Band parameters of group IV semiconductors in wurtzite structure

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Metastable crystal phases of group IV semiconductors present in low aspect ratio nanostructures exhibit great potential to overcome current limitations in semiconductor industry. Their chemical and structural similarity to diamond structure is a key factor in incorporation such structures in current group IV technology, at the same time leaving much room for tailoring physical properties by means of size effect and polytypes mixing. Usual pathway for modeling heterostructures and low dimensional systems are **kp** and tight binding models which are computationally efficient and require minimal set of parameters. It is known however, that the accuracy of these models relies strongly on their parametrization and the stable phase values, present in the literature, cannot be transferred to other crystal phases. On the other hand *ab initio* methods provide great accuracy without empirical parameters but are computationally more expensive which limits their use in complex systems modeling.

The goal of presented work is the parametrization of six band **kp** model for lonsdaleite crystal phase which is the second most common phase after diamond. We use high accuracy *ab initio* methods to derive physical properties of group IV materials and then transfer our results to **kp** model. In particular the effects of strains on crystal and band structures are investigated in detail and described by elastic tensor and absolute deformation potentials respectively. Our parameters set together with already known parameters for diamond structure allows for efficient modeling of heterostructures containing different polytypes.