutions of their respective bulk Hamiltonian. A transformation between these basis sets has been devised to allow for expansion in one consistent and complete set. This transformation is described without full knowledge of the basis function, as this would defeat the purpose of the envelope function method. We employ only the known interband momentum matrix elements to obtain the transformation coefficients. With this method it is not only possible to describe the electronic structure in heterostructures in a more rigorous way, it is also possible to describe band-to-band transitions through these heterostructures. In particular, we studied the transmission coefficients through broken-gap heterostructure. A large discrepancy was found with the effective mass approach, which predicts full transmission at a certain energy. Our method correctly predicts additional reflections due to the interface betweeen the two materials.

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