Enhanced Seebeck coefficient due to quantum confinement in gated 2d nanomembranes

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The effective control on electron and phonon transport due to confinement, interface and quantum effects has made nanostrutures as a good way to achieve high figure-of merit (ZT). Maximizing the power factor $S^2\sigma(S$ is seebeck coefficient and σ is electrical conductivity) and restricting the phonon transport can improve ZT. Mahan and Sofo [1] proposed that a delta-shaped Transport Distribution Function (TDF) $\sigma(E) = \tau(E)g(E)v^2(E)$ can significantly improve S thereby improving the overall ZT through electron filtering. Achieving a delta-shaped TDF, however, proved difficult as the sharp features in the density-of-states (DOS) $g(E)$ are readily cancelled by related features in the scattering rate $\tau^{-1}(E)$.

In this work, we studied ways to achieve such a delta-shaped TDF by gate-tuning the subband spacing and scattering mechanisms in a gated 2-dimensional silicon nanomembrane. The 2-d nature of the system leads to a step-like electronic DOS $g_n^b(E) = m_n^*/(\pi\hbar^2)\Theta(E - E_n^b)$ with one step contributed by each subband n in each ladder b. Inelastic scattering rates are proportional to the DOS; however, inelastic and intersubband scattering can only begin to occur when the carrier accumulates enough energy so $\tau_{inel.}^{-1}(E) \propto g(E \pm \Delta E)$ where ΔE is the energy being exchanged–either the difference in subband energies for intersubband scattering or the optical phonon energy $\hbar\omega_{op}$ for optical transitions. Hence these mechanisms, when inelastic scattering is dominant, delay the onset of the step in the scattering rate relative to the DOS and thus lead to a delta-shaped TDF.

To explore the practical possibility of achieving the delta shaped Transport distribution function a back gated undoped silicon nanoribbon (SiNR) on oxide is simulated. The oxide acts as capacitor which induces charges that participates in transport of both charge and energy and applied voltage controls the subband seperation. The subband energies are calculated by self-consistently solving the Poisson and 1-D Schrödinger equation. The S of a nanostructure is given [2] by $L^{(1)}/L^{(0)}$ where the transport integrals are

$$L^{(\alpha)} = -e^2 \sum_{n,b} \int_0^\infty \frac{\partial f_{FD}}{\partial E} \sigma(E)(E + E_n^b - E_F)^\alpha dE$$

and E_n^b is energy of the n'th subband, $g_n^b(E)$ is density of states, $\tau_n^b(E)$ is energy dependent relaxation time, and $v_x(E)$ is velocity along the x direction. The electron relaxation times are calculated by considering surface roughness, elastic acoustic phonon scattering, and inelastic optical phonon (both intra and intersubband) scattering mechanisms. We computed S and observed a significant enhancement, especially at low temperatures when optical phonon scattering is the dominant mechanism (restricting the other scattering mechanisms) as shown in Fig. 1. In a confined nanostructure, the discrete energy bands limits the states available for electron to occupy which in turn limits phonon energies that can participate in scattering. Fig. 2 shows optical phonon energies that can provide enhancement in S at low temperatures. Enhancement occurs when the optical phonon energy is comparable to the subband energy difference. This filters out only a narrow energy window between two successive subbands, resulting a higher Seebeck coefficient as seen in Fig. 2. We thus produce a delta shaped Transport Distribution Function (TDF) as shown in Fig. 3 with a peak at lower subbands and decreasing rapidly towards the high energies. Tuning the energy difference between the subbands to match the optical phonon energies by varying the gate voltage is demonstrated in Fig. 4. The observed enhancement is more evident at low temperatures

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because of the suppression of phonon absorption. The enhancement in S can be further increased by reducing the effective mass, as it is inversely proportional to step height in the 2-d density of states, increasing the height of the peak in the TDP and giving a higher S as shown in Fig. 5.

In summary, we simulated gated 2-d systems and showed that enhanced thermoelectric properties are achieved by tuning the subband separation to match the optical phonon energy and creating a delta shaped transport distribution function.

