

Transferable tight binding model for strained group IV and III-V heterostructures

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Modern semiconductor devices have reached critical device dimensions in the range of several nanometers. Devices such as superlattice-FETs[1], Ultra Thin Body(UTB)-FETs and FinFETs consist of strained materials with different lattice constant. Quantitative analysis of those devices requires the reliable prediction of the bandgaps, effective masses in strained heterostructures. The Empirical Tight Binding (ETB) methods are appropriate for atomistic device modeling due to their numeric efficiency[2]. However, the accuracy of ETB calculations depends on the transferability of the ETB parameters. In this work, transferable ETB parameters of strained IV and III-V group semiconductors are generated from *ab-initio* calculations[3], [4]. The ETB parameters show good transferability when applied to strained bulk materials as well as ultra-thin superlattices.

ETB parameters are obtained through *ab-initio* mapping process[4]. During the parameterization process, ETB parameters and basis functions are adjusted to match the corresponding *ab-initio* band structures and wave functions. In this work, *ab-initio* bands of the strained bulk materials and superlattices are calculated using VASP. Hybrid functional HSE06 is used to produce correct band gaps. Group IV and III-V materials are parameterized using the sp³d⁵s* ETB model. The parameterized group IV and III-V materials include Si, Ge, Si_{0.5}Ge_{0.5} and compounds XY with X = Al, Ga and In, Y = P, As and Sb. To have transferable ETB parameters, following constraints are imposed. a) Onsites of each atom depend only on the atom type instead of materials. b) Both strained and unstrained ETB band structures are fitted to *ab-initio* results. c) Variation of interatomic coupling parameters among different materials is less than 0.3eV. The strain

effect is included using strain induced onsite and interatomic couplings which depend on the change of bond lengths of the first nearest neighbours and bond angles between the first nearest neighbours.

Band structures of Selected semiconductors (bulk Si, Ge, Si_{0.5}Ge_{0.5}, AlAs, GaAs and InAs) are shown in Fig. 1. The ETB band structures match the corresponding hybrid functional calculations results well. Compared with corresponding HSE06 results, band edge at high symmetry points are within 0.05eV and important effective masses have less than 10% error. Fig. 2 and 3 show InAs and Si conduction and valence band edge splitting under strains produced by stress along 001 and 111 directions. The splitting of conduction and valence band edges at high symmetry points such as Γ , L and X are correctly captured by the strain model. Fig. 4 and Fig. 5 show the band structure of GaAs/AlAs and Si/Ge superlattices respectively. The TB band structure agree with the HSE06 bands, demonstrating good transferability of ETB parameters for group IV and III-V semiconductors.

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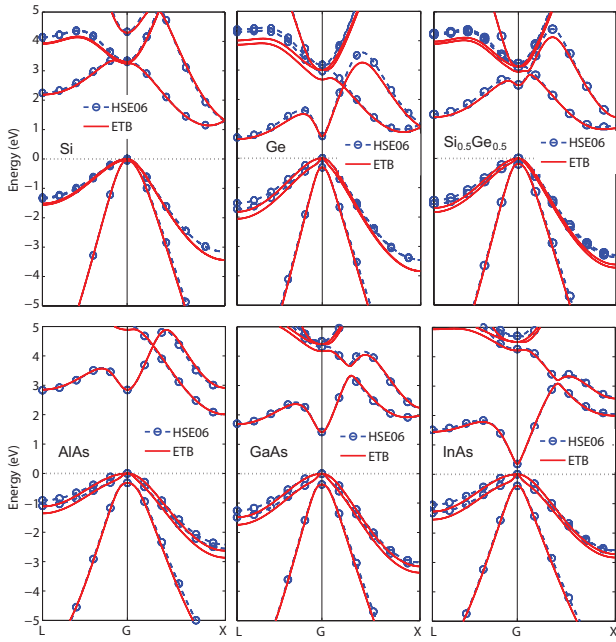


Fig. 1. Bulk band structure of Si, Ge, SiGe, AlAs, GaAs and InAs. ETB bands shows good agreement with the hybrid functional bands(HSE06).

