Quantum
Mechanical &
Electromagnetic
Systems
Modelling Lab

Uncertainty Quantification of Charge Transfer through a Nanowire Resonant-Tunnelling Diode with an ADHIE-FDTD Method.

Pieter Decleer & Dries Vande Ginste.

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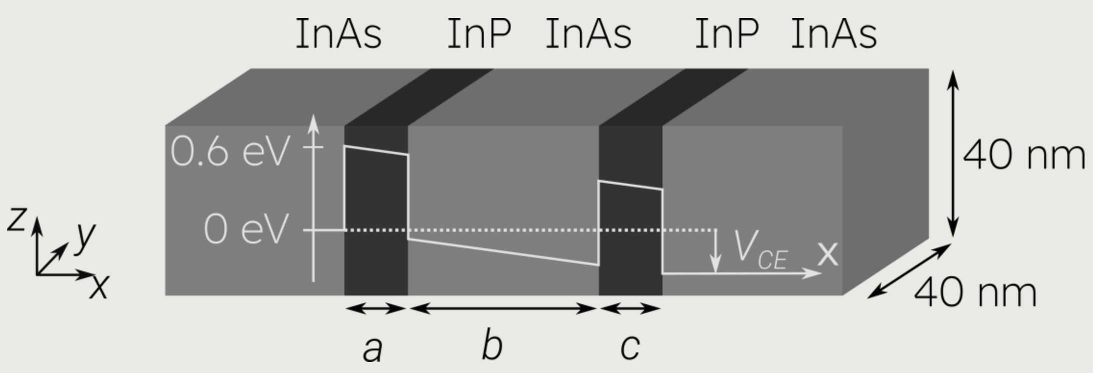
The Nanowire Resonant-Tunnelling Diode.

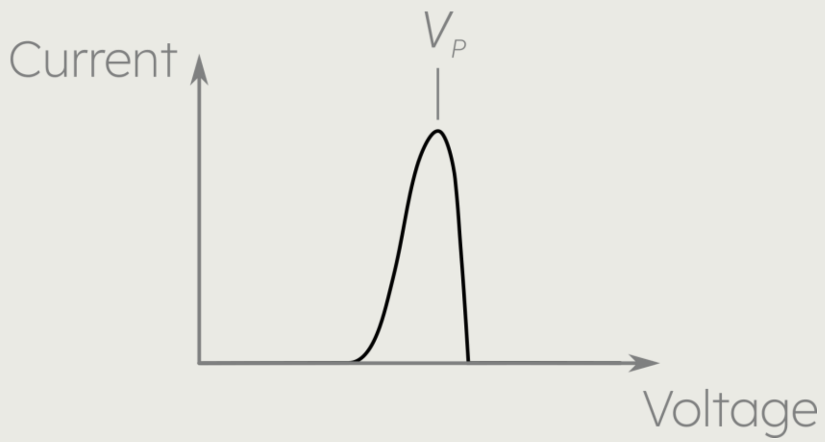


Double barrier structure allows only specific energies to pass.

IV-characteristic exhibits peak at certain voltage V_P.

Imperfections and variability of geometrical parameters cause aberrant behavior.

Assess how manufacturing defects influence performance.



Solving the time-dependent Schrödinger equation.

The Finite-Difference Time-Domain (FDTD) method

The time-dependent Schrödinger equation

$$j\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2}\nabla\cdot\left(\frac{1}{m}\nabla\psi\right) + V\psi$$

Discretized with the regular FDTD method

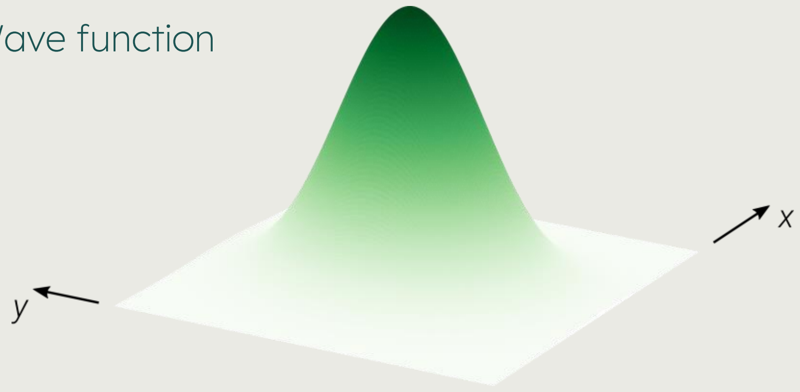
$$\psi^{n+1} = \Delta t\hat{H}\psi^n$$

Fast time stepping, but:

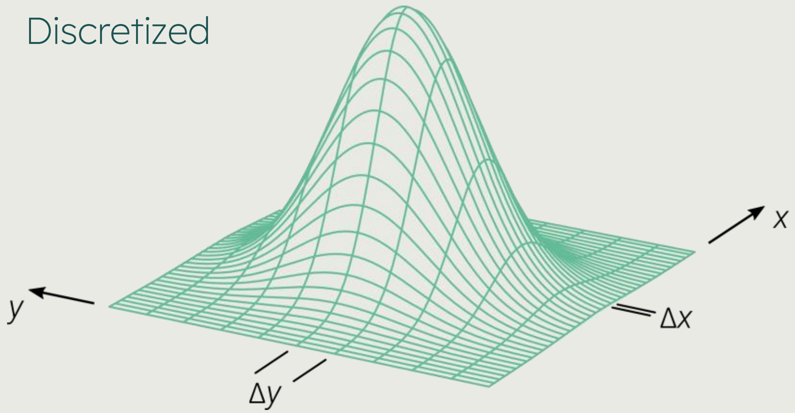
$$\Delta t < \frac{2\hbar}{\frac{2\hbar^2}{m}\left(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}\right)+V}$$

Stability criterion requires small Δt due to small Δx.

Wave function



Discretized



Solving the time-dependent Schrödinger equation.

The Alternating-Direction Hybrid Implicit-Explicit (ADHIE)-FDTD method.

Discretized with the ADHIE-FDTD method which treats different directions differently

$$\hat{L}\psi^{n+1} = \Delta t \hat{R}\psi^{n}$$

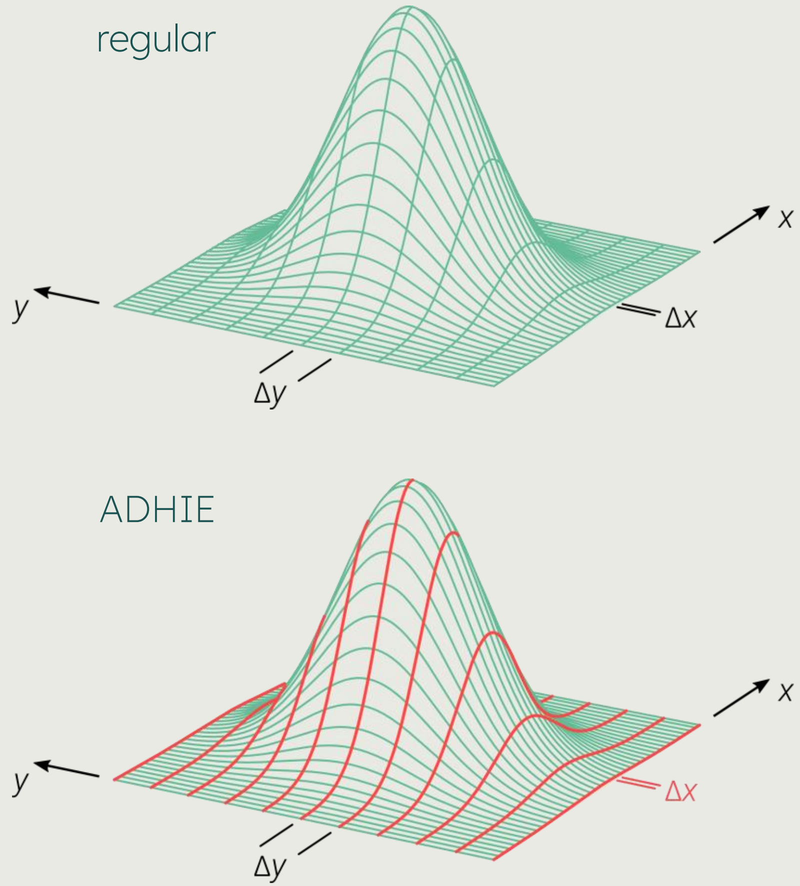
Have to solve a linear-system of equations, but relaxed stability criterion:

$$\Delta t < \frac{2\hbar}{\frac{2\hbar^2}{m}\frac{1}{\Delta y^2} + V}$$

Small steps Δx can be eliminated.

