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Semiconductor Nanowire and Nanoribbon Thermoelectrics: A Comprehensive Computational Study

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Final Report

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14. ABSTRACT Through detailed microscopic simulation, this project advances our understanding of the transport of charge and heat in Si, SiGe, and graphene nanostructures, with the objective of furthering their applications in thermoelectric cooling and energy harvesting. Main findings include: (1) Room-temperature thermoelectric figure of merit, ZT, of ultrathin silicon nanowires varies slowly with thickness, having a soft maximum of about 0.4 at the nanowire thickness of 4 nm. The benefit of nanostructuring is much less dramatic than previously suggested; (2) We find a significantly enhanced thermoelectric power factor in gated Si nanomembranes, and explain that it occurs due to include quantum confinement, low scattering due to the absence of dopants, and, at low temperatures, a significant phonon-drag contribution; (3) In Si nanomembranes, in-plane thermal conductivity is minimal on {001}, due to the strong coupling of TA modes to {001} surfaces. Highest in-plane conductivity is achieved in [100]/(011) SOI, with benefits for passive cooling applications. (4) Thermal transport in suspended graphene nanoribbons is edge-dominated and highly anisotropic, but isotropic in realistic-sized supported nanoribbons owing to strong substrate scattering.					
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Abstract

This project advances our understanding of the transport of charge and heat in semiconductor nanostructures, with the objective of furthering their applications in thermoelectric cooling and energy harvesting. Specifically, this project focuses on the physics of electrons (carriers of charge) and phonons (quanta of lattice vibrations, main carriers of heat) in group IV semiconductor nanowires and nanoribbons. Thermoelectric applications require efficient transport of charge (high electrical conductivity) and inefficient transport of heat (low thermal conductivity). Group IV semiconductors are ubiquitous in electronic industry and have excellent electrical and thermal conductivities, which generally makes them poor candidates as thermoelectrics. However, by introducing nanostructured barriers to the motion of phonons, thermal conductivity can be (beneficially) degraded with seemingly little penalty in electronic conductivity. Employment of group IV semiconductors in thermoelectric applications is an enticing idea, because of the maturity of their processing, wide availability, and low cost. However, the question still remains whether their thermoelectric performance can be improved to a degree significant enough to render them competitive with heavy-atom semiconductors like Bi_2Te_3 .

The central goal of this project was to develop theoretical understanding and computational tools that would enable detailed microscopic simulation of the dynamics of electrons and phonons in Si, SiGe, and graphene nanostructures, and answer how good their potential really is for thermoelectric applications. Main findings include: (1) Room-temperature thermoelectric figure of merit, ZT , of ultrathin silicon nanowires varies slowly with thickness, having a soft maximum of about 0.4 at the nanowire thickness of 4 nm. The benefit of nanostructuring is much less dramatic than previously suggested; (2) We find a significantly enhanced thermoelectric power factor in gated Si nanomembranes, and explain that it occurs due to include quantum confinement, low scattering due to the absence of dopants, and, at low temperatures, a significant phonon-drag contribution; (3) In Si nanomembranes, in-plane thermal conductivity is minimal on {001}, due to the strong coupling of TA modes to {001} surfaces. Highest in-plane conductivity is achieved along [100] on the low-symmetry (011) SOI, which benefits passive cooling applications. Thermal conductivity can be minimized in [100] wires with (001) and (010) surface facets; (4) Thermal transport in suspended graphene nanoribbons is edge-dominated and highly anisotropic, but much more isotropic in realistic-size supported nanoribbons owing to strong substrate scattering.

Final Report: Project Highlights

1) Thermoelectric properties of ultrathin silicon nanowires

E. B. Ramayya, L. N. Maurer, A. H. Davoody, and I. Knezevic, *Physical Review B* **86**, 115328 (2012).

We calculated the room-temperature thermoelectric properties of highly doped ultrathin silicon nanowires (SiNW) of square cross section (3×3 to 8×8 nm²) by solving the Boltzmann transport equations for electrons and phonons on an equal footing, using the ensemble Monte Carlo technique for each. We account for the two-dimensional confinement of both electrons and phonons and all the relevant scattering mechanisms, and present data for the dependence of electrical conductivity, the electronic and phononic thermal conductivities, the electronic and phonon-drag Seebeck coefficients, as well as the thermoelectric figure of merit (ZT) on the SiNW rms roughness and thickness. ZT in ultrascaled SiNWs does not increase as drastically with decreasing wire cross section as suggested by earlier studies. The reason is surface roughness, which (beneficially) degrades thermal conductivity, but also (adversely) degrades electrical conductivity and offsets the Seebeck coefficient enhancement that comes from confinement.

