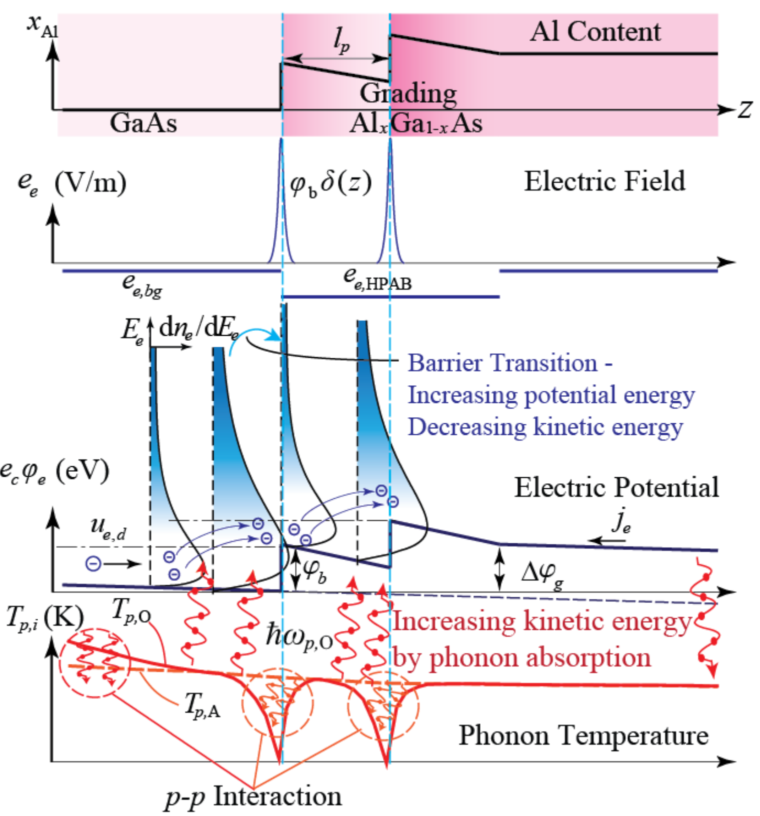
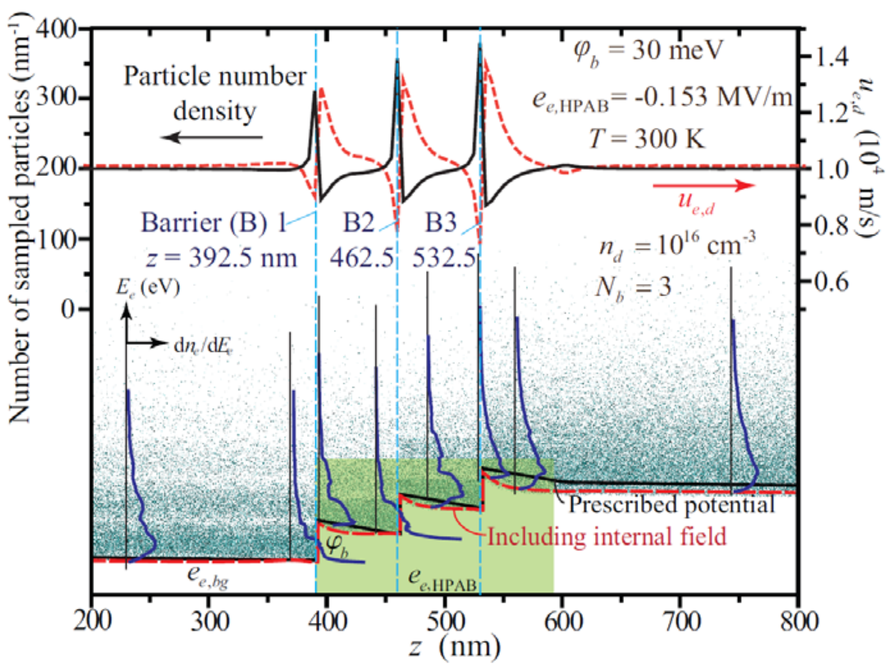
Heterobarrier for Converting Hot-phonon Energy to Electric Potential

We show that hot phonons emitted in energy conversion or resistive processes can be converted to electric potential in heterobarrier structures. Using phonon and electron interaction kinetics and self-consistent ensemble Monte Carlo (MC), we find the favorable conditions for unassisted absorption of hot phonons and design graded heterobarriers for their direct conversion into electric energy. Tandem barriers with nearly optical-phonon height allow for substantial potential gain without current loss. We find that 19% of hot phonons can be harvested with an optimized GaAs/Al$_x$Ga$_{1-x}$As barrier structure over a range of current and electron densities, thus enhancing the overall energy conversion efficiency and reducing waste heat.



