A Study of Alloyed Nanowires from Two Perspectives: Approximate Dispersion and Transmission

Gerhard Klimeck, Timothy B. Boykin, Mathieu Luisier, Neerav Kharche, and Andreas Schenk

Citation: AIP Conf. Proc. **893**, 711 (2007); doi: 10.1063/1.2730088
View online: http://dx.doi.org/10.1063/1.2730088
View Table of Contents: http://proceedings.aip.org/dbt/dbt.jsp?KEY=APCPCS&Volume=893&Issue=1
Published by the American Institute of Physics.

A Study of Alloyed Nanowires from Two Perspectives: Approximate Dispersion and Transmission

Gerhard Klimeck[1,2], Timothy B. Boykin[3], Mathieu Luisier[4], Neerav Kharche[1], Andreas Schenk[4]

[1] *Network for Computational Nanotechnology, Purdue University, West Lafayette, IN 47906, USA*
[2] *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109, USA*
[3] *Department of Electrical and Computer Engineering, University of Alabama, Huntsville, AL 35899, USA*
[4] *Integrated Systems Laboratory, ETH Zürich, 8092 Zürich, Switzerland*

Abstract. Local atomic arrangement in heterostructures or disorder due to alloying, surface roughness and impurities strongly influence the bandstructure and charge transport. With decreasing diameters down to nanometer scales, disorder can no longer be treated in an average manner using the virtual crystal approximation (VCA) and the need for atomistic simulations arises. This work looks at the nanoscale devices from two different perspectives. The materials science perspective in which average bandstructure of the whole nanowire is computed using the nanoelectronic modeling tool (NEMO-3D) and the zone-unfolding algorithm. The device physics perspective, where the transmission coefficient is calculated with an atomistic non-equilibrium Green's function (NEGF) approach. Both approaches use 20 band $sp^3d^5s^*$ empirical tight-binding model with spin orbit coupling. The connection between dispersions and transmission coefficients of AlGaAs random alloy nanowires is highlighted. Both, transmission coefficients and average bandstructures show reduced bandgaps and noisy behavior. Their complimentary and mutually supporting nature provides a significant insight into the physics of charge transport through disordered systems.

Keywords: nanowire, tight binding, transmission, transport, NEGF, disorder, alloy
PACS: 71.20.-b, 71.23.-k, 73.21.Cd

INTRODUCTION AND APPROACH

Theoretical approaches to study transport through semiconductor nanostructures can be classified into two broad classes: bandstructure and transport. Most often effective-mass or **k.p** models are used [1], however, more complete, multi-band calculations based on methods such as pseudopotentials[2] tight-binding[3], or the bond-orbital model[4] have appeared recently. Disorder is known to influence electronic structure at the nano-scale[5]. To study the effects of alloy-disorder in nanowires we perform atomistic random-alloy calculations of approximate bandstructures as well as the transport characteristics of $Al_{0.15}Ga_{0.85}As$ nanowires.

In this work, we calculate approximate bandstructure in freestanding [100] directed $Al_{0.15}Ga_{0.85}As$ nanowires and compare them to transmission coefficient calculations. All calculations have been done in 20-band $sp^3d^5s^*$ tight-binding model with spin-orbit coupling [6]. The nanowire geometry is specified in terms of zincblende conventional unit cubes (lattice parameter a_0=0.565 nm) $n_x \times n_y \times n_z$, where n_i is the number of cubes in i-direction. Eigenspectrum (eigenvalues and wavefunctions) of 40×6×6 $Al_{0.15}Ga_{0.85}As$ nanowire supercell is computed using NEMO_3D [5]. The supercell is periodic in the transport (x-direction) and the wire mantle surfaces are passivated [7]. Small cell bandstructure for a 1×6×6 cell is then projected out of the supercell eigenspectrum using our zone-unfolding method [8].

Transmission coefficients through the same nanowire are computed using a hybrid method combining a recursive NEGF method and a wavefunction calculation [9]. In these calculations the semi-infinite emitter (collector) region is identical to the first (last) slab of the nanowire.

RESULTS

Figure 1(a) shows bandstructures of an $Al_{0.15}Ga_{0.85}As$ random alloy nanowire calculated using conventional VCA method and unfolding 40×6×6 supercell eigenspectrum. The random alloy calculation

CP893, *Physics of Semiconductors, 28th International Conference*
edited by W. Jantsch and F. Schäffler

results in significantly lower conduction band minima than VCA calculation. Transmission coefficients through the same nanowire supercell are shown in figure 1(b). The VCA transmission shows an ideal step like behavior, however, the transmission coefficient from random alloy calculations shows a noisy behavior as a consequence of random placement of Al atoms in AlGaAs nanowire. Features in transmission are related to the approximate bandstructure and vice versa. Each band corresponds to two transmission channels for up and down spins. The lowest approximate band at $k=0$ produces a transmission turn on near 1.92 eV. More channels turn on at about 1.97 eV due to approximate bands near π/a_0.

