DFT Calculation and Spectral Analysis of Electronic Structure of Dislocations in Germanium

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INTRODUCTION

Germanium has an absorption edge at a wavelength of 1.55 μm and can be grown epitaxially on silicon, and hence is a promising material for the development of advanced photonic devices such as photo detectors, optical interconnects and infrared lasers. There is a 4.2% lattice mismatch between Si and Ge and the interfacial layer will be strained below a certain critical thickness, and will contain defects or dislocations above this growth limit. Defects near the Si/Ge interface lead to 'trap states' – additional states in the band gap – with effects on carrier transport, generation/recombination statistics and optical absorption. Accurate calculation of the electronic structure of such states is an important component in accurate device modelling and performance.

Ab initio simulation methods such as DFT may be used to calculate the electronic structure of Ge supercells containing defects. However, the use of supercells for simulation requires additional analysis to interpret the bandstructure and identify the energy and character of bound states in the bandgap.

MODEL

Defects in germanium may be misfit dislocations a – a mismatched plane creating a line of dangling bonds – or threading dislocations which glide along the [111] direction of the cubic cell and terminate misfit dislocations (Figure 1) [1]. DFT implemented in the CASTEP [2] software was used to calculate the bandstructure for Ge supercell containing a pair of misfit dislocations. Simulation parameters were validated by calculating a bandstructure for bulk Ge using the rhombohedral primitive unit cell, producing excellent agreement with band edges at the Γ, X and L points, outlined in Table 1.

Bandgap	**Experimental (eV)**	**Simulated (eV)**
E_L	0.66	0.628
E_X	1.2	0.972
E_Γ	0.8	0.808

Table 1: Simulated and Experimental Bandgaps for Ge

Simulation supercells were formed by repeating units of the rhombohedral unit cell of germanium, with some atoms removed to create two evenly-spaced misfit dislocations per cell. The natural propagation direction of misfit dislocations is preserved by the chosen supercell shape, allowing them to be only one unit cell deep hence enabling a larger separation of dislocations for a fixed supercell volume (i.e. number of atoms) so that neighbouring dislocations do not interact strongly. Figure 2 shows a repeated 6x4x1 supercell of Ge containing misfit dislocations.

The Brillouin Zone of a supercell is contracted with respect to the primitive cell; this produces folded bandstructures (Figure 3). It is possible to identify a number of states in the bandgap visually, however further spectral analysis of these states is required.

ANALYSIS AND RESULTS

Spectral analysis of folded states calculates the contribution of primitive cell states to a supercell state [3]. A wave vector of the primitive cell, *k*, will fold into a wavevector *K* in the supercell if there is a supercell reciprocal lattice vector G_0 such that:

$$\vec{K} = \vec{k} - \vec{G}_0$$

However, there is no unfolding of a given supercell wavevector into a single primitive cell wavevector:

$$\vec{k}_i = \vec{K} + \vec{G}_i \qquad i=1, 2 \ldots\ldots\ldots n$$

Instead, the proportion of 'Bloch character' of a primitive cell state retained within a supercell state, P_{Km}, may be calculated by projecting a supercell state with wavevector K_m onto all the Bloch states k_in of the primitive cell:

$$P_{\vec{K}m}(\vec{k}_i) = \sum_n |\langle \vec{K}m | \vec{k}_i n \rangle|^2$$

This provides a spectral decomposition of each state identified at a given point in the folded supercell bandstructure (in this case at Γ) and allows accurate identification of the origin and energy of bandgap bound states in the defected cell (Figure 4).

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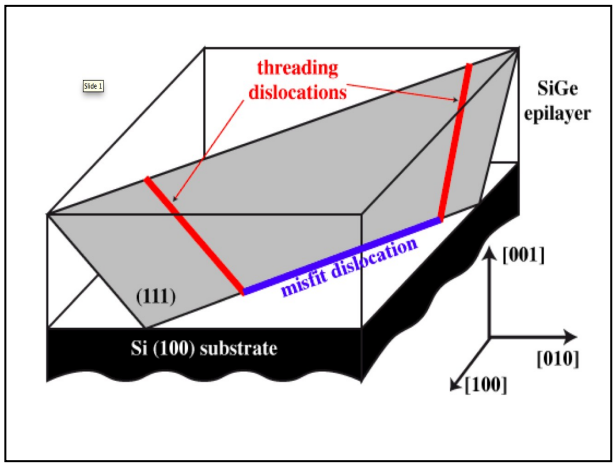

Fig. **1**. Misfit dislocation and threading dislocations in the Si/Ge interface.

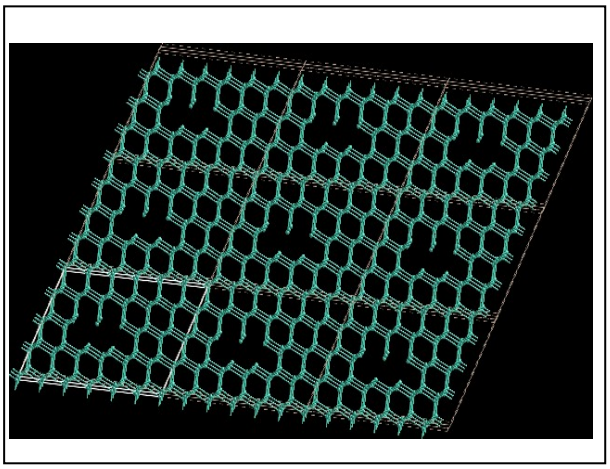

Fig. 2. Repeated 6x4x1 Ge supercell with misfit dislocations.