Spatial distributions of x_{Al}, **electric field** and **potential,** and **optical and acoustic phonon temperatures** in the hot-phonon absorbing barrier structure (HPAB).



Sampled **particle number density**, $u_{e,d}$, and **particle-energy distribution** over the simulation cell.

Hot phonon (Nonequilibrium, overpopulated)

- Phonons are emitted by various decays, recombination and drags in energy conversions, and many resistive processes (e.g., in electronic circuits).
- Among the phonon modes, optical phonon emission is the dominant energy relaxation channel in semi-conductors. The optical phonon emission rate can be larger than its decay rate, then **this optical mode is overpopulated over the equilibrium.**

Hot phonon absorption barrier (HPAB)

- Designed for converting phonon energy to electric potential using barrier structure
- Potential barriers cause an **adverse current**

→ To compensate this adverse effect, large, forward local electric field formed by x_{Al} grading ($e_{e,HPAB}$) is introduced in the barrier.

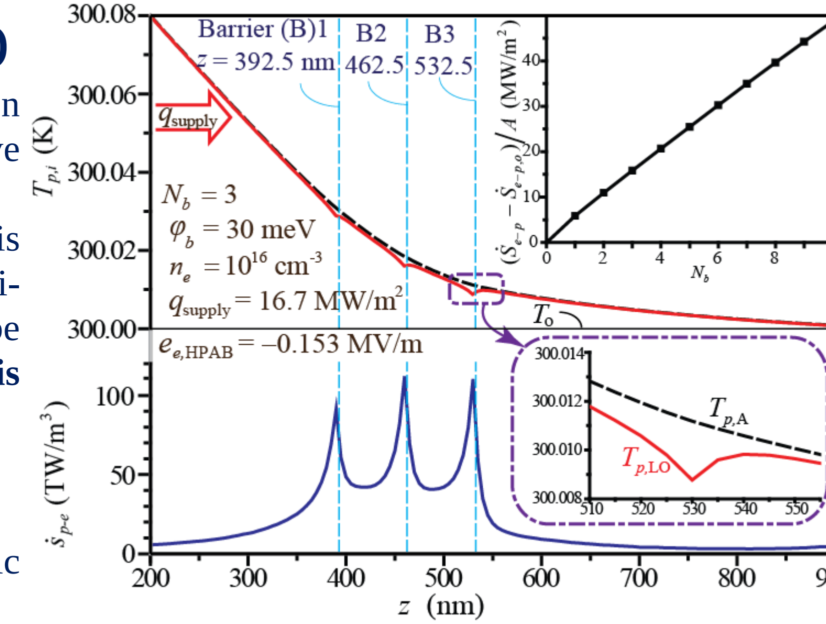
- Phonon absorption populates electrons with high energy and momentum before or after barrier transition, and this energy is converted to electric potential

Self-consistent ensemble Monte Carlo

- Simulation of the **electron transport and phonon absorption/emission in HPAB** with electron and phonon interaction kinetics
- Large **ensemble** of sampled electrons are coupled to the **Poisson equation** (for internal charge redistribution)
- Simulation results are obtained by **ensemble average of the sampled particles** (0.5 to 1 ns).

Distribution of electron properties

- Electrons are accumulated behind barriers and low-energy electrons are highly populated near barriers.
- Potential profile near barriers is bent by this nonuniform charge distribution, but this effect is not significant for small n_e ($< 10^{17}$ cm^{-3}).



Distributions of phonon temperatures ($T_{p,A}$ and $T_{p,LO}$) and **phonon energy absorption rate** ($\dot{s}_{p-e}$)

T_p and $\dot{s}_{p-e}$ Distribution

- Larger nonequilibrium between phonon modes at barriers.
- T_p variation is not significant. [Due to the large phonon density compared to electron ($n_d < 10^{-17}$ cm^3), LO phonon depletion is not significant and is made up by up-conversion of acoustic phonons]

