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Modeling Assisted Atomic Precision Advanced Manufacturing (APAM) Towards Room Temperature Operation

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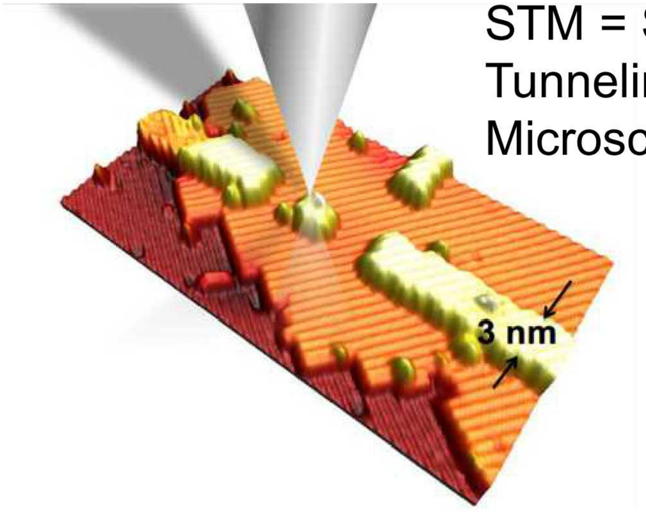
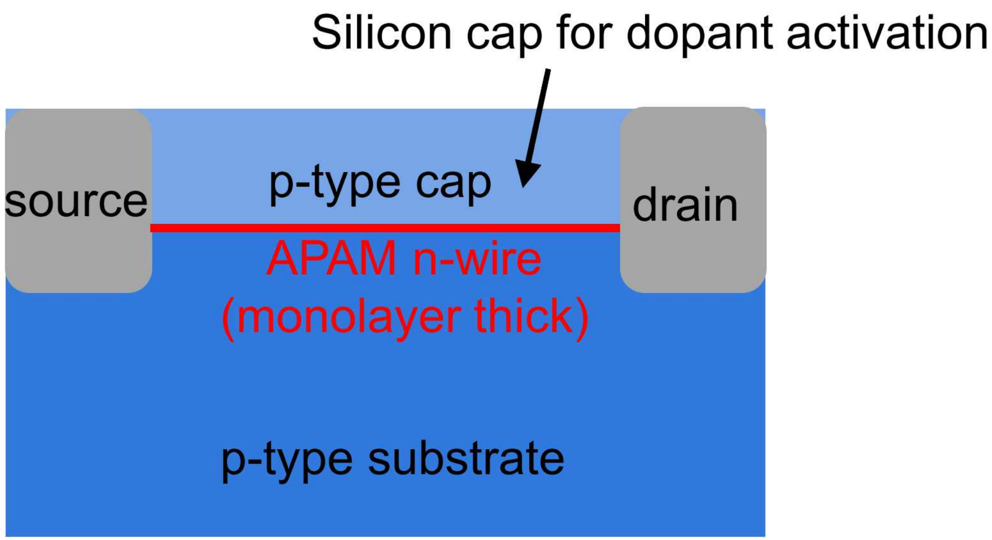
Atomic Precision Advanced Manufacturing (APAM)

APAM is a process of area-selective dopant incorporation at the atomic scale



STM = Scanning Tunneling Microscope

Example of APAM device



APAM key properties (vs. standard processing)

- Atomic precision
- Extremely high density of dopants

APAM can unlock revolutionary opportunities in microelectronics from the atomic physical limit