For a given carrier density and with increasing confinement, the energy separation between the conduction band edge and the Fermi level increases, resulting in an increase in the average energy carried by electrons; therefore, the electronic Seebeck coefficient increases as the wire cross section decreases. The phonon-drag component of the Seebeck coefficient is negligibly small in SiNWs because of a very short phonon mean-free path. Overall, the power factor does not show orders-of-magnitude increase with decreasing wire cross section, as predicted by earlier theoretical studies, because the decrease in electrical conductivity with decreasing thickness offsets the increase in the Seebeck coefficient. Also, as in bulk silicon, the electronic contribution to thermal conductivity is more than an order of magnitude smaller than the contribution from phonons. The ZT in SiNWs calculated from this thermoelectric simulation is 20–40 times larger than that in bulk silicon: the enhancement in ZT occurs primarily because of the decrease in the lattice thermal conductivity due to strong phonon-boundary scattering and not due to an enhancement in the power factor. Overall, room-

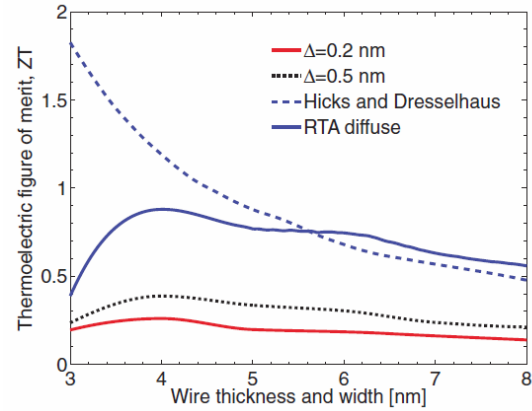


Fig. 1: Variation of ZT with the SiNW cross section. ZT incorporating thermal conductivity from phonon Monte Carlo with real-space roughness is presented for rms roughness = 0.2 nm (red solid curve) and = 0.5 nm (dotted black curve). ZT obtained from the RTA assuming completely diffuse boundary scattering for phonons (specularity parameter equal to zero; solid blue curve) overestimates ZT.

temperature ZT of ultrathin SiNWs varies slowly with thickness, having a soft maximum of about 0.4 at the nanowire thickness of 4 nm.