Much higher time step Δt.

Decreases simulation time from 2364s to 167s (14x faster).



Solving the time-dependent Schrödinger equation.

Transmission and current.

Transmission probability calculated with:

$\Psi_{ana}(E)$: Energy spectrum of incoming wave function.

$\Psi_{calc}(E, V_{CE})$: The Fourier transform of time-domain wave function behind barrier for applied voltage V_{CE}.

$$T(E, V_{CE}) = \left| \frac{\Psi_{\text{calc}}(E, V_{CE})}{\Psi_{\text{ana}}(E)} \right|^2$$

Current according to [1]:

$$I(V_{CE}) = \frac{2e}{\pi\hbar}\sqrt{E_0}\int_{E_0}^{\infty} T(E, V_{CE})(E - E_0)^{-\frac{1}{2}} \left(\frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} - \frac{1}{1 + \exp\left(\frac{E - E_F - eV_{CE}}{k_B T}\right)} \right) \mathrm{d}E$$

[1] R. Ragi, R. V. T. da Nobrega, and M. A. Romero, "*Modeling of peak voltage and current of nanowire resonant tunnelling devices: case study on InAs/InP double-barrier heterostructures*," Int. J. Numer. Model. Electron. Networks, Devices Fields, vol. 26, no. 5, pp. 506–517, Sep. 2013.

Variability Analysis.

Transmission probability.

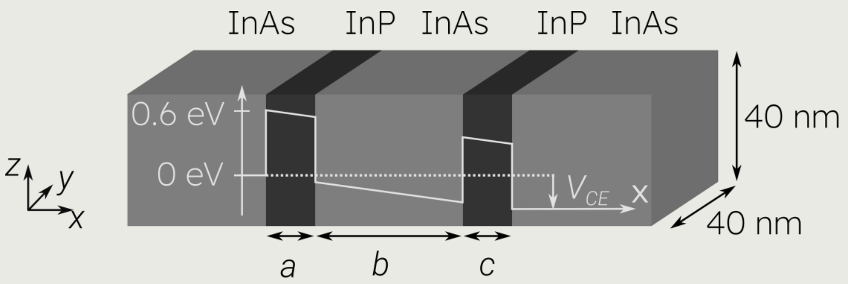
Monte Carlo analysis

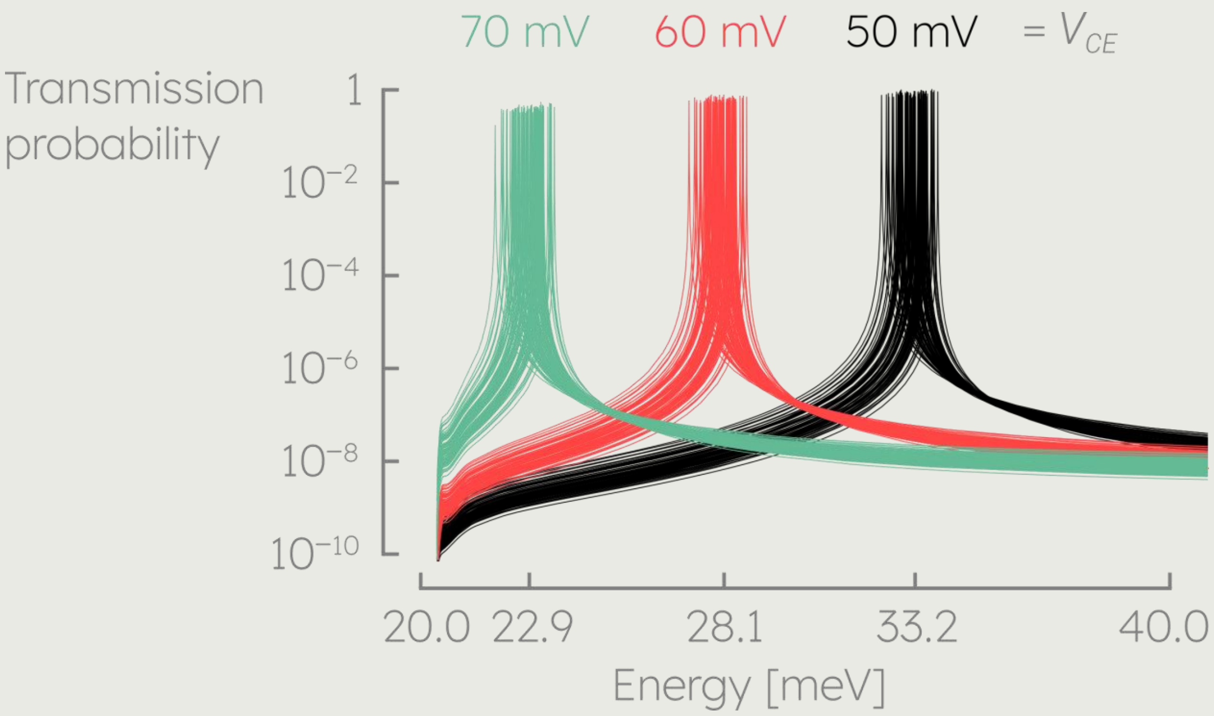
Sample barrier thicknesses *a* and *c* from bivariate Gaussian distribution with:

$$\mu_a = \mu_c = 5.0\text{nm}, \quad \sigma_a = \sigma_c = 0.1\text{nm} \quad \text{and} \quad \rho = 0.8$$

Perform simulation for every sample at every applied voltage V_{CE}.

Calculate the transmission probability at voltage V_{CE}.





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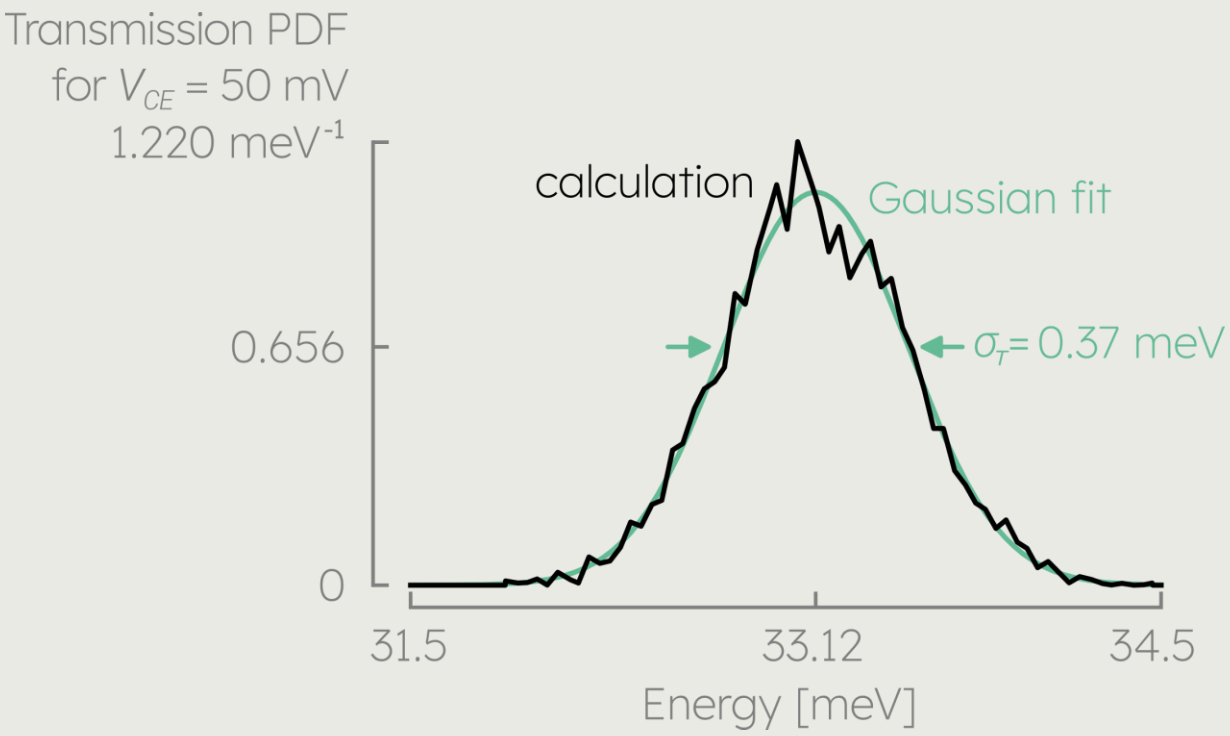
Calculate the transmission probability at voltage V_{CE}.

Determine the position of the transmission peak.

$$\text{mean } \mu_T = 33.12 \text{ meV and std } \sigma_T = 0.37 \text{ meV}$$

Need many thousands of samples.