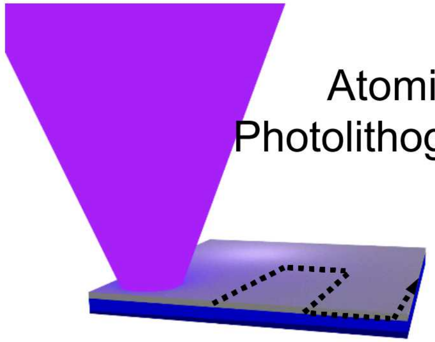
Challenges of Current APAM Technology

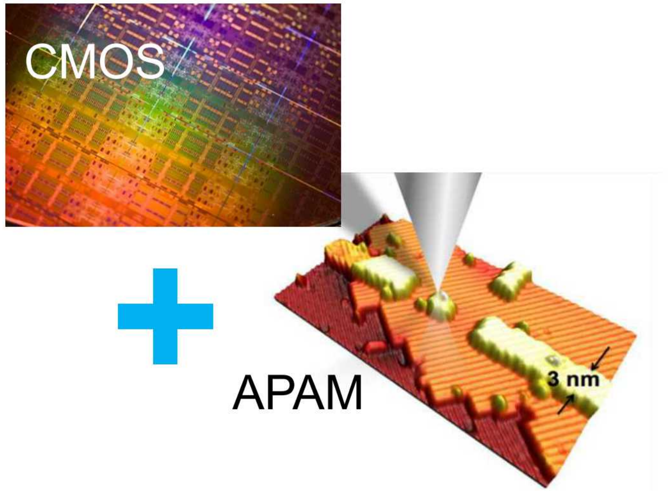
Key challenges of current APAM technology:

- X APAM devices work only at cryogenic temperature
- X APAM p-type devices remain an outstanding challenge
- X APAM needs be integrated with CMOS
- X STM lithography too slow for any production

An interdisciplinary experimental and modeling team at Sandia National Laboratories work closely together to address these challenges:

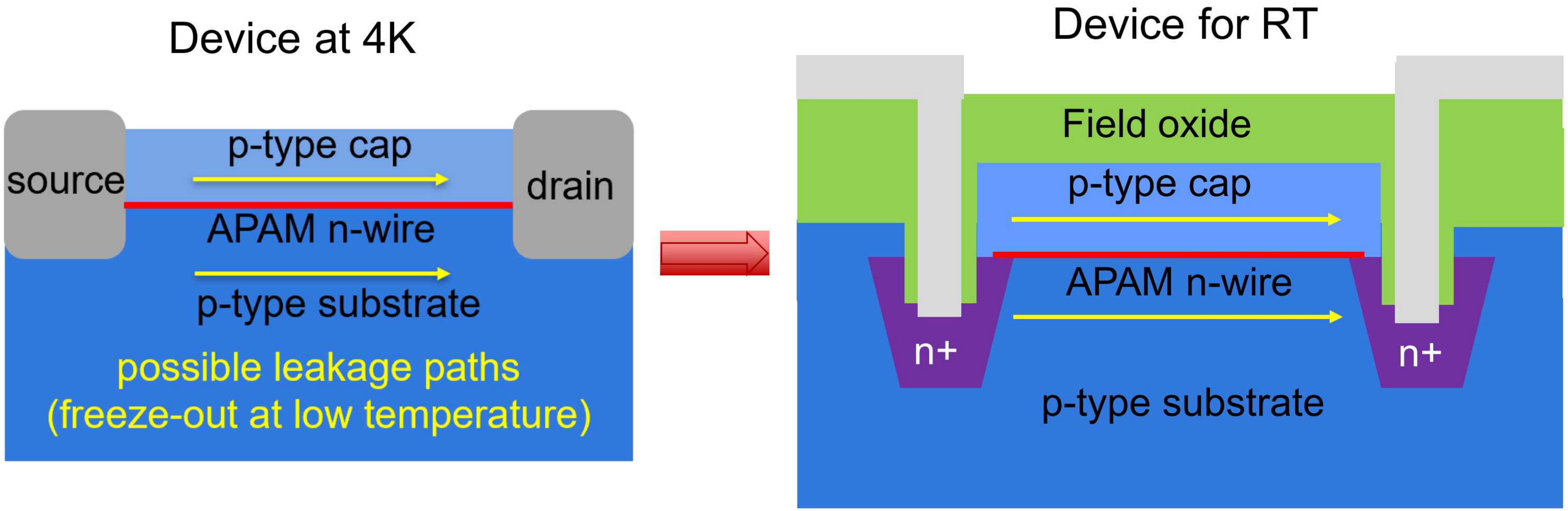
- ✓ Enable APAM device operation at room temperature (RT)
- ✓ Discover acceptor dopants for APAM
- ✓ Demonstrate APAM-CMOS integration
- ✓ Discover photolithography technology for production scale


Atomic Photolithography



Pathway Toward Enabling APAM Device RT Operation

Implement oxide isolation and leverage p-n junction depletion to minimize leakage paths for RT operation



What is the cap layer doping and thickness requirement to minimize cap leakage at RT?

Device modeling can greatly help to answer this question

Should we use quantum or semiclassical device simulation?

