GaN Nanowires for Thermoelectric Applications

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In recent years, gallium nitride (GaN) has gained a lot of attention as a material with characteristics especially suitable for high-frequency, high-power devices. Use of an integrated spot cooling thermoelectric device is a good solution for heating problem in high-power devices. The need for GaN device integration brings up the use of GaN as the thermoelectric (TE) material in GaN-based integrated circuits. Efficiency of a TE device is characterized by the TE figure of merit $ZT = S^2\sigma T/\kappa$, where S is the Seebeck coefficient, σ is electrical conductivity, T is the temperature, and κ is thermal conductivity. A paper by Hicks and Dresselhaus [1] predicted that using nanostructured materials can increase the Seebeck coefficient, as well as cause a significant reduction of thermal conductivity while electrical conductivity stays almost the same. In this work, we have investigated the potential of GaN nanowires (NWs) as TE devices over the temperature range of 300 K to 1000 K.

We considered a single-valley, non-parabolic band structure for the wurtzite GaN. We developed a coupled Poisson-Schrödinger solver to calculated electron wavefunctions across the wire. Then we calculated the electron scattering rate based on the calculated wavefunctions. The important electron scattering mechanisms in GaN NWs are acoustic phonon scattering, impurity scattering, surface roughness scattering, polar optical phonon (POP) scattering, and piezoelectric scattering. The obtained scattering rates are used in a Monte Carlo (MC) kernel to calculate electron mobility [2].

Major phonon scattering processes in the thermal conductivity calculation are normal and Umklapp phonon-phonon scattering, surface roughness scattering, and isotope (mass difference) scattering. We used Holland's model to calculate the normal and Umklapp scattering rates [3]. Ensemble MC technique is used to simulate thermal conductivity in GaN NW.

We solved the 1D Boltzmann transport equation (BTE) within the relaxation time approximation (RTA) to calculate the electronic Seebeck coefficient. The phononic Seebeck coefficient is found to be orders of magnitude smaller than the electronic Seebeck coefficient, and thus negligible.

Results of the simulations are shown in Fig. 1-6. As we see in Fig. 1-3, both thermal conductivity and the electron mobility decrease as the temperature increases, wire thickness decreases, and the doping density increases. The Seebeck coefficient shows non-monotonic trends in Figs. 4 and 6. This behaviour is different from that of bulk materials and is a result of energy quantization in NWs. According to Figs. 4-6, optimum doping density is 3×10^{18} cm^{-3}, optimum wire thickness is 4 nm. ZT increases as temperature increases.

In conclusion, we calculated the TE figure of merit over a wide range of doping densities, temperatures, and wire thicknesses, through MC simulation of the electron mobility and thermal conductivity and the RTA technique calculation of the Seeck coefficient. The results showed that ZT can be increased by an order of magnitude with respect to bulk when used at high temperatures, having the proper doping density and the wire thickness.

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References

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[2] E. B. Ramayya, D. Vasileska, S. M. Goodnick, and I. Knezevic, *Electron transport in silicon nanowires: The role of acoustic phonon confinement and surface roughness scattering*, J. Appl. Phys. **104**, 063711 (2008).

[3] M.G. Holland, *Analysis of lattice thermal conductivity*, Physical Review **132**, 2461 (1963).

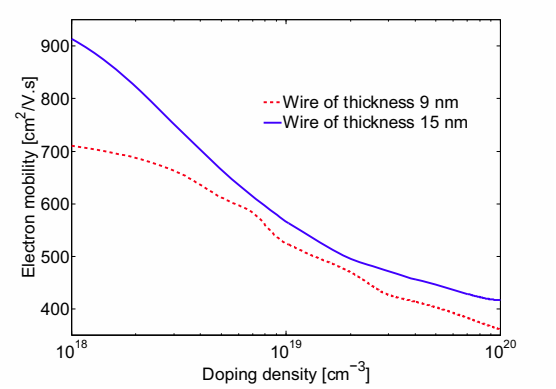

Fig. 1. Electron mobility of nanowires as a function of doping density. The rms roughness of the interface is $\Delta = 0.3$ nm. Wire temperature is $T = 300$ K.