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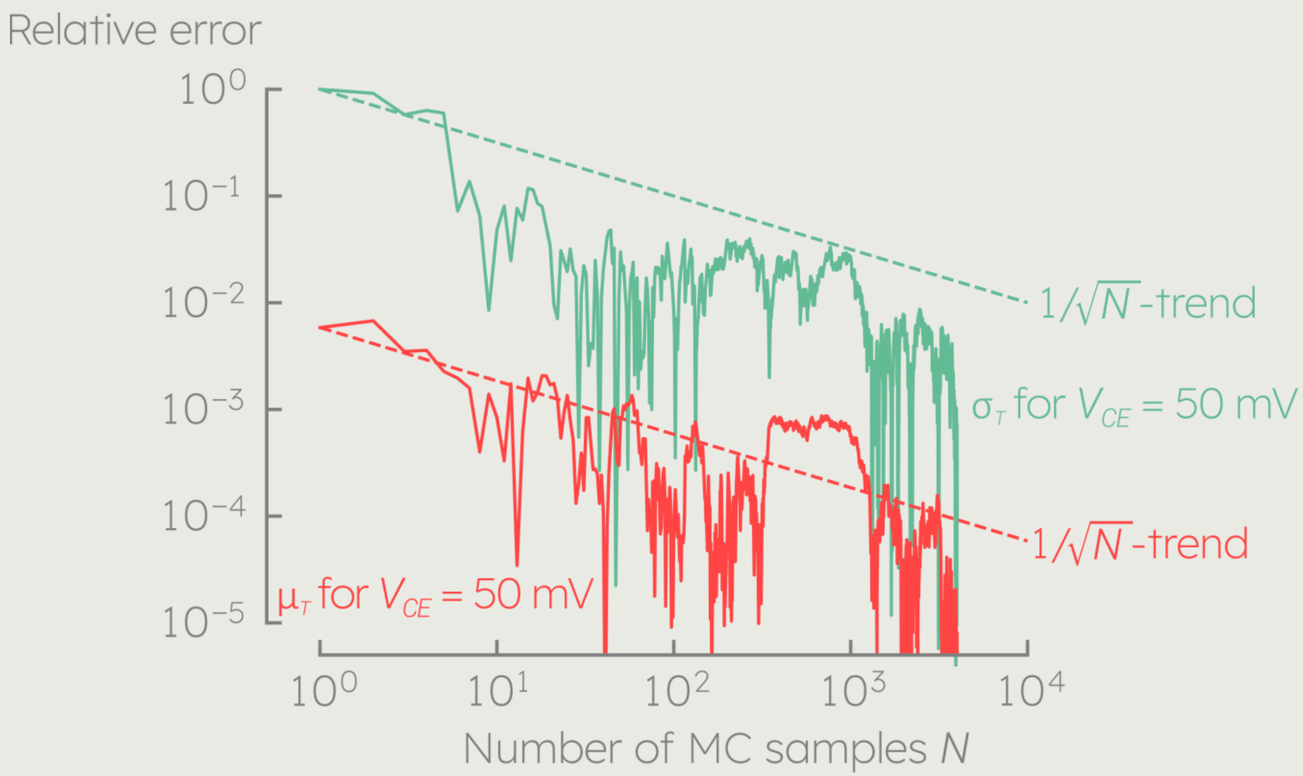
Relative error goes down as $1/\sqrt{N}$.

Not possible without ADHIE.