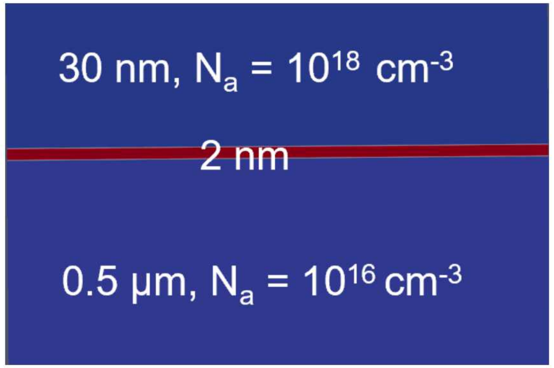
Can semiclassical simulation be used for APAM devices?

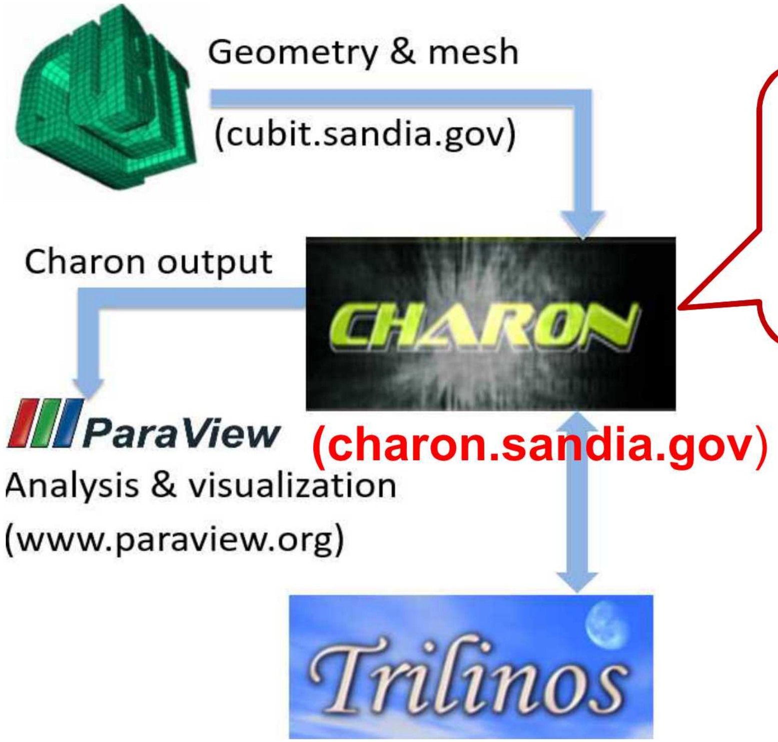
Full quantum transport simulation is extremely computing intensive for complex realistic devices

Can semiclassical simulation be used for APAM devices? (since it is fast for complex devices)

To address this question, we simulated a simplified APAM wire using **Charon** & compared with measured data

