A plane-wave based, generalised formulation of continuum elasticity and multiband k·p-models

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Multiband k·p-models have been used successfully for the theoretical modelling of semiconductor nanostructures of different shapes, sizes, and for a wide range of materials. These models offer a computationally efficient approach to the electronic properties of quantum dots, wires, and wells on the basis of a continuum representation of the system under consideration. We will present a general formulation of k·p-models, that allows to study arbitrary nanostructure geometries, sizes, and material compositions employing an n-band Hamiltonian. The details of the Hamiltonian as well as the nanostructure geometry and composition are defined in user-generated input files, which adds great flexibility to taylor the calculation to the question of interest. In this manner, simulations using the well-established eight-band k·p-model as well as more sophisticated 14-band approaches or simple one-band effective mass models are straightforwardly possible. To account for elastic and piezoelectric properties, a continuum elasticity model has also been implemented. The resulting strain and piezoelectric potentials can then be considered in the calculation of the electronic properties. Both the continuum elasticity model as well as the multiband k·p-formalism were implemented in a plane-wave framework within the existing S/PHI/nX physics simulation package. This allows to make use of existing, highly efficient minimisation algorithms and to apply a reciprocal space representation for gradient operations, allowing for a significant boost in efficiency. The specific issues that occur in a plane-wave based implementation of these two continuum models will be furthermore discussed in example simulations that have been performed with our approach.

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