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.

**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 semiconductors. 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 ($e_{p,HPAB}$) 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$^{-3}$).

**Variations of HPAB efficiency**
- $\eta_{HPAB}$ with respect to $n_{e,d}$
  - $\eta_{HPAB}$ first increases with $n_{e,d}$ due to increase in $P_{e}$ ($\Delta \phi_{p-e}$) and then decreases because of smaller $\Delta \phi_{p-e}$ (The maximum efficiency $\eta_{HPAB,max}$ is 18.8% when $u_{e,d}$ = 6.2 × 10$^{4}$ m/s and $\varphi_{b}$ = 30 meV).

**HPAB operational regime**
- $\eta_{HPAB}$ with respect to $n_{e}$ and $J_{L}$
  - $\eta_{HPAB}$ increases with $n_{e}$ and $J_{L}$.

**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.