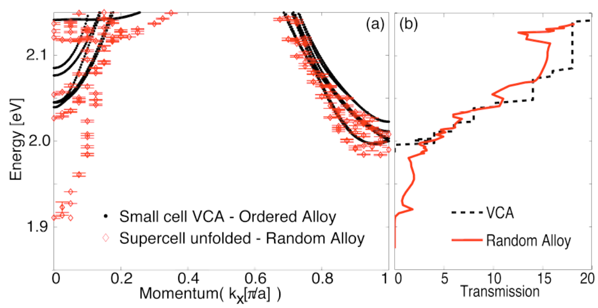

FIGURE 1. (a) Conduction bands of the 40×6×6 $Al_{0.15}Ga_{0.85}As$ nanowire as calculated with the VCA (small solid symbols) and as projected out of random-alloy supercell eigenstates (large, open symbols with error bars). Note in particular that the randomalloy calculation gives a significantly lower minimum at k = 0. (b) Transmission characteristics. Dotted line: VCA nanowire; this nanowire is effectively a pure nanowire made of a pseudo-material, and shows step-like transmission. Solid line: random-alloy supercell wire.

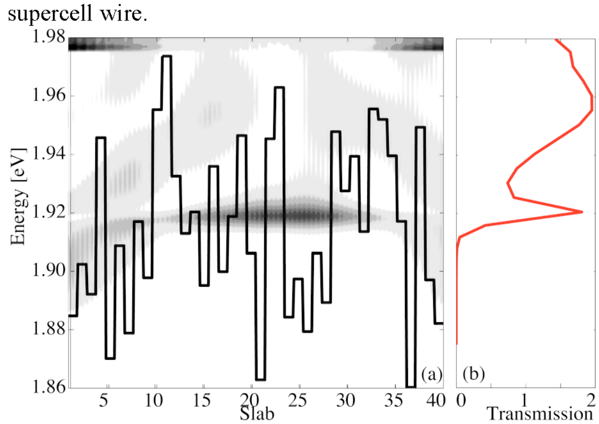

FIGURE 2. (a) Logarithm of the DOS (shaded region) neglecting spin, for the random-alloy nanowire superimposed over the wire conduction-band edge profile (thick line). (b) Transmission coefficient. The injected state is spin-up. The concentration of the DOS corresponds to the resonance peak in the transmission coefficient.

Figure 2(a) shows the local conduction band minima for each slab (1×6×6 cell) and a density of states of the same 40×6×6 AlGaAs nanowire. The transmission spike at about 1.92 eV in figure 2(b) corresponds to a localised density of states seen in figure 2(a).

In summary, we have found that approximate bandstructures from random alloy supercell calculations and atomistic NEGF transport calculations are complimentary and mutually supporting. Both methods provide better insight into the disordered nanowire device physics.

ACKNOWLEDGMENTS

The work at Purdue was supported by the National Science Foundation, Grant No. EEC-0228390 and ONR. nanoHUB.org computational resources were used in this work. The work at UAH was supported by Jet Propulsion Laboratory, California Institute of Technology and ONR.

REFERENCES

1. L. C. Lew Yan Voon, B. Lassen, R. Melnik, and S. Willatzen, J. Appl. Phys. vol. 96, no. 8, pp. 4660, 2004; L. C. Lew Yan Voon, and S. Willatzen, J. Appl. Phys., vol. 93, no. 12, pp. 9997, 2003; S. Jaziri and R. Ferreira, J. Appl. Phys., vol. 84, no. 2, pp. 893-900, 1998; M. Tsetseri and G. P. Tribera, Phys. Rev. B vol. 69, no. 7, art. 075313, 2004; H. T. Johnson, L. B. Freund, C. D. Akyüz, and A. Zaslavsky, J. Appl. Phys., vol. 84, no. 7, pp. 3714, 1998.
2. A. Francheschetti and A. Zunger, Phys. Rev. B, vol. 52, no. 20, pp. 14 664-14 670, 1995.
3. S. Pescetelli, A. Di Carlo, and P. Lugli, Phys. Rev. B, vol. 56, no. 4, pp. R1668-R1671, 1997; A. Di Carlo, S. Pescetelli, A. Kavokin, M. Vladimirva, and P. Lugli, Phys. Rev. B, vol. 57, no. 16, pp. 9770- 9779, 1998; M. P. Persson and H. Q. Xu, Phys. Rev. B, vol. 70, no. 16, art. 161310(R), 2004; Y.-J. Ko, M. Shin, S. Lee, and K. W. Park, J. Appl. Phys., vol. 89, no. 1, pp. 374, 2001.
4. L.-X. Li and Y.-C. Chang, J. Appl. Phys., vol. 84, no.11, pp.6162, 1998; L.-X. Li, S. Sun, and Y.-C. Chang, J. Appl. Phys., vol 89, no. 4, pp. 2251-2260, 2001.
5. G. Klimeck, F. Oyafuso, T. B. Boykin, R. C. Bowen, and P. von Allmen, *Computer Modeling in Engineering and Science*, **3**, 601-642 (2002).
6. Jean-Marc Jancu, Reinhold Scholz, Fabio Beltram, and Franco Bassani, Phys. Rev. B vol. 57, pp. 6493, 1998.
7. S. Lee, F. Oyafuso, P. von Allmen, and G. Klimeck, Phys. Rev. B vol. 69, pp. art. 045316, 2004.
8. T.B. Boykin and G Klimeck, Phys. Rev. B vol. 70, no. 11, pp. art. 115215, 2005; T.B. Boykin, N. Kharche, G. Klimeck, and M. Korkusinski (subm. IEEE Nano).
9. M Luisier, et al., (accepted in Phys. Rev. B).