Equivalent Model for Tunneling Simulation of Direct-Gap Semiconductor Nanowires

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It is important to develop a method to reduce the order of Hamiltonian describing the electronic state of a device to improve the speed of quantum transport simulation [1]. We have developed a method that uses adaptive moment estimation with automatic differentiation to construct a small equivalent Hamiltonian which reproduces the real band structure within a transport energy window of a target system [2]. In this study, we extend the method and construct an equivalent model that reproduces not only the real band structure but also the complex band structure of a direct-gap semiconductor nanowire for quantum transport simulation of tunneling transistors. The performance of the equivalent model was evaluated by calculating the band-to-band tunneling probability of direct-gap semiconductor nanowires.

We have considered a III-V semiconductor nanowire whose schematic diagram is given in Fig. 1(a). In the equivalent model, the system is represented by a pseudo-one-dimensional chain, as schematically shown in Fig. 1(b) [2]. The parameter matrices D and S of the equivalent model were determined using the adaptive moment estimation with automatic differentiation [3] to reproduce the real and complex band structure of the target system (see Fig. 2). Figure 3(a) shows the band structure of a GaAs nanowire with a square cross section of 1.41 nm per side, calculated with the $sp^3d^5s^*$ tight-binding approximation model (TBM) whose Hamiltonian size is 600×600. The band structure of the equivalent model (EM), which was constructed to reproduce the TBM band structure, is shown in Fig. 3(b). The size of EM is 48×48. We see that EM correctly reproduces the real band structure (right panel, E-k diagram) and complex band structure (left panel, E-κ diagram, the values of k are also plotted in color) within the transport window.

We have calculated the band-to-band tunneling probability with the non-equilibrium Green's function method. We have applied Eckart-type potential shown in the inset of Fig. 4(b). Figure 4(a) shows the energy dependence of transmission function $T(E)$, and 4(b) the tunnel distance dependence of the tunnel probability. The results of an InAs nanowire are also plotted in the figures. In both cases, we see that EM correctly reproduces the TBM results.

[1] G. Mil'nikov, N. Mori, and Y. Kamakura, Physical Review B **85**, 035317 (2012). [2] J. Okada, F. Hashimoto, and N. Mori, Japanese Journal of Applied Physics, **60** SBBH08 (2021). [3] TensorFlow, https://github.com/tensorflow/tensorflow

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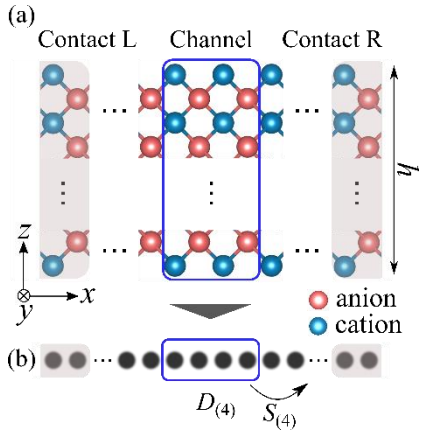

Fig. 1: Schematic diagram of a ⟨100⟩ wurtzite semiconductor nanowire. (a) Tight-binding approximation model (TBM) and (b) equivalent model (EM) representation.

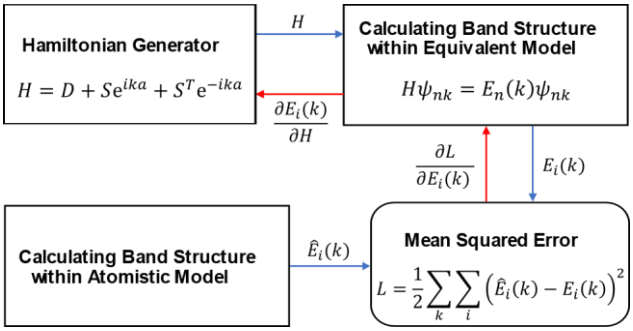

Fig. 2: Processes to reproduce the target band structure through minimization of the loss function L. Red arrows represent the automatic differentiation.