REFERENCES

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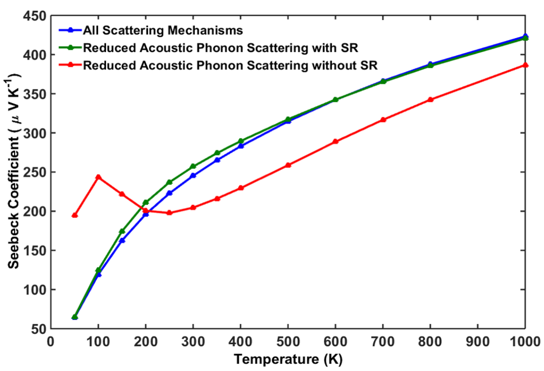

Fig. 1. S at several temperatures with a V_{gate}= 5V for all scattering mechanisms, reduced acoustic phonon scattering, with and without surface roughness scattering.

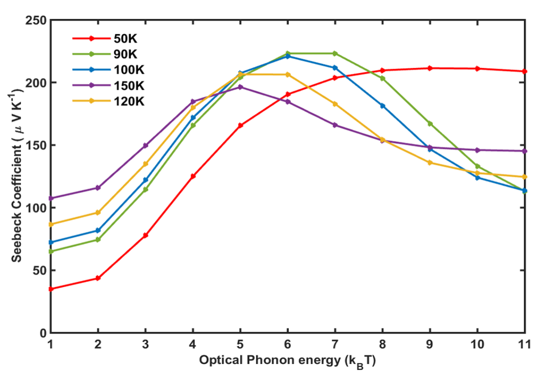

Fig. 2. S variation with optical phonon energies showing the peak being positioned near the valley bottom subband energy difference with V_{gate}=5 V

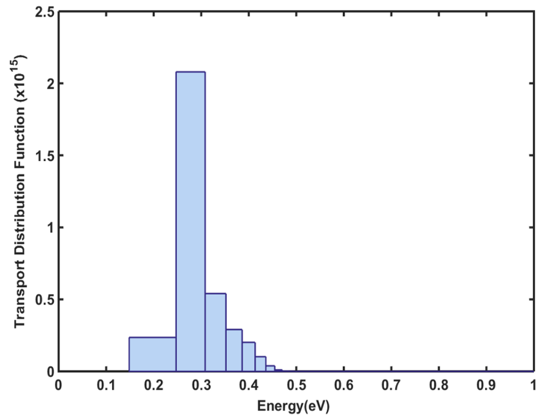

Fig. 3. Delta-shaped Transport Distribution Function (TDF) formed at T=100K, V_{gate}=5V and optical phonon energies comparable to the subband energy gap.

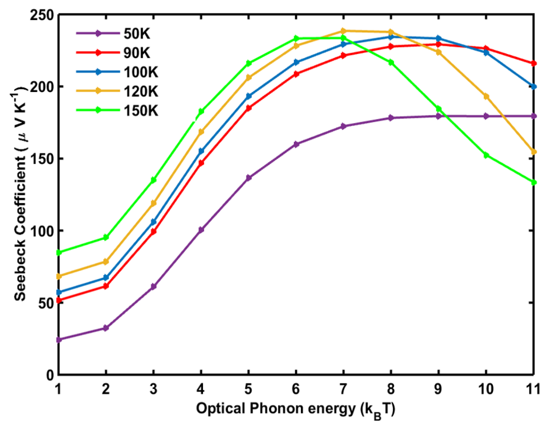

Fig. 4. The shift in the phonon energies due to the change in the energy gap between subbands being introduced by applying a higher gate voltage V_{gate}= 7V at low temperatures.

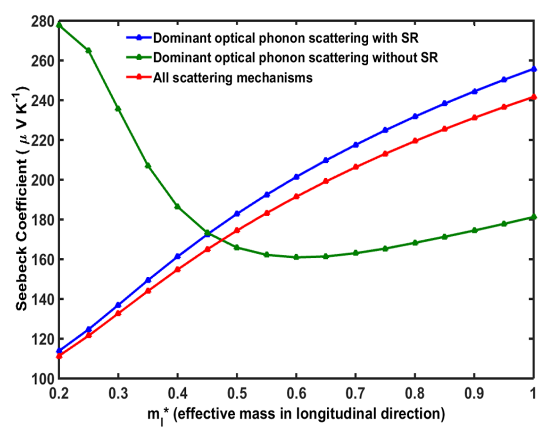

Fig. 5. Variation in S with the longitudinal effective mass(m_l^*) at T=100K with $E_{optical}$=0.043eV and V_{gate}=5V.