Thermoelectric Properties of Periodic Quantum Structures in the Wigner-Rode Formalism

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ABSTRACT

Improving the thermoelectric Seebeck coefficient, while simultaneously reducing thermal conductivity, is required in order to boost thermoelectric (TE) figure of merit (ZT) and further increase the efficiency of TE energy conversion. One approach to improve the Seebeck coefficient is electron filtering where "cold" (low energy) electrons are restricted from participating in transport by an energy barrier [1, 2]. However, the impact of electron tunneling through thin barriers and resonant states on TE properties has been given less attention. In our work, we simulate energy filtering through a series of potential barriers in silicon. The affect of their shape and periodicity on TE performance is studied. We developed a comprehensive transport model that includes energy relaxation and quantum effects from potential barriers using Wigner-Rode formalism.

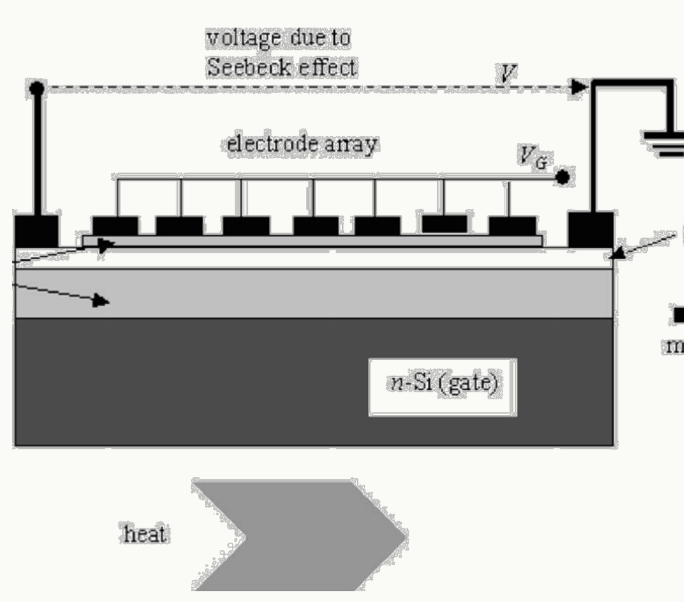
INTRODUCTION

➢ The efficiency of thermoelectric devices is given by the figure of merit,

$$ZT = \sigma S^2 \frac{T}{k_{ph}+k_e}$$

➢ Structures with rapid potential variations are reported to achieve a higher Seebeck Coefficient[3,4,5].

➢ To model such devices, carrier-potential interactions has to incorporated in to transport equation using Wigner-Boltzmann transport equation (WBTE).



➢ Using relaxation time approximation for collision operator and with a small perturbation to distribution function, WBTE is given as

$$\left(v_r \nabla_r + \frac{\hbar k}{m}\nabla_r\right) f_w(r,k,t) = Qf_w(r,k,t) + \left(\frac{\partial f_\omega}{\partial t}\right)_c$$

where $Qf_w(r,k,t) = \int dk'\, \mathrm{V_w}(\mathrm{r}, \mathrm{k}-\mathrm{k}')\, f_w(r,k,t)$ and

Wigner Potential $V_w(r,k) = \frac{1}{i\hbar(2\pi)^d}\int dr'\, e^{ir'k}\left(\mathrm{V}\left(\mathrm{r}+\frac{\mathrm{r}'}{2}\right) - \mathrm{V}\left(\mathrm{r}-\frac{\mathrm{r}'}{2}\right)\right)$

MODEL

➢ Rode's method is used to solve WBTE for a doped bulk silicon with rapid varying periodic potential using the full band data from empirical psuedo potentials.

