Tight-Binding Modeling of Intermediate Valence Compound SmSe for Piezoelectronic Devices

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INTRODUCTION

Scaling of MOSFET physical dimensions has enabled exponential growth of the total transistor number in a single chip. Today heat dissipation issues prevent any performance increases through clock frequency increases, since the supply voltage cannot be lowered. These fundamental power consumption issues have spurred the exploration of alternative switching mechanisms[1].

The Piezoelectronic Transistor (PET) has been proposed as a post-CMOS device for fast, low power switching[2, 3]. In this device the piezoresistive channel is filled with carriers through pressure induced via the expansion of a piezoelectric element. The mixed-valence compound SmSe is a good choice of PET channel material because of its pressure-induced Metal Insulator Transition (MIT). Performance prediction and optimization of a realistic, nano-scaled PET based on SmSe requires the understanding of quantum confinement, tunneling, and metal interface effects. To achieve this, a computationally efficient empirical tight binding (ETB) model is necessary. In this work, TB parameters are developed for SmSe and used in quantum transport simulations to explore the atomistic nature of material properties and the scaling limit of PET channel lengths.

METHODS

Our parameterization of ETB features a basis transformation from DFT e.g. plane wave representation to an orthogonal TB basis i.e. Löwdin orbitals[4] and subsequent refinement by numerical optimization. First principle calculations within generalized gradient approximation with spin-orbit coupling and Hubbard-like, localized potential (GGA+SO+U) are performed with ELK [5]. Wavefunctions and bandstructure at the minimum-energy lattice constant are obtained. The DFT Hamiltonian is then constructed and transformed to the TB Hamiltonian[6]. Values of onsite energy and two center integrals for the TB basis are extracted following Slater and Koster notations[4]. Parameters are then refined with the simplex algorithm. Effects of strain are accounted for by additional parameters representing bond bending and stretching[7]. DFT bandstructures under hydrostatic strain are used as fitting targets. NEGF is employed to study the ballistic transport in SmSe with NEMO5 [8]. Currents are evaluated for different strains in a 6nm SmSe channel.

DISCUSSION

The TB model is determined based on the analysis of a decomposition of DFT DOS into atom species and orbitals (Fig.1a-c). The TB model with second nearest neighbor coupling is implemented with *spdfs** orbitals. Spin-orbit (SO) coupling for *p,d and f* orbitals are included for both atoms. The *4f* band splitting, which is included in DFT as Hubbard-type *U* has been considered in our model through *4f* SO coupling. In the energy range relevant to transport, the band dispersion is accurately reproduced as shown in Fig.1d. Detailed analysis shows that conduction band minimum energy and dispersion at the band minimum are mainly affected by second nearest neighbor Sm-Sm coupling of *d*-orbitals.

The MIT in SmSe is believed to originate from the bandgap reduction under pressure. Fig.2a shows the extracted indirect bandgap for SmSe under hydrostatic strain and uniaxial strain along

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the (100) direction. Although the TB parameters are fitted to bandstructure under hydrostatic strain, the good match obtained for uniaxial strain without modification of the parameters confirms good transferability of the TB parameters.

Figure 3a demonstrates the simulation domain in form of a thin film. The equilibrium Fermi level position is determined self-consistently (Fig.3a) and a 0.05V bias is applied in the drain contact. A ballistic current calculation shows that modulation of the resistance by 3 orders of magnitude is achieved by hydrostatic strain of 3% (Fig.3d). In the Hubbard model the *f*-electrons are supposed to be highly localized[9]. However, both DFT and TB bandstructure show a small effective mass at the top of valence band at Γ (Fig.1d) which gives rise to hole currents and increases the conductance (Fig.3d). The band width of *f*-band is found to be controlled by the nearest neighbor *p-f* coupling between Se and Sm atoms.

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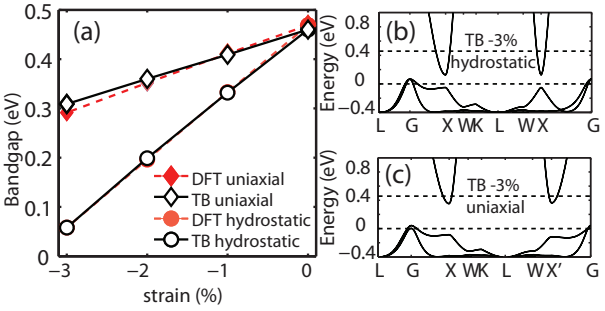

Fig. 2. Comparison of band gap modulations with strain calculated by DFT and TB. (a) Band gap extracted from DFT and TB band structure under hydrostatic and uniaxial strain. (b) TB band structure with 3% compressive hydrostatic strain in each direction. (c) TB band structure with 3% compressive uniaxial strain in growth direction. Dashed lines show bulk band edges in (b, c).

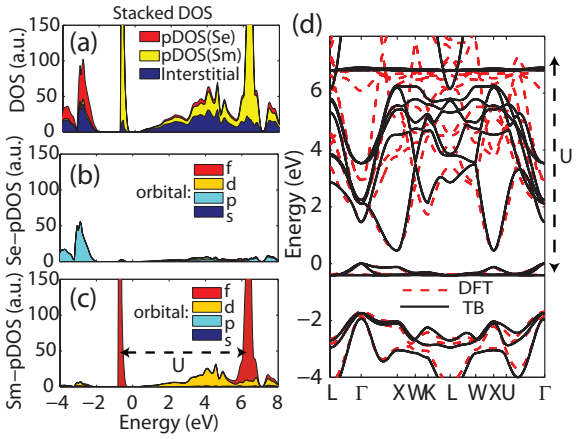

Fig. 1. Stacked DFT DOS and DFT/TB bandstructure comparison. (a) DOS within muffin-tin radius of Sm/Se and interstitial DOS. (b) DOS within Se atom decomposed by angular momentum. (c) DOS within Sm atom decomposed by angular momentum. (d) Band structure by *spdfs**+SO TB model without strain (black) and DFT band structure without strain (red). E=0 at top of valence

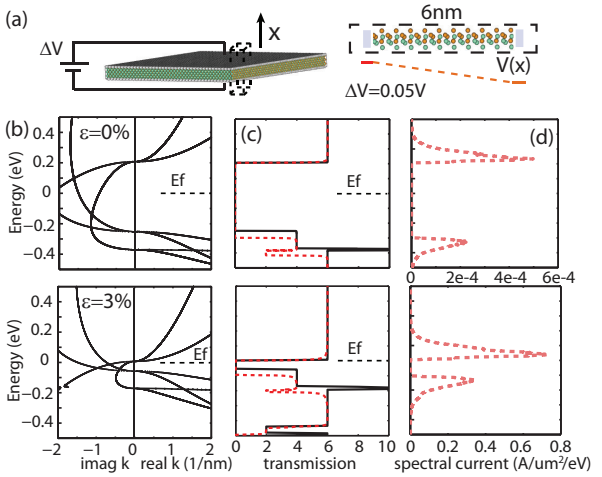

Fig. 3. Transport simulation for SmSe with hydrostatic strain. (a) Device configuration and supercell of simulation domain. (b) Real and imaginary band structure for 0% and 3% hydrostatic strain. (c) Transmission with 0V and 0.05V linear drop potential. (d) Vd=0.05V, spectral current with linear drop potential.