Simulated APAM wire



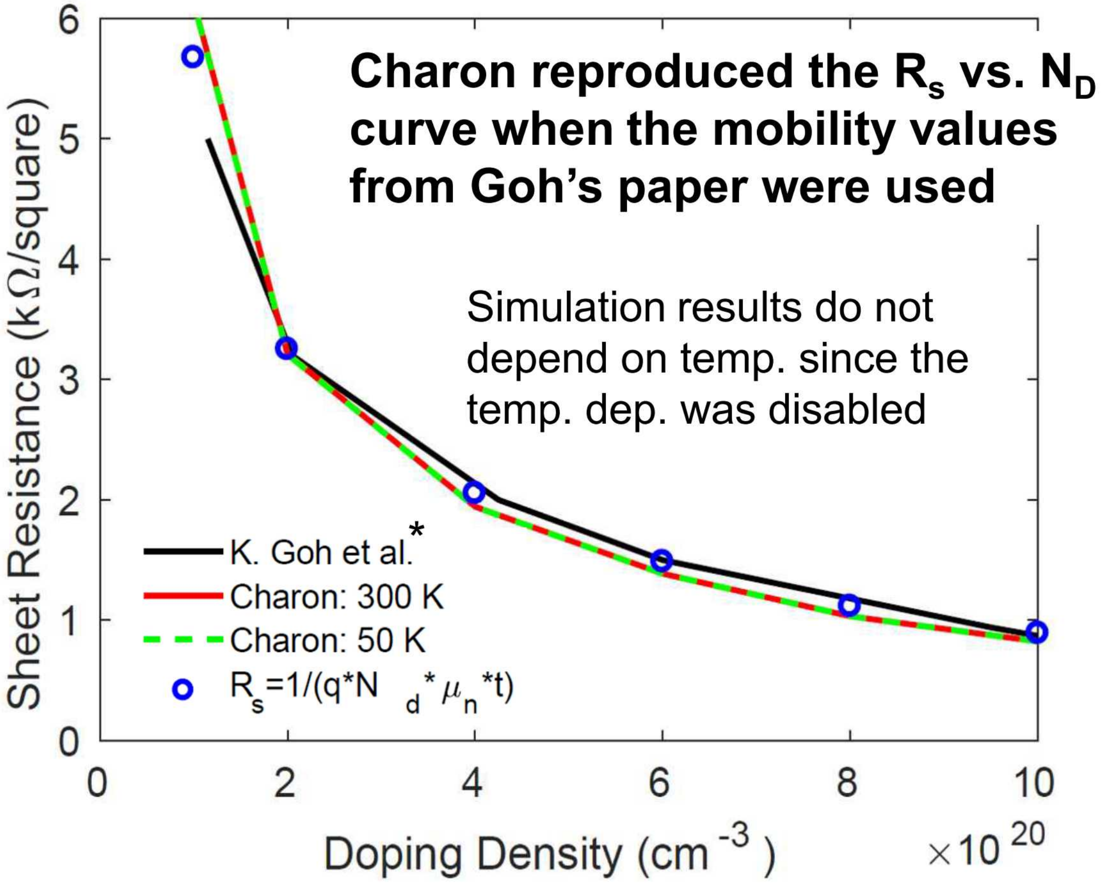


Charon is Sandia's semiclassical TCAD device simulator (2D/3D, MPI-parallel)

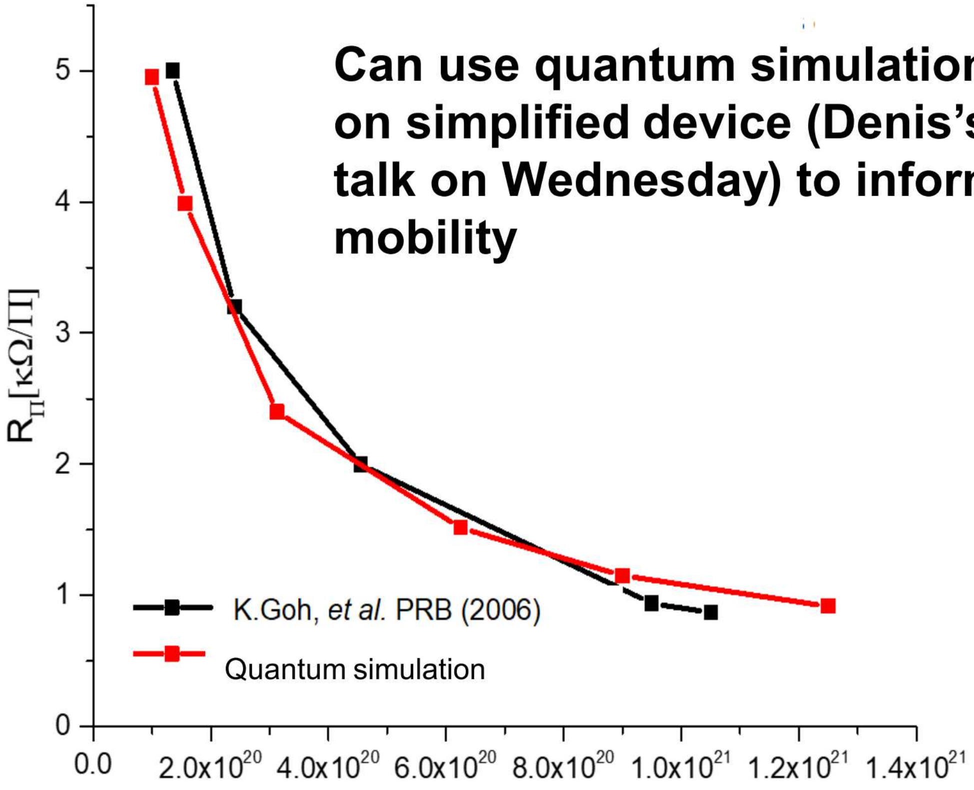
Can semiclassical simulation be used for APAM devices?