➢ The scattering mechanisms implemented are

- Acoustic phonon deformation potential scattering
- Impurity Scattering
- Inter-valley phonon scattering
- Boundary scattering

➢ A fast varying cosine shaped potential can be written in the form

$$V_q(r) = V_0\cos(K_0 r) \text{ where } K_0 = \frac{2\pi}{L_p}$$

and quantum evolution term is obtained as

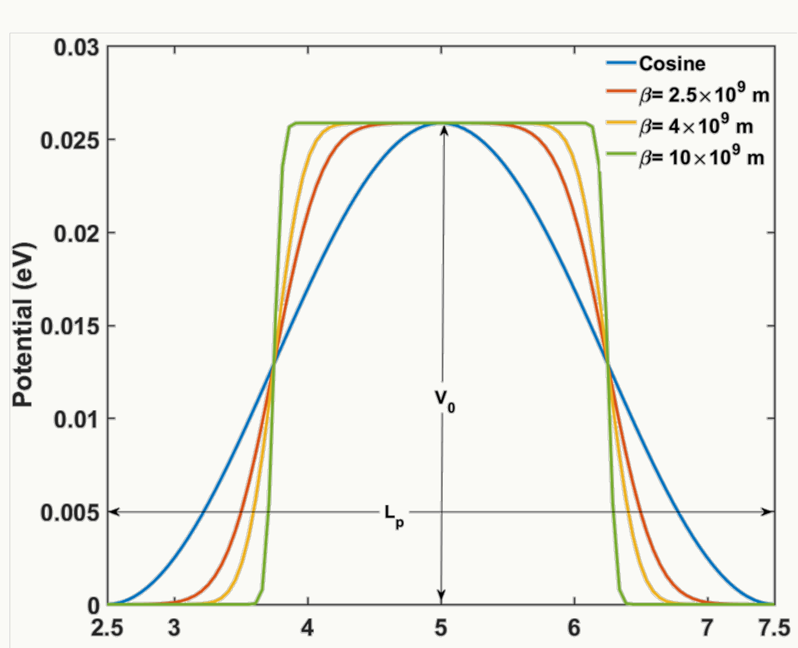
$$Qf_w(r,k) = \frac{V_0 \sin(K_0 r)}{\pi\hbar}\left[f_\omega\left(r, k - \frac{K_0}{L_p}\right) - f_\omega\left(r, k + \frac{K_0}{L_p}\right)\right]$$

➢ A more general fast varying periodic potential can be written in the form[6]

$$V_q(r) = \sum_{n=-\infty}^{\infty} V_p(r - nL_p)$$

➢ A square potential with smoothening V_p can be written

$$\frac{V_0}{2}\left[-\mathrm{erf}(\beta(r-a)) + \mathrm{erf}(\beta(r+a))\right]$$



➢ In Rode's iterative method, the distribution of carriers is written as a sum of equilibrium component (Fermi-Dirac statistics) and a small perturbation to it.

$$f_w(\vec{k}) = f_o(\vec{k}) + \sum_{n=1} g_n(\vec{k}) P_n(\cos\theta)$$

➢ A rapid varying potential applied in r direction, then the perturbation in the carrier distribution is calculated by a self-consistent iteration as

$$g_{i+1}(k) = \left(I(k) + eFf_0(k)'/\hbar - v_r\frac{\partial f_w}{\partial r} + Qf_w(r,k,t)\right)/S_0$$

where $S_o = S_0^{inel}(k) + S_0^{el}(k)$

and $I(k) = \int dk' \frac{q(Z-2)D_{kf}^2\left(N_{po}+\frac{1}{2}\pm\frac{1}{2}\pm f_0\right)}{\rho\omega_f} g_i(k')\delta(E_i \pm \hbar\omega_0 - E(k'))$

➢ To calculate $I(k)$ we use Spherical Averaging Method (SAVE), where δ function is calculated by counting the states inside the sphere with in a radius R_S.

