Non-linear strain theory for low-dimensional semiconductor structures

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Abstract

We present a continuous non-linear strain theory and demonstrate its plausibility on modelling low-dimensional semiconductor nanostructures. The main advantages of this theory are its non-linearity, continuous nature (computationally inexpensive), and anisotropy (includes the crystal structure). The theory allows us to account explicitly for internal strain and for realistic interface boundary conditions. The discussion is restricted to cases where the strain is nearly constant on the length scale of the primitive lattice cell except at interfaces where discontinuities are allowed. The main idea behind the theory presented here is to include as much information on the atomic structure in the continuous limit as it is necessary in order to accurately describe nanoscale systems. To illustrate the importance of non-linear effects and the inclusion of internal strain, we present some simple calculation for quantum wells with diamond crystal structure oriented in the [1 1 1] direction.

Keywords: Strain; Inhomogeneities; Crystalline structures

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