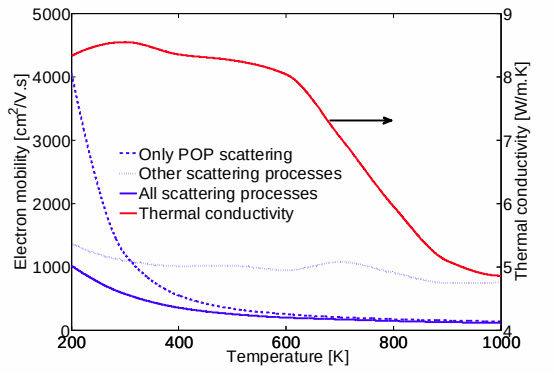

Fig. 2. Electron mobility and thermal conductivity of a 9 nm thick nanowire as a function of temperature. The rms roughness of the wire interface is $\Delta = 0.3$ nm. The doping concentration is $N = 1 \times 10^{19}$ cm^{-3}.

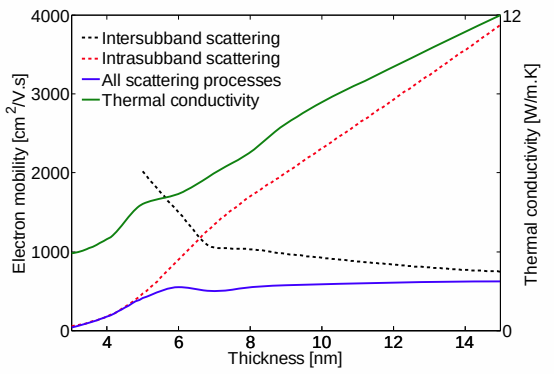

Fig. 3. Electron mobility and thermal conductivity of nanowires as a function of thickness at temperature $T = 300$ K. The rms roughness of wire interface is $\Delta = 0.3$ nm. The doping concentration is $N = 1 \times 10^{19}$ cm^{-3}.

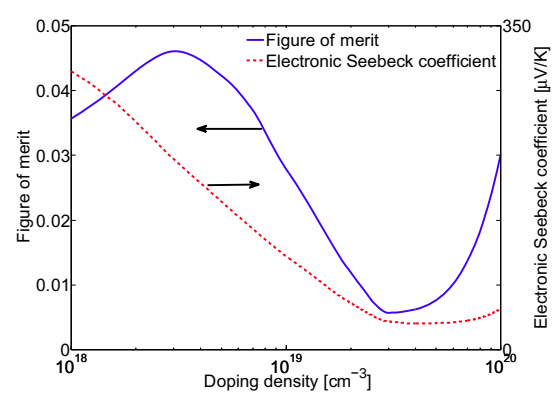

Fig. 4. The electronic Seebeck coefficient and the thermoelectric figure of merit as a function of the doping density for a wire of 9 nm thickness. The rms roughness of interface is $\Delta = 0.3$ nm. Wire temperature is $T = 300$ K.

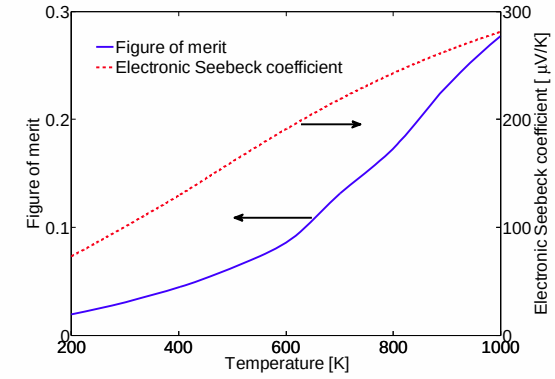

Fig. 5. The electronic Seebeck coefficient and Thermoelectric figure of merit as a function of temperature for a wire of 9 nm thickness. Wire surface roughness is $\Delta = 0.3$ nm. The doping concentration is $N = 1 \times 10^{19}$ cm^{-3}.

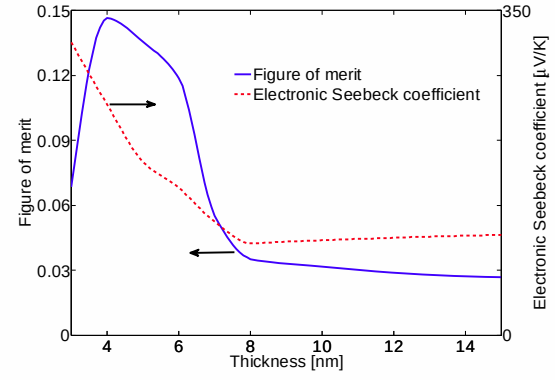

Fig. 6. The electronic Seebeck coefficient and the thermoelectric figure of merit as a function of the wire thickness at temperature $T = 300$ K. The rms roughness of wire interface is $\Delta = 0.3$ nm. The doping concentration is $N = 1 \times 10^{19}$ cm^{-3}.