➢ Then $g(k)$ is used to calculate mobility and Seebeck coefficient using the expression

$$\mu_e = \frac{\int\int v(k) g_i(k)\delta\big(E - E(k)\big)dk\, dE}{eF\int\int f(k)\delta\big(E - E(k)\big)dk\, dE}$$

$$S = \frac{\int\int v(k) g_i(k)(E - E_f)\delta\big(E - E(k)\big)dk\, dE}{T\int\int v(k) g_i(k)\delta\big(E - E(k)\big)dk\, dE}$$

RESULTS

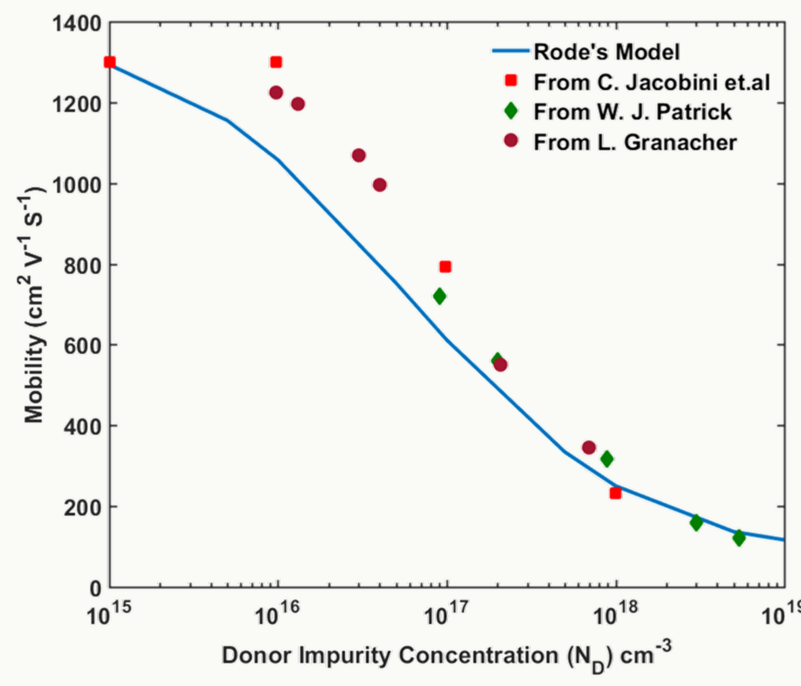


Fig 1. Effect of impurity concentration on mobility of electrons at $T = 300\,K$.

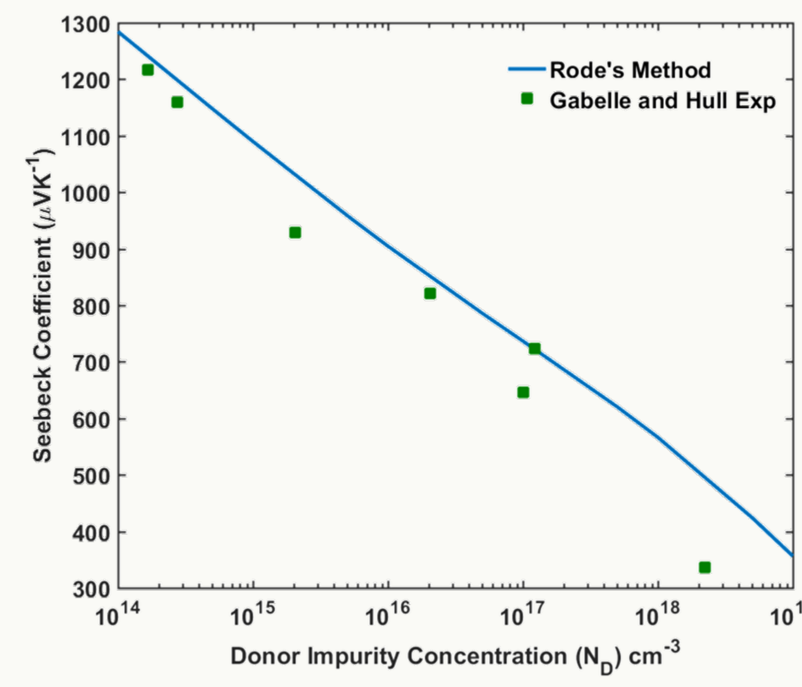


Fig 2. Effect of impurity concentration on Seebeck coefficient at $T = 300\,K$.