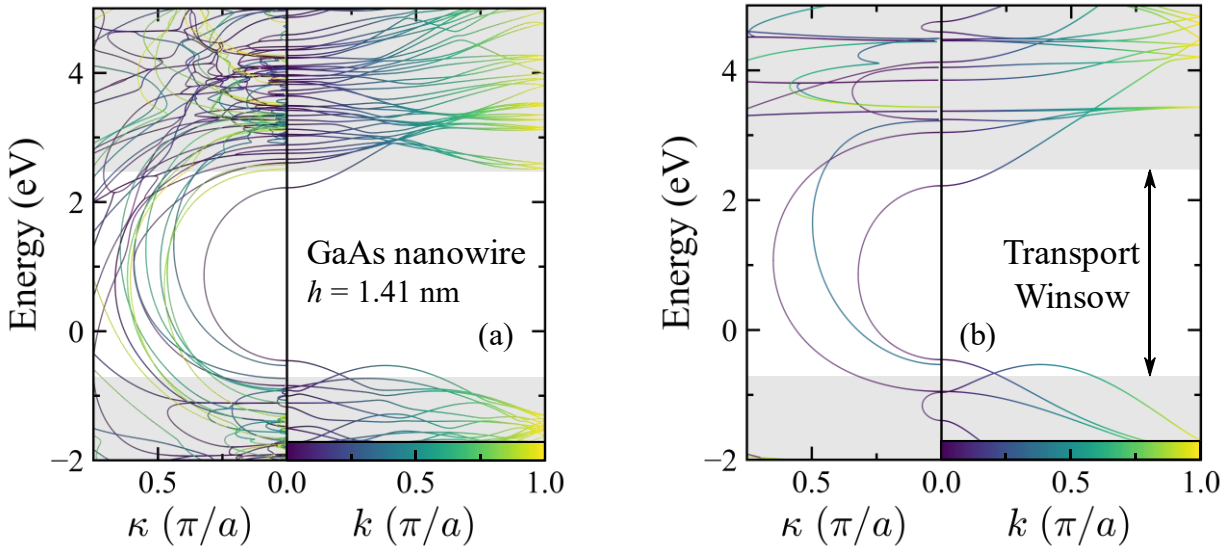

Fig. 3: (a) Band structure of a 1.41 nm × 1.41 nm GaAs nanowire calculated with TBM whose Hamiltonian size is 600 × 600. (b) Band structure calculated with EM whose Hamiltonian size is 48 × 48.

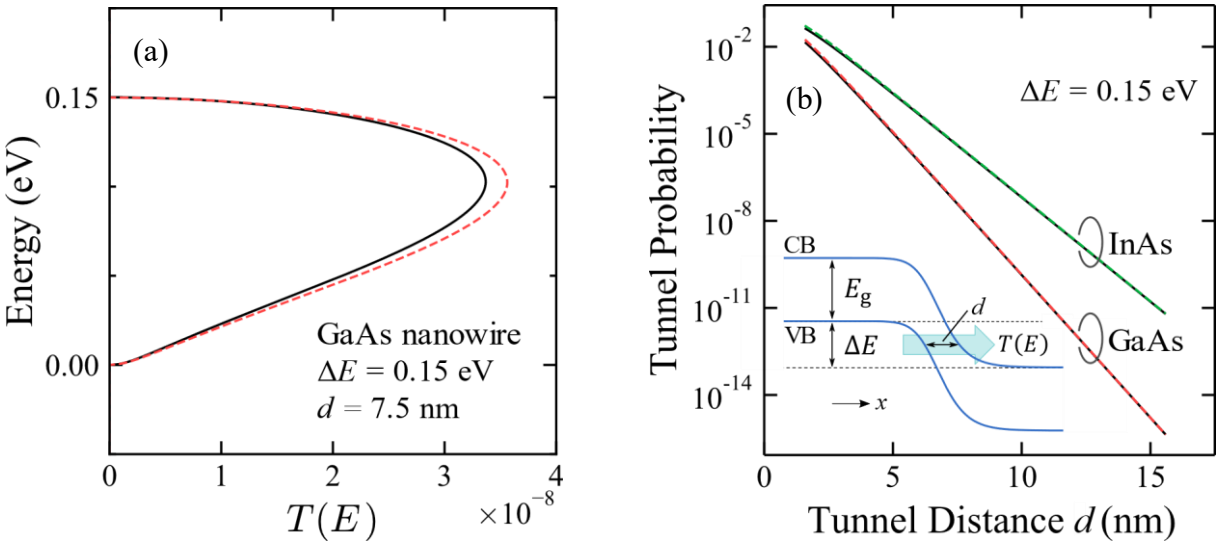

Fig. 4: (a) The energy dependence of transmission function calculated with TBM (solid line) and with EM (dashed line). (b) The tunnel distance dependence of tunnel probability calculated with TBM (solid line) and with EM (dashed line). Inset shows the potential profile.

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