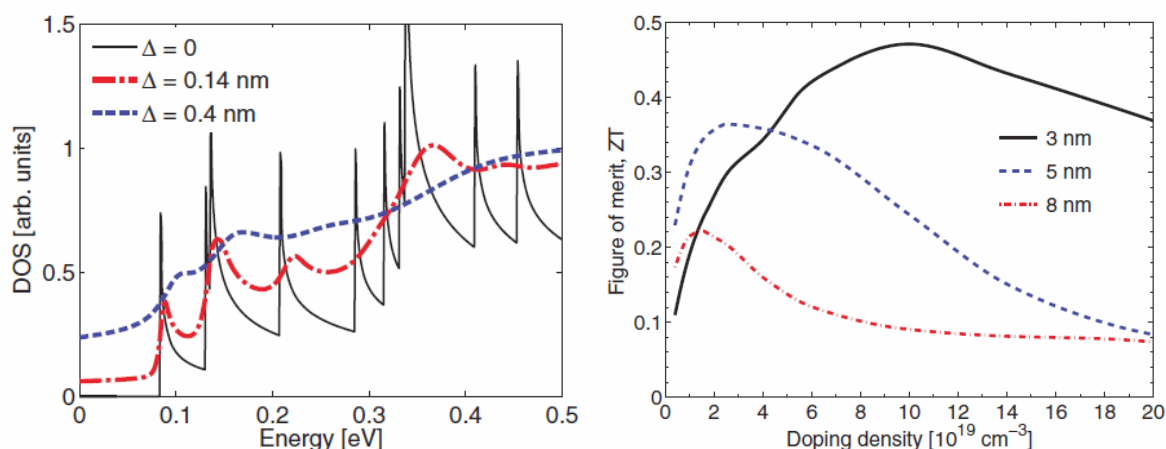


Fig. 2: (Left) Density of states (DOS) of a $5 \times 5 \text{ nm}^2$ SiNW (black solid curve) and the effective DOS in the presence of appreciable surface-roughness scattering, for $\Delta = 0.14 \text{ nm}$ (red dashed-dotted curve) and $\Delta = 0.4 \text{ nm}$ (blue dashed curve). Roughness smears the high peaks in the DOS, thereby negating potential benefits that quantum confinement could have on the Seebeck coefficient. (Right) Variation of ZT with the doping density for different SiNW thicknesses. $\Delta = 0.5 \text{ nm}$.

2) Quantitative determination of contributions to the thermoelectric power factor in Si nanostructures

H. J. Ryu, Z. Aksamija, D. M. Paskiewicz, S. A. Scott, M. G. Lagally, I. Knezevic, and M. A. Eriksson, *Physical Review Letters* **105**, 256601 (2010).

We report thermoelectric measurements on a silicon nanoribbon in which an integrated gate provides strong carrier confinement and enables tunability of the carrier density over a wide range. We find a significantly enhanced thermoelectric power factor that can be understood by considering its behavior as a function of carrier density. We identify the underlying mechanisms for the power factor in the nanoribbon, which include quantum confinement, low scattering due to the absence of dopants, and, at low temperatures, a significant phonon-drag contribution. The measurements set a target for what may be achievable in ultrathin nanowires.

We have presented measurements and calculations of the hole thermopower and power factor in gated silicon $[\bar{1}10]/(100)$ nanoribbons. With increasing sheet density, tuned by a back gate, the power factor of the nanoribbons is significantly enhanced, because of the combined effects of quantum confinement, a hole mobility that does not decrease with increasing carrier density, and (especially at low temperatures) phonon drag. We have used an essentially metallic gate to demonstrate such enhancements and to facilitate understanding and comparison to theory. In a practical system, recent advances such as surface transfer doping could be used to provide carriers, in place of either bulk doping or a metallic gate, and in analogy with the field effect of a gate.

Critically, such surface transfer doping will also produce a large electric field between the surface and the carriers in the interior of a nanowire, and thus the benefits of quantum confinement are expected to remain in such an approach.

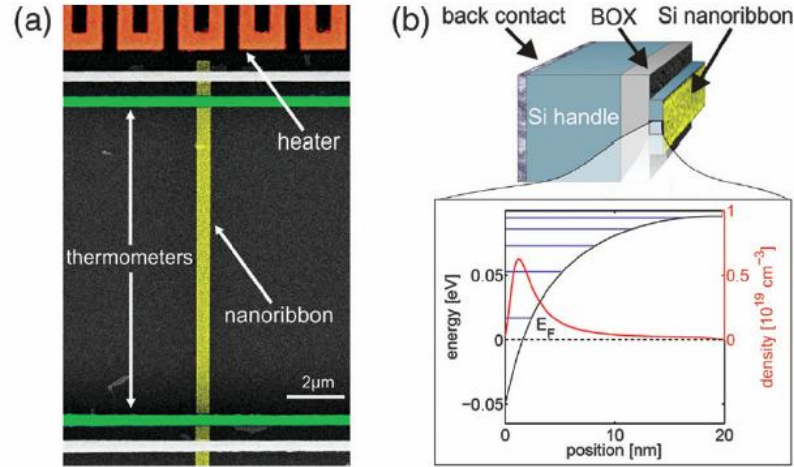


Fig. 3: Gated Si nanoribbon thermoelectric device. (a) Colorized scanning electron micrograph of a device with the same structure as the one measured here. The surface is (110), and the nanowire is oriented along the $[\bar{1}10]$ direction. (b) Perspective schematic diagram of the sample. Inset: The red curve shows the charge distribution in the nanoribbon when the sheet density $n_s = 10^{12} \text{ cm}^{-2}$. The horizontal lines are the subbands derived from the heavy-hole band; the subbands derived from the light-hole and split-off bands are omitted from the plot, for clarity. The Fermi level is at zero energy.