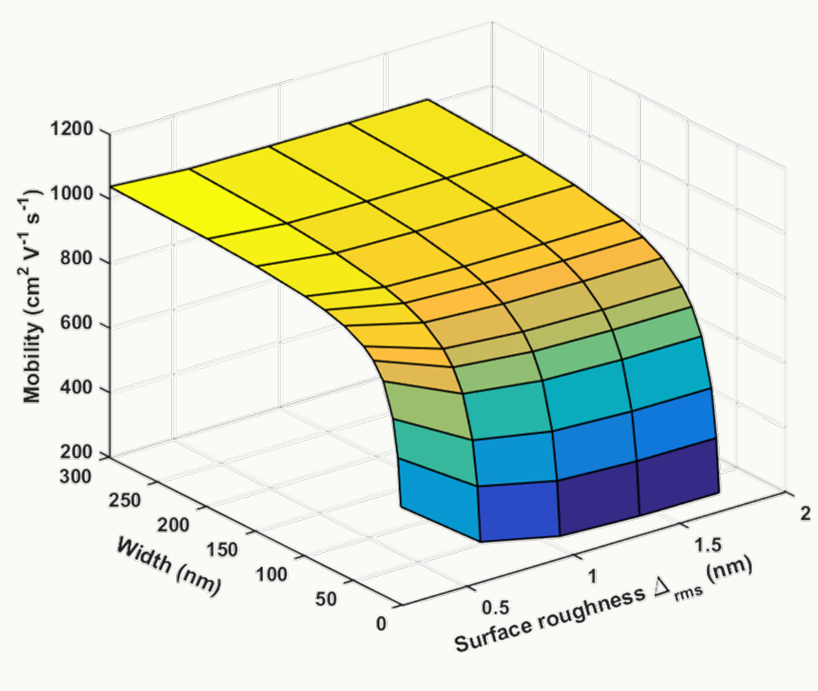


Fig 3. Effect of boundaries on mobility at $N_d = 10^{16}\,cm^{-3}$ and $T = 300\,K$.

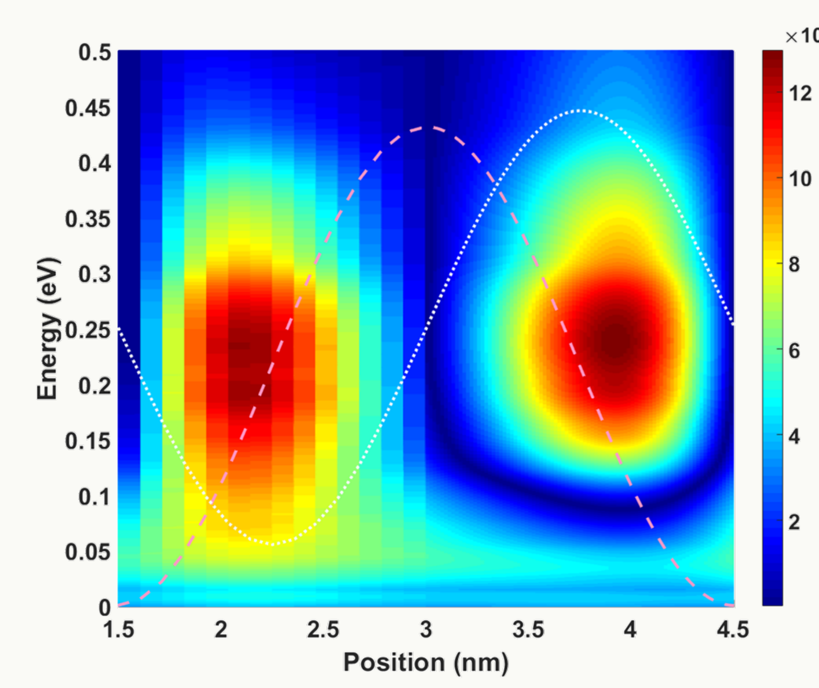


Fig 4. $\sigma(E)$ at $V_0 = 1\,k_BT$ and $L_p = 3\,nm$.