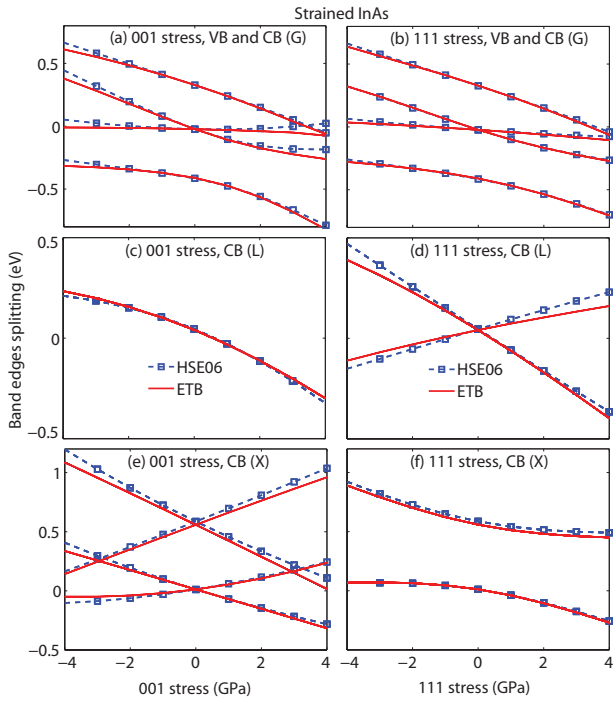


Fig. 2. Band edge at high symmetry points(Γ ,L,X) splitting of strained InAs under 001 and 111 stress. The 0 energy of (a) and (b) corresponds to the unstrained top valence bands; while the 0 energy of the (c),(d) and (e),(f) correspond to lowest unstrained conduction band at L and X points respectively. Compared with the HSE06 result, the ETB model capture the band edge splitting at high symmetry point under different strains.

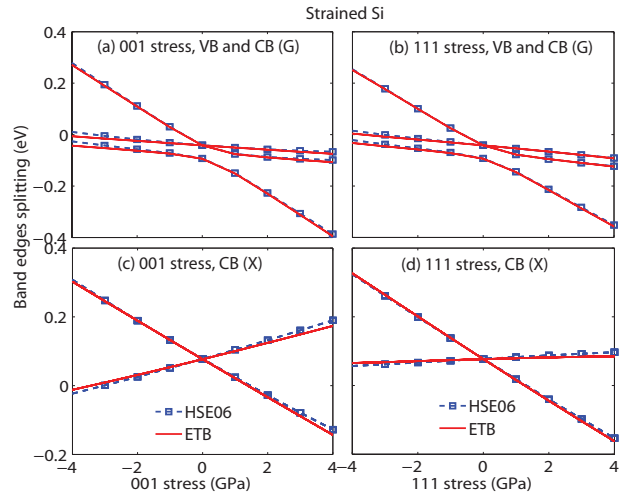


Fig. 3. Band edge at high symmetry points(Γ ,X) splitting of strained Si under 001 and 111 stress. The 0 energy of (a) and (b) corresponds to the unstrained top valence bands; while 0 of the (c),(d) correspond to lowest unstrained conduction band at X points.

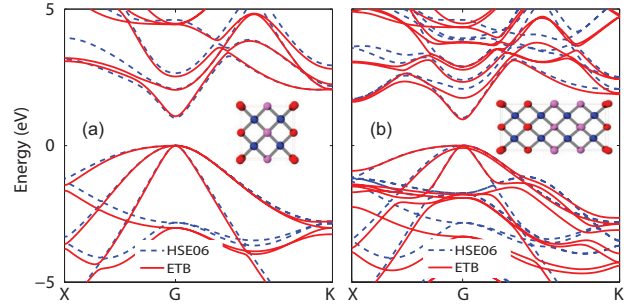


Fig. 4. Band structure of GaAs/InAs superlattices(HSE06 vs ETB). Band structure of GaAs/InAs superlattices with 4 atomic layers (a) and 8 atomic layers (b) in the primitive unit cell. The ETB parameters are transferable when applied to ultra thin superlattices.

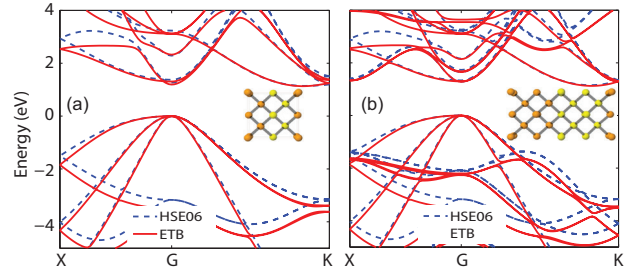


Fig. 5. Band structure of Ge/Si superlattices(HSE06 vs ETB). Band structure of Ge/Si superlattices with 4 atomic layers (a) and 8 atomic layers (b) in the primitive unit cell. The TB parameters are transferable when applied to ultra thin superlattices.