Electronic Structure of Interface Defects in Epitaxially Grown Germanium on Silicon

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Defects in the germanium/silicon epitaxial interface result in trap states which affect carrier recomination and transport, and thus device performance. Density functional theory (DFT) offers one method for characterising these states.

BACKGROUND

A number of devices rely on epitaxially grown germanium on silicon, including photodetectors, Stark modulators and lasers. There is a 4.2% lattice mismatch between these materials, hence germanium grown epitaxially on silicon will contain defects within some distance from the interface [1]. Line defects are either misfit dislocations—lines of dangling bonds where a mismatched plane terminates parallel to the heterointerface—or threading dislocations which occur where the side edges of the misfit dislocation terminate and usually glide along the (111) plane [2]. Defect structures create 'trap states'—allowed energy states within the forbidden band gap. Traps may act as recombination centres or inhibit transport over the interface, which can limit the repetition rate of devices such as photodetectors and may contribute to noise currents from detrapping of carriers outside the normal operating regime of a device. DFT offers one means of characterising the electronic structure of defects and hence the available states for carrier recombination and transport.

METHOD

The CASTEP simulation software [3] is used to calculate the electronic bandstructure for germanium and epitaxial interfaces of germanium grown on silicon, both for pure bulk and for cells containing extended misfit dislocations. CASTEP relies on periodic boundary conditions, and hence a misfit placed within a supercell will be replicated across the structure. However, first-principles calculations impose practical limits to the number of atoms which may be simulated, and one challenge is to ensure the calculated electronic states due to a dislocation are not unduly influenced by an adjacent periodic dislocation. A rhombohedral cell of germanium, in which the dislocation propagates along the [100] direction, was used to increase the spatial separation between dislocations while retaining practical numbers of atoms for simulation. In this orientation, a supercell one unit. cell deep in the plane of the dislocation may be created, allowing greater spatial separation in the remaining directions for the same volume of supercell. A repeated supercell constructed from 12×8×1 rhombohedral cells is shown in Fig. 1. The electronic bandstructure for bulk germanium without defects has been calculated using CASTEP, applying a norm-conserving pseudopotential and PW91 exchange-correlation functional. This has been repeated using 6×4×1 and 12×8×1 rhombohedral cells containing a single extended misfit dislocation. Comparison of these electronic structures allows identification of electronic states due to extended misfit dislocations in germanium.

DISCUSSION

For a supercell constructed of multiple primitive cells, the effective Brillouin zone represents only a portion of that of the primitive cell, and band folding takes place. A calculated bandstructure for bulk germanium using a 6×4×1 rhombohedral cell, demonstrating the reduced-scheme representation of a single band, is shown in Fig. 2. The electronic bandstructure for a 6×4×1 supercell containing a misfit dislocation is shown in Fig. 3. A number of additional energy states are observed in the bandgap for the material containing defects relative to the electronic structure for bulk material. This calculation may be repeated for various sizes of supercell and for the Ge/Si heterointeface.

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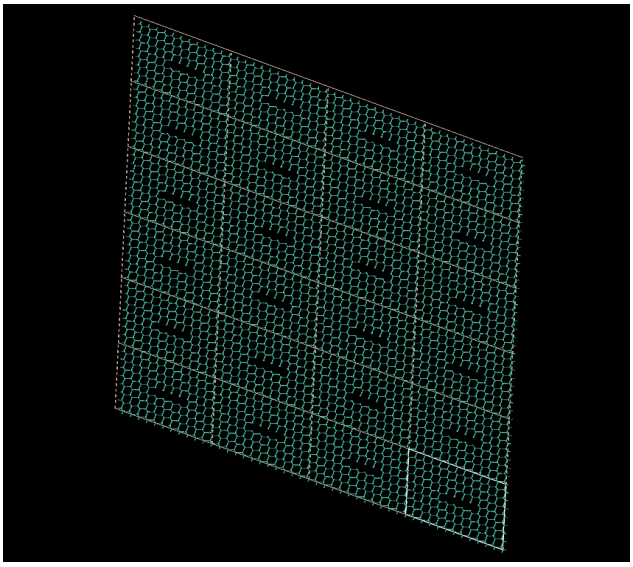

Fig. 1. Repetition of a 12 rhombohedral supercell of germanium containing a misfit dislocation.

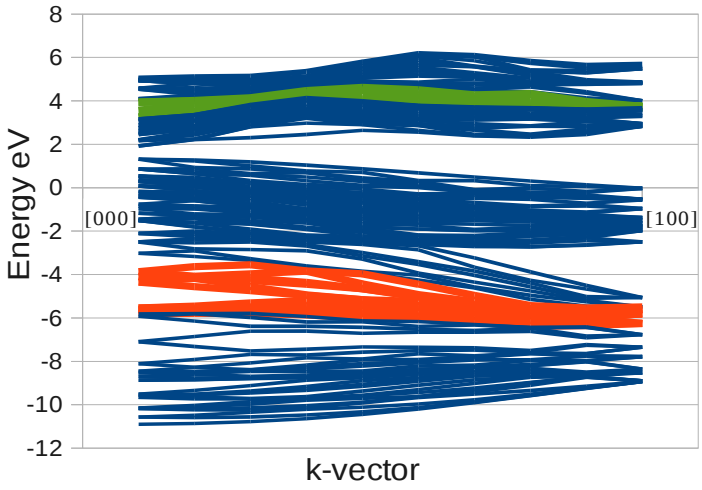

Fig. 2. Reduced-scheme bandstructure for a supercell of bulk germanium, with one folded valence band and one folded conduction band indicated.

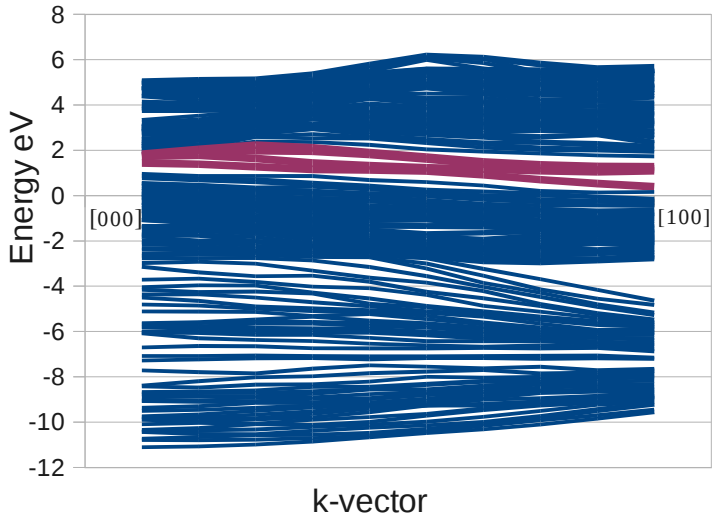

Fig. 3. Electronic bandstructure for a 6×4×1 supercell containing an extended misfit dislocation. The additional states due to the dislocation are highlighted.