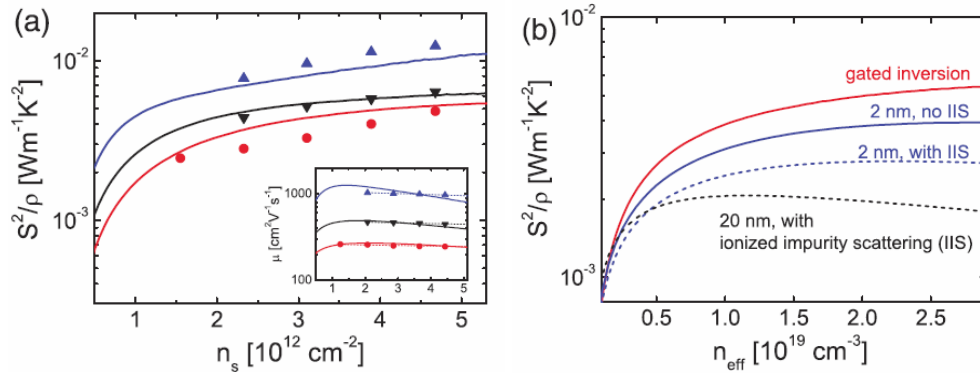


Fig. 4: Power factor S^2/ρ . (a) Solid symbols show the power factor at $T = 300$ (red), 200 (black), and 100 K (blue). Solid curves show the total calculated power factor, including both diffusion and phonon-drag components. Inset: mobility as a function of n_s ; solid lines: calculation; dashed lines: linear fit. (b) S^2/ρ as a function of the effective three-dimensional hole density n_{eff} at $T = 300$ K for four cases. Dashed black: doped nanoribbon of thickness 20 nm. Dashed blue: doped nanoribbon of thickness 2 nm. Solid blue: doped nanoribbon of thickness 2 nm with ionized impurity scattering (IIS) removed from the calculation. Solid red: gated nanoribbon corresponding to the experiment. For the cases with doping, $n_{\text{eff}} = N_A$; for the gated nanoribbon, $n_{\text{eff}} = n_s/w$, where w is the effective thickness of the inversion layers.

3) Anisotropy and boundary scattering in the lattice thermal conductivity of silicon nanomembranes

Z. Aksamija and I. Knezevic, *Physical Review B* 82, 045319 (2010).

We have calculated the full thermal conductivity tensor in (001), (011), and (111) silicon-on-insulator (SOI) nanomembranes based on solving the Boltzmann transport equation while accounting for the full phonon dispersion, momentum-dependent boundary scattering, as well as three-phonon and isotope scattering. In-plane thermal conductivity is minimal on {001} Si nanomembranes, due to the strong coupling of TA modes to {001} surfaces. Highest in-plane conductivity is achieved along [100] on the low-symmetry (011) SOI. Therefore, for applications requiring efficient passive cooling (i.e., high thermal conductivity), such as in digital electronic circuits, [100]/(011) should offer twice the thermal conductivity of Si(001) at room temperature even in relatively thick (10 nm) nanomembranes. The rougher the samples, the more pronounced the surface-orientation dependence of the in-plane thermal conductivity becomes. Overall, the strong interplay between the phonon dispersion anisotropy and boundary scattering enables one to have the surface facet orientation as an additional degree of control over thermal conduction in nanostructures. In rectangular or square wires, which can be fabricated by lithography and etching from Si nanomembranes, thermal conductivity is expected to be lowest for [100] wires with (001) and (010) surface facets. Intentional roughening, feature size reduction, and surface decoration of nanowires are likely to bring the most detriment to thermal conductivity if applied to these wires.