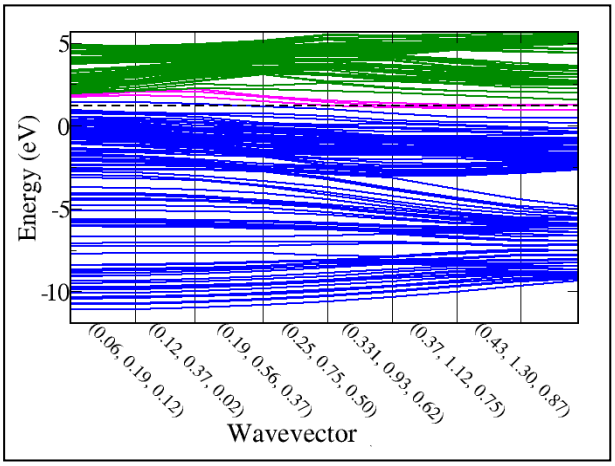

Fig. 3. Folded bandstructure for 6x4x1 defected supercell of Ge, demonstrating additional bandgap states.

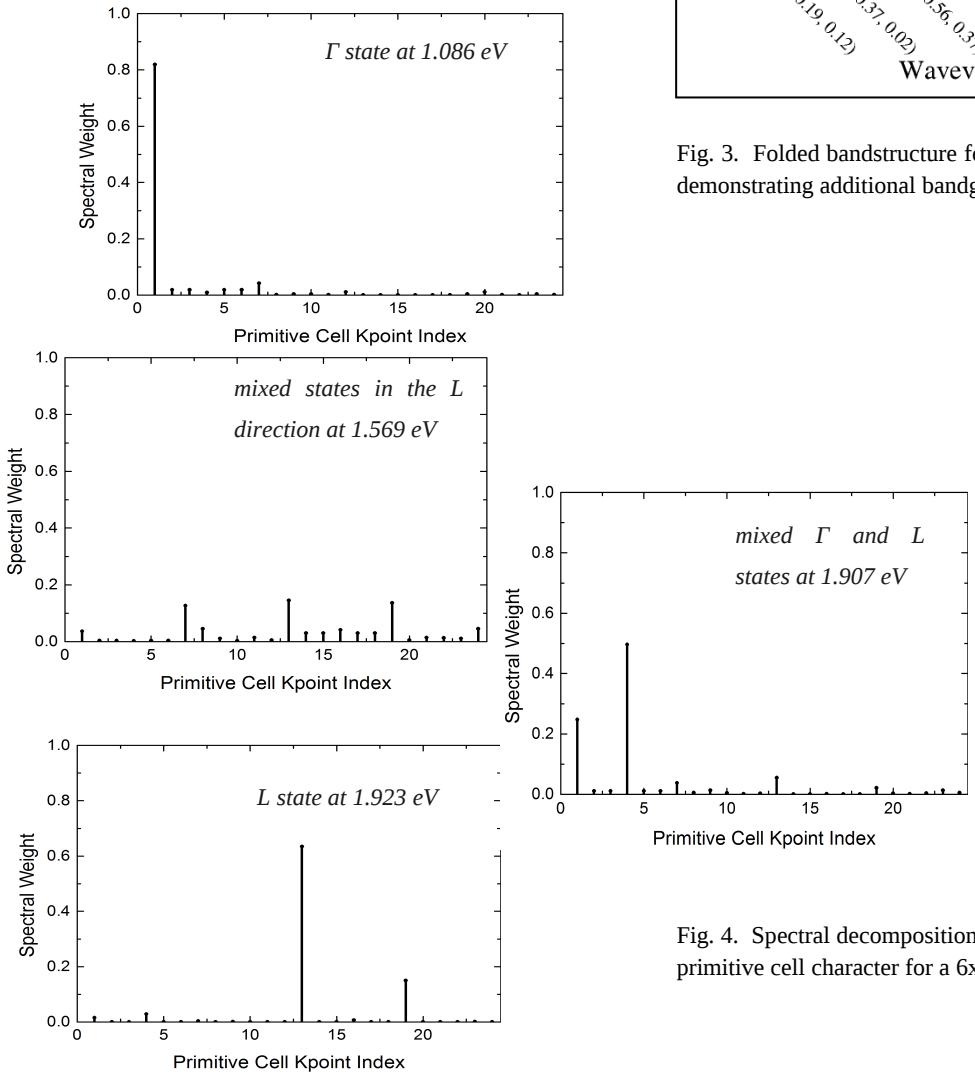

Fig. 4. Spectral decomposition of supercell Γ bandgap states into primitive cell character for a 6x4x1 supercell of defected Ge.