Charon reproduced the R_s vs. N_D curve when the mobility values from Goh's paper were used

Simulation results do not depend on temp. since the temp. dep. was disabled



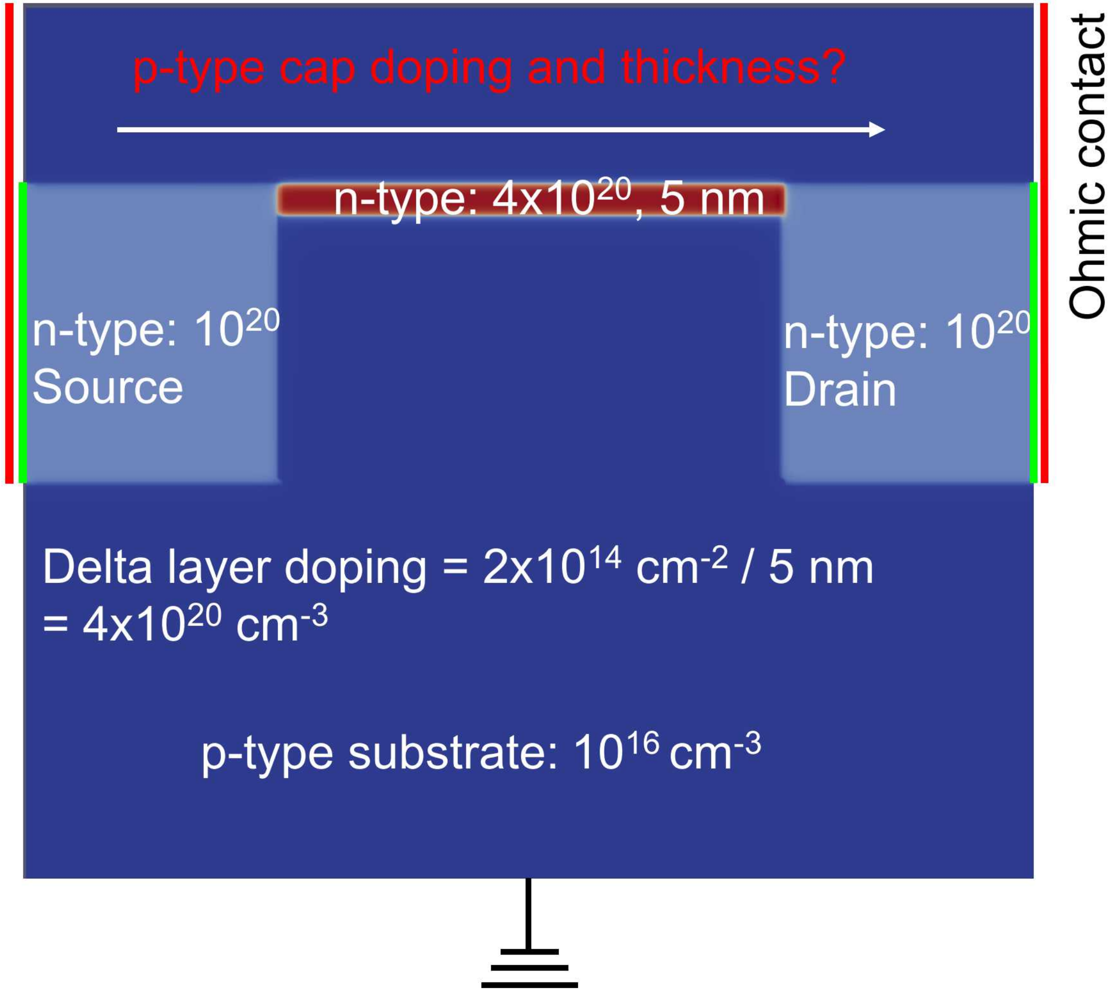
Can use quantum simulation on simplified device (Denis's talk on Wednesday) to inform mobility



Semiclassical simulation can be used for modeling APAM devices as long as the proper mobility values are used.

* K. E. J. Goh, L. Oberbeck, M. Y. Simmons, A. R. Hamilton, M