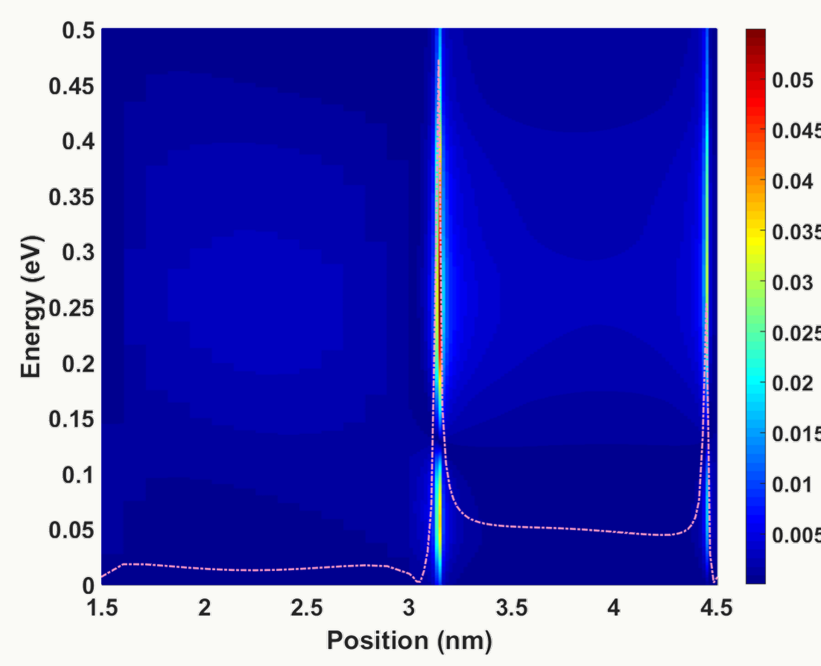


Fig 5. $S(E)$ at $V_0 = 1\,k_BT$ and $L_p = 3\,nm$.

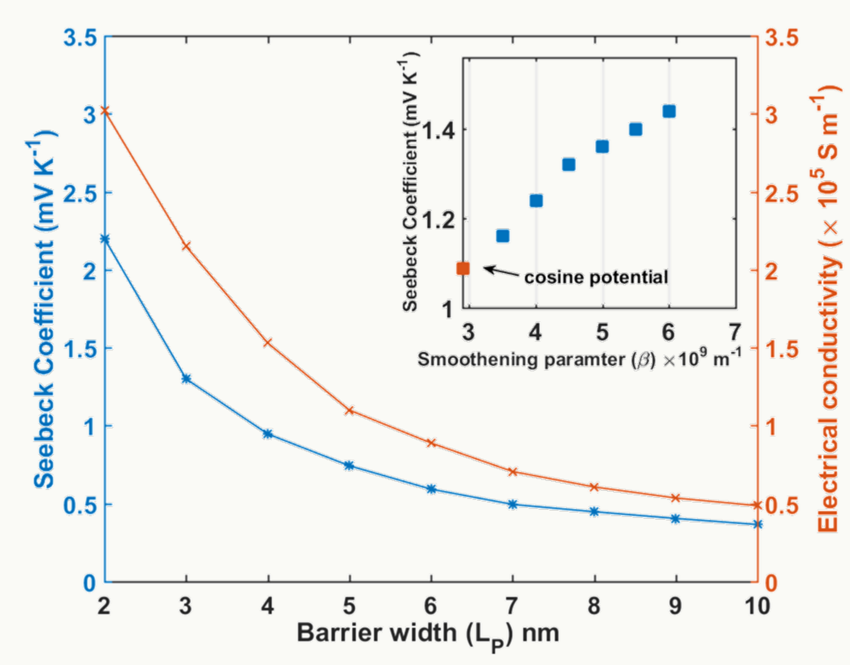


Fig 6. $N_D = 4\times10^{19}\,cm^{-3}$, $V_0 = 1\,k_BT$ at $T = 300\,K$.

CONCLUSION

➢ An extensive model that includes both quantum and semi-classical effects is implemented to study electron transport in the presence potential barriers.

➢ This helped us to understand the extend of quantum effects like tunneling in periodic structures and ways to enhance thermoelectric performance in those structures.

➢ Future work:

1. Improve the model scope to simulate the entire spectrum of potentials.
2. Extend the model to simulate multi barrier structures like RTD's.

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