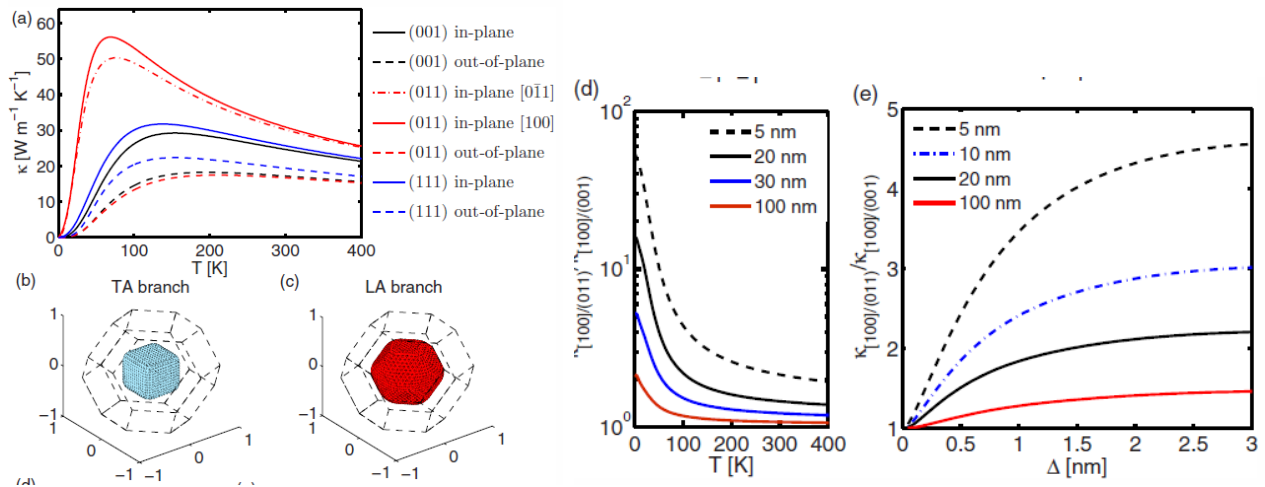


Fig. 5: Lattice thermal conduction in thin SOI membranes. (a) Eigenvalues of the thermal conductivity tensor for a 20-nm-thick SOI with rms surface roughness 0.45 nm. Maximal in-plane thermal conductivity eigenvalue is along [100] on (011) SOI and it is minimal on (001) SOI due to the very strong scattering of TA modes from (001) boundaries. (b) & (c) Energy isosurfaces for TA and LA modes, respectively. Dashed lines denote the Brillouin-zone edges. The TA constant-energy surfaces are boxlike with box faces perpendicular to $\langle 001 \rangle$ directions. The LA mode energy isosurfaces have faces perpendicular to $\langle 111 \rangle$ and $\langle 001 \rangle$ directions. (d) & (e) Ratio of the highest to the lowest in-plane thermal conductivity, $\kappa_{[100]/(011)} / \kappa_{[100]/(001)}$, for SOI with thicknesses in the 5–100 nm range, as a function of (d) temperature (surface-roughness rms height is 0.4 nm) and (e) rms roughness height (at room temperature).

4) Lattice thermal conductivity of graphene nanoribbons: anisotropy and edge roughness scattering, *Applied Physics Letters* **98**, 141919 (2011); **Thermal transport in graphene nanoribbons supported on SiO₂**, *Physical Review B* **86**, 165426 (2012). (Z. Aksamija and I. Knezevic)

We present a calculation of the thermal conductivity of graphene nanoribbons (GNRs), based on solving the Boltzmann transport equation with the full phonon dispersions, a momentum-dependent model for edge roughness scattering, as well as three-phonon and isotope scattering. For suspended GNRs, the interplay between edge roughness scattering and the anisotropy of the phonon dispersions results in thermal conduction that depends on the chiral angle of the nanoribbon. Lowest thermal conductivity occurs in the armchair direction and highest in zig-zag nanoribbons. Both the thermal conductivity and the degree of armchair/zig-zag anisotropy depend strongly on the width of the nanoribbon and the rms height of the edge roughness, with the smallest and most anisotropic thermal conductivities occurring in narrow GNRs with rough edges.

For supported GNRs, transport is characterized by a complex interplay between line edge roughness (LER) and internal scattering, as captured through an effective LER scattering rate that depends not only on the surface roughness features, but also on the strength of internal scattering mechanisms (substrate, isotope, and umklapp phonon scattering). Substrate scattering is the dominant internal mechanism, with a mean free path (mfp) of approximately 67 nm. In narrow supported GNRs ($W < 130$ nm, i.e., roughly twice the mfp due to substrate scattering), phonon transport is limited by LER and spatially anisotropic. For intermediate widths ($130 \text{ nm} < W < 1 \mu\text{m}$) a competition between LER and substrate scattering governs transport, while thermal transport in wide GNRs ($W > 1 \mu\text{m}$) is dominated by substrate scattering and spatially isotropic. Thermal transport in supported GNRs can be tailored by controlling the ribbon width and edge roughness. Narrow ribbons act as longitudinal heat conduits, wide ribbons as omnidirectional heat spreaders.