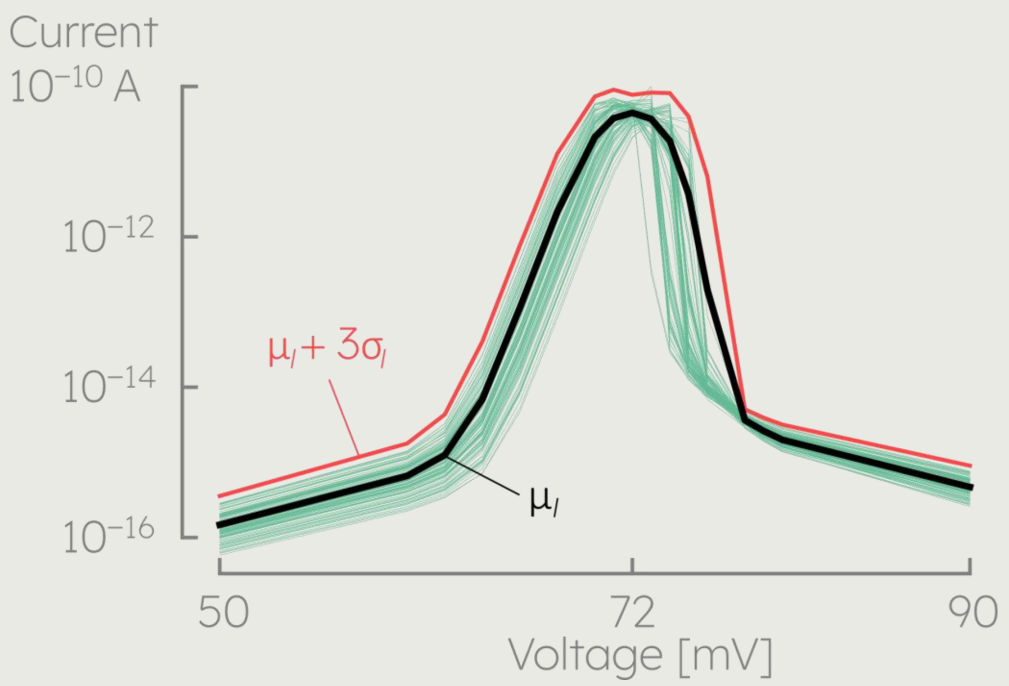


Variability Analysis.

Current-Voltage.

Mean current μ_I exhibits peak at 72 mV.

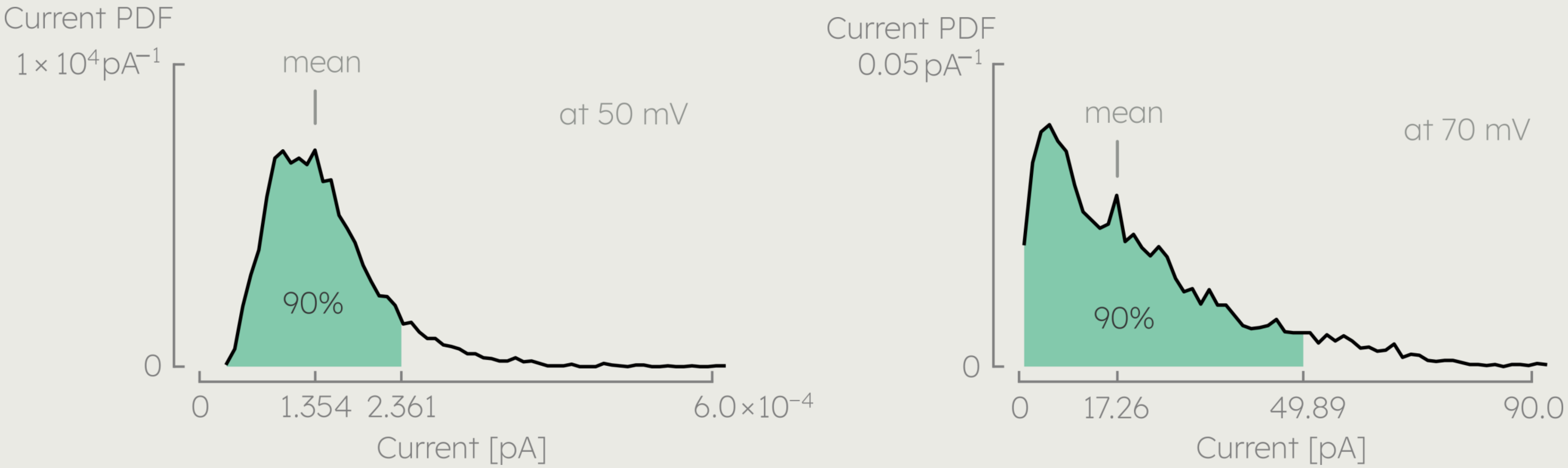
$\mu_I + 3\sigma_I$ line is much higher than μ_I, indicating a considerable variability of the current through the RTD.



Variability Analysis.

Current-Voltage.

Current probability density function at different applied voltages V_{CE}.



Conclusions.

Charge transport through nanowire resonant-tunnelling diode.

Simulated with the novel ADHIE-FDTD method.

Performed variability analysis of barrier thickness with Monte Carlo.

A complete statistical description is needed to understand and design more robust devices.

Showed that ADHIE-FDTD is fast enough to run several thousands of simulations.

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