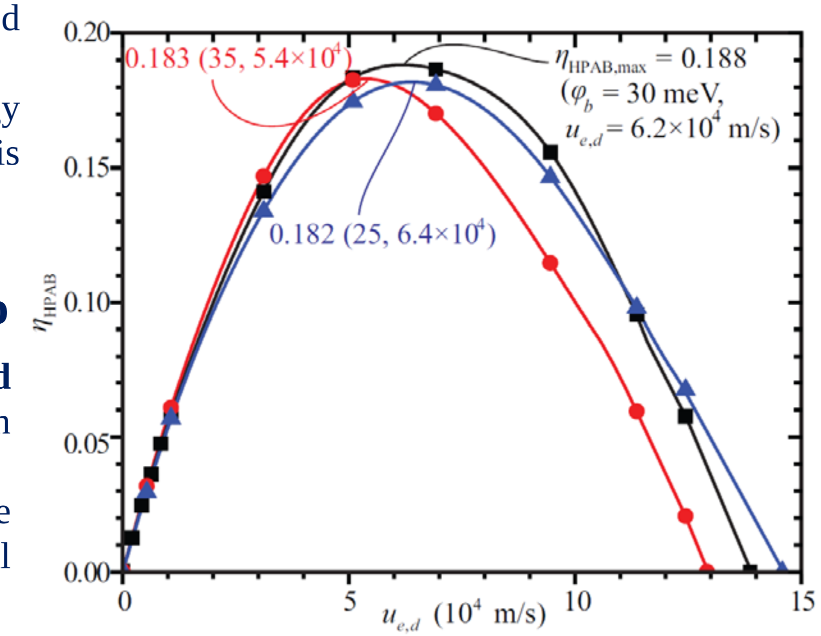
Local phonon energy absorption rate (W/m³)

$$\dot{s}_{p-e} = \sum_j \int_{E_e} [\dot{\gamma}_{p\to e,j}(E_e) - \dot{\gamma}_{e\to p,j}(E_e)] E_{p,j} \frac{dn_e(E_e)}{dE_e} dE_e$$

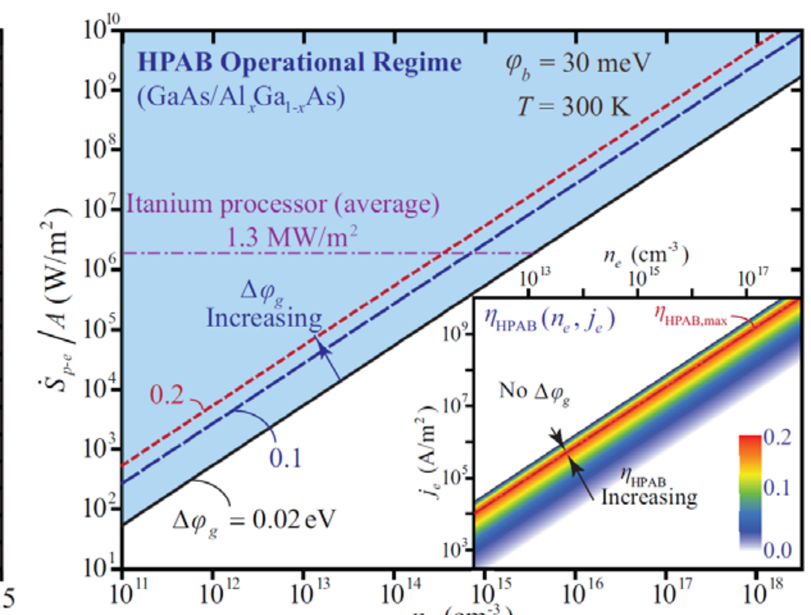
[j: interaction mechanism]

- **Low-energy electrons: Absorption favorable.** (Large low-E_e electron population near barriers)
- **Large phonon absorption & field acceleration**

→ Recovering the distribution to equilibrium



Variations of HPAB efficiency η_{HPAB} with respect to $u_{e,d}$. η_{HPAB} first increases with $u_{e,d}$ due to increase in P_g ($= \Delta\varphi_g j_e$) and then decreases because of smaller $\Delta\varphi_g$ (The maximum efficiency $\eta_{HPAB,max}$ = 18.8 %, when $u_{e,d}$ = 6.2 × 10⁴ m/s and φ_b = 30 meV.)



- **HPAB operational regime** and **variations of phonon energy absorption rate** $\dot{S}_{p-e}/A$ with respect to n_e, *for* $\Delta\varphi_g$ = 0.02, 0.1, and 0.2 eV, and $u_{e,d} < 10^4$ m/s. Inset shows **variations of η_{HPAB} with respect to n_e and j_e**. $\dot{S}_{p-e}/A$ (for a given $\Delta\varphi_g$ and j_e corresponding to $\eta_{HPAB,max}$) increases with n_e.

- It is estimate **up to 19% of the phonon energy conversion** with proper phonon flux and current
- **HPAB reverses the phonon role**, generally hindering electron transport, by harvesting hot phonons. By integrating HPAB in electronic devices, **reduced heat dissipation** by effective removal of excess phonons, as well as **additional electric power generation** (or recovery) will be achieved.