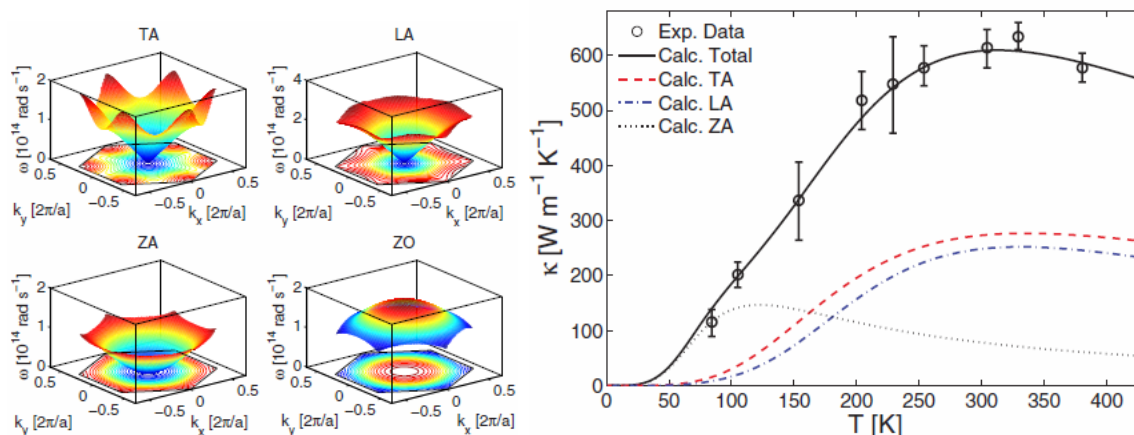


Fig. 6: (Left) Phonon dispersion relationship of single-layer graphene calculated using the 4NNR model, showing the TA, LA, ZA, and ZO branches over the first Brillouin zone of graphene. The dispersions are strongly anisotropic, causing phonon group velocities given by the gradients of the radial frequency to be strongly dependent on the direction of the phonon wave vector. The remaining two optical branches (TO and LO) are not depicted due to their negligible contribution to thermal transport. (Right panel) Comparison of lattice thermal conductivity of a wide ($W = 2 \mu\text{m}$) graphene ribbon supported on SiO₂ with experimentally measured data. Dashed lines are calculated contributions by individual phonon branches and the solid line is the total, showing excellent agreement with experiment throughout the temperature range. At low temperatures, the dominant contribution is from the out-of-plane acoustic (ZA) mode, which gets suppressed by the strong substrate interaction above 100 K, where in-plane modes take over.

Publications

JOURNAL PUBLICATIONS

1. Z. Aksamija and I. Knezevic,
"Thermal transport in graphene nanoribbons supported on SiO₂,"
Physical Review B 86, 165426 (2012).
2. E. B. Ramayya, L. N. Maurer, A. H. Davoody, and I. Knezevic,
"Thermoelectric properties of ultrathin silicon nanowires,"
Physical Review B 86, 115328 (2012).
3. N. Sule and I. Knezevic,
"Phonon-limited electron mobility in graphene using electronic tight-binding Bloch waves,"
Journal of Applied Physics 112, 053702 (2012).
4. Z. Aksamija and I. Knezevic,
"Lattice thermal conductivity of graphene nanoribbons: anisotropy and edge roughness scattering,"
Applied Physics Letters 98, 141919 (2011).
>> Paper recognition: Selected for the April 25, 2011 issue of Virtual Journal of Nanoscale Science & Technology (<http://www.vjnano.org>, volume 23, issue 16).
5. H. J. Ryu, Z. Aksamija, D. M. Paskiewicz, S. A. Scott, M. G. Lagally, I. Knezevic, and M. A. Eriksson,
"Quantitative determination of contributions to the thermoelectric power factor in Si nanostructures,"
Physical Review Letters 105, 256601 (2010).
6. Z. Aksamija and I. Knezevic,
"Anisotropy and boundary scattering in the lattice thermal conductivity of silicon nanomembranes,"
Physical Review B 82, 045319 (2010).
>> Paper recognition: Selected for the August 9, 2010 issue of Virtual Journal of Nanoscale Science & Technology (<http://www.vjnano.org>, volume 22, issue 6).
7. Feng Chen, E. B. Ramayya, C. Euaruksakul, F. J. Himpsel, G. K. Celler, Bingjun Ding, I. Knezevic, and M. G. Lagally,
"Quantum confinement, surface roughness, and the conduction band structure of ultrathin silicon membranes,"
ACS Nano 4, 2466–2474 (2010).
8. Z. Aksamija and I. Knezevic,
"Thermoelectric properties of silicon nanostructures,"
Journal of Computational Electronics 9, 173-179 (2010).
9. E. B. Ramayya and I. Knezevic,
"Self-consistent Poisson-Schrödinger-Monte Carlo Solver: electron mobility in silicon nanowires,"
Journal of Computational Electronics 9, 206-310 (2010). (invited article)

