Mode space tight binding model for ultra-fast simulations of III-V nanowire MOSFETs and heterojunction TFETs

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As transistors are scaled into the nanoscale regime, III-V channel materials and gate-all-around (GAA) nanowire (NW) MOSFETs and TFETs can be used to achieve performance boost and low power operation [1,2]. Quantum effects play a crucial role in affecting device performance. Atomistic tight binding (TB) simulations within the NEGF framework has emerged as a powerful and versatile technique for full band transport studies that goes beyond the limitation of effective mass (EME) approximation [3,4]. Atomistic transport simulations in realistic nanostructures having a few tens of thousands of atoms typically translate into Hamiltonian matrices that have a rank of ~10^6 and require substantial computational resources.

Using an incomplete basis or low rank approximation, the mode space (MS) approach has been widely used to significantly speed up EME models while keeping accuracy in a reduced energy window [5-7]. A direct transcription of the MS technique to TB models usually fails. In a full band model, the device Hamiltonian is no longer a bounded operator. Thus, the basis transformed model is plagued with unphysical modes (UM) (Fig. 2), even if the chosen basis reproduces well the physical modes of interest (Fig. 1) [3].

A solution to this problem was proposed and its applicability to Si NWs demonstrated. The technique enlarges the MS basis by adding new basis vectors specially "tailored" to remove one by one the unphysical branches in the MS model [3].

In this work, we have implemented such a MS algorithm in Nemo5 [4] and explored its suitability to various III-V homo- and hetero- junction NW devices. We found that in III-V materials, the number of unphysical modes to eliminate is very high (typically above 100) compared to the Si case reported in [3] which has only a few UM. Nevertheless, we demonstrate here the possibility to clean III-V MS basis from the UM and achieve a significant speed up ratio (Fig. 3 and 4).

The first step that consists in creating an initial MS basis by sampling the NW slab eigenmodes at selected *E-k* points is the crucial step upon which relies the successful derivation of an optimized basis. A successful initial sampling is illustrated in Fig.1 for a [100] InAs NW in a sp^3s^* basis including Spin Orbit coupling (SO) and the number of UM after 5 and 75 optimization steps is shown in Fig. 2 and 3, respectively. As shown in Fig. 1, the key point is to start with sampling a small number of eigenmodes within a reduced energy window and optimize this basis first. It is usually not possible to optimize a larger basis directly. If needed a larger energy range can then be achieved by performing a second initial sampling (e.g. adding new basis vectors at higher energy) to the first optimized basis (i.e. the optimized basis of Fig. 3) and perform a second optimization.

Using the procedure illustrated in Fig. 1 to 3, MS basis for [100] InAs and GaSb NWs with a square cross-section of size d = 5.45 nm were derived from an initial sp^3s^* SO TB basis and slab Hamiltonian sizes in the MS were 5% and 6%, respectively, from their original size. The MS basis sets were used to simulate an InAs MOSFET and an InAs-GaSb heterojunction TFET. *I-V* curves obtained from the MS models match well those obtained in the full model (Fig. 4). Using the MS models, speed up factors larger than 150 were achieved, when compared to the initial TB models,

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for both the MOSFET and TFET cases, using a cluster having 96 cores.

In conclusion, the achievement of significant speed up factors demonstrates the potential of MS tight binding models and offers unprecedented possibilities for the full band simulation of nanostructures.

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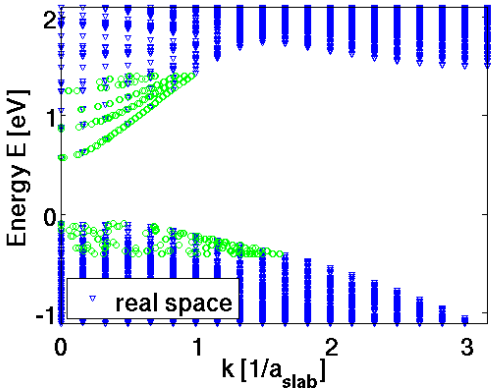

Fig. **1**. Band structure (*E-k* dispersion in the first half of the Brillouin Zone) of a [100] InAs NW slab (d = 5.45 nm) computed from the original (Real Space) TB model in a sp^3s^* basis including SO coupling (▼). The *E-k* points used to construct the initial MS basis (from the related eigenvectors) are indicated by green circles.

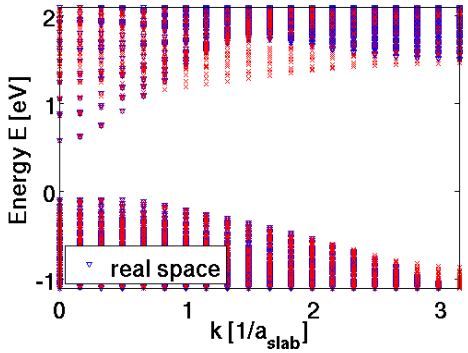

Fig. 3. Band structure of the MS model (×) of Fig. 1 after 75 optimization steps. The original band structure (▼) obtained using RS basis is also shown for comparison. The lowest part of the conduction band and higher part of the valence band are free of the UM and correctly reproduce the band structure obtained using RS basis. The MS model is suitable for transport in a reduced energy window. The MS basis size is only a few % of the original NW slab TB model.

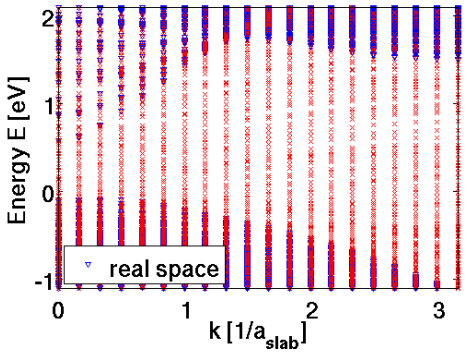

Fig. 2. Band structure obtained using MS basis (×) for the same structure as in Fig. 1 after 5 optimization steps, i.e. adding 5 new basis vectors to remove 5 unphysical modes. The original band structure (▼) obtained using Real Space (RS) basis is also shown. Many UM are still present in the MS model, which is not suitable for transport studies.

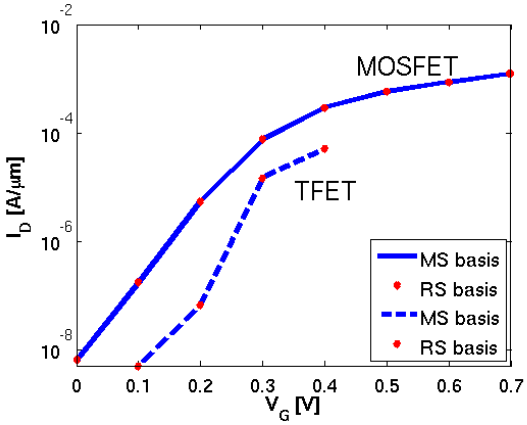

Fig. 4. $I_D(V_G)$ characteristics of a [100] d = 5.45nm 15 nm long InAs NW MOSFET and InAs-GaSb TFET computed from the original (RS) TB model in a sp^3s^* basis including SO coupling and from the reduced InAs MS basis of Fig. 3. For the TFET case a GaSb MS basis was also derived. Using the MS models, good matching of the *I-V* characteristics together with large speed up factors were achieved when compared to the original model.