PAPERS IN REVIEW

10. Z. Aksamija and I. Knezevic,
"Lattice thermal conductivity in Si_{1-x}Ge_x/Si_{1-y}Ge_y superlattices: Competition between interface and internal scattering,"
Physical Review B, submitted.

11. A. H. Davoody, E. B. Ramayya, and I. Knezevic,
"Thermoelectric properties of GaN nanowires,"
 Phys. Rev. B, submitted.
12. L. N. Maurer, Z. Aksamija, E. B. Ramayya, A. H. Davoody, and I. Knezevic,
"Roughing It: Phonon Transport at the Nanoscale in the Presence of Rough Boundaries,"
 Phys. Rev. B, submitted.

FULL PAPERS IN CONFERENCE PROCEEDINGS

1. Z. Aksamija and I. Knezevic, *"Anisotropy and Edge Roughness Scattering in the Lattice Thermal Conductivity of Graphene Nanoribbons"*, ECS Transactions 35, 195 (2011).
2. Z. Aksamija and I. Knezevic, *"Thermoelectric Properties of Silicon-On-Insulator Nanostructures"*, ECS Transactions 35, 267 (2011).
3. I. Knezevic, *"Computational Design of Semiconductor Nanostructures for Optoelectronic, Electronic, and Thermoelectric Applications,"* Proceedings of IEEE NANO 2010 (<http://www.ieeenano2010.org>), Modeling and Simulation Section, Seoul, Korea (August 17-20, 2010). Available online through IEEE Xplore. <http://dx.doi.org/10.1109/NANO.2010.5698047>
4. Z. Aksamija and I. Knezevic, *"Thermoelectric properties of silicon nanostructures,"* Proceedings of IEEE NANO 2010 (<http://www.ieeenano2010.org>), Modeling and Simulation Section, Seoul, Korea (August 17-20, 2010). Available online through IEEE Xplore. <http://dx.doi.org/10.1109/NANO.2010.5697827>
5. D. Vasileska, K. Raleva, S. M. Goodnick, Z. Aksamija, and I. Knezevic,
"Thermal modeling of nanodevices,"
 Proceedings of the 14th International Workshop on Computational Electronics (IWCE 2010)
 Available online through IEEE Xplore, <http://dx.doi.org/10.1109/IWCE.2010.5677916>
6. E. B. Ramayya and I. Knezevic, *"Ultrascaled Silicon Nanowires as Efficient Thermoelectric Materials,"* Proceedings of the 13th International Workshop on Computational Electronics (IWCE 2009), Beijing, China, May 27-29, 2009, pp. 129-132. Available online through IEEE Xplore. <http://dx.doi.org/10.1109/IWCE.2009.5091160>

Personnel, Theses, and Awards

PERSONNEL

Irena Knezevic (PI, partial salary support and travel covered on this grant)

Edwin B. Ramayya (PhD student, RA support and travel)

Jie Chen (MS student, RA support)

Amirhossein Davoody (PhD student, RA support and travel)

Zlatan Aksamija (postdoctoral CIFellow, <http://cifellows.org/>,
<http://www.cra.org/crc/press.release.10.15.09.php>)

AWARDS

2011 Best Dissertation Award (UW ECE) -- Edwin Ramayya

2008 Best Paper Award Finalist (IEEE NANO 2008) -- Edwin Ramayya

E. B. Ramayya, D. Vasileska, S. M. Goodnick, and I. Knezevic, "*Thermoelectric Properties of Silicon Nanowires*"

DISSERTATIONS AND THESES

Edwin Ramayya, PhD 2010

PhD dissertation: "*Thermoelectric properties of ultrascaled silicon nanowires*"

PDF available at

http://homepages.cae.wisc.edu/~knezevic/pdfs/EdwinBoscoRamayya_AsPrinted.pdf

Amirhossein Davoody, MS 2011

MS project report "Thermoelectric Properties of Ultrascaled GaN Nanowires"

PDF available at <http://144.92.161.87/handle/1793/56412>

Invited and Contributed Talks

INVITED TALKS

1. *Title TBD, "Energy Conservation and Waste Heat Recovery,"* Institute for Pure and Applied Mathematics (IPAM), UCLA, November 18 – 22, 2013.
2. *"Phonon transport in silicon and graphene nanostructures,"* XIV International Conference on Phonon Scattering in Condensed Matter (Phonons 2012), University of Michigan Ann Arbor, MI, USA (July 8-13, 2012)
3. *"Computational Design of Semiconductor Nanostructures for Optoelectronic, Electronic, and Thermoelectric Applications,"* IEEE NANO 2010 (<http://www.ieeenano2010.org>), Modeling and Simulation Section, Seoul, Korea (August 17-20, 2010).
4. *"Design of Nanostructured Materials for Electronic, Thermoelectric, and Optoelectronic Applications,"* 2010 March Meeting of the American Physical Society, Portland, OR (March 15-19, 2010).
5. *"Computational Design of Semiconductor Nanostructures for Electronic, Thermoelectric, and Optoelectronic Applications,"* University of Houston, Electrical and Computer Engineering (March 5, 2010).
6. *"Thermoelectric properties of silicon nanowires"* Boston University, Electrical and Computer Engineering Department (May 1, 2009)

CONTRIBUTED CONFERENCE PRESENTATIONS

1. L. Maurer, Z. Aksamija, E. Ramayya, A. H. Davoody, and I. Knezevic, "Phonon Surface Scattering in Monte Carlo Simulations," APS March Meeting 2013, Baltimore, Maryland, March 18–22, 2013.
2. Z. Aksamija and I. Knezevic, "Reduced Thermal Conductivity in SiGe Alloy-based Superlattices for Thermoelectric Applications," 2012 Materials Research Society (MRS) Fall Meeting, Boston, MA (November 2012)
3. Z. Aksamija and I. Knezevic, "Thermal Transport in Suspended and Supported Graphene Nanoribbons", 49th Annual Technical Meeting of the Society of Engineering Science (SES), Atlanta, GA (October 10-12, 2012).
4. Z. Aksamija and I. Knezevic, "Thermal Transport in Suspended and Supported Graphene Nanoribbons", International Conference on Simulation of Semiconductor Processes and Devices (SISPAD'12), Denver, CO (September 2012).
5. Z. Aksamija and I. Knezevic "Simulation of Thermal Transport in Semiconductor Nanostructures on Heterogeneous Systems", XSEDE12 Conference, Chicago, IL (July 2012).
6. Z. Aksamija and I. Knezevic "Reduced Thermal Conductivity in SiGe Alloy-based Superlattices for Thermoelectric Applications", 14th International Conference on Phonon Scattering in Condensed Matter (PHONONS 2012), Ann Arbor, MI (July 2012).
7. Z. Aksamija and I. Knezevic "Thermal Conductivity in SiGe Alloy-based Superlattices for Thermoelectric Applications", 6th International Silicon-Germanium Technology and Device Meeting (ISTDM 2012), Berkeley, CA (June 2012).
8. Z. Aksamija and I. Knezevic "Thermal transport in graphene-based nanostructures", American

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9. Z. Aksamija, E. Ramayya, and I. Knezevic, "Modeling of Thermal Conductivity and Thermoelectric Power Factor in Ultrathin SOI Nanomembranes and Silicon Nanowires", International Semiconductor Research Symposium (ISDRS), University of Maryland, College Park, MD (Dec. 7-9, 2011)
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14. Z. Aksamija and I. Knezevic, "Anisotropy and Edge Roughness Scattering in the Lattice Thermal Conductivity of Graphene Nanoribbons", Electro-Chemical Society Meeting (ECS-219), Montreal, Canada (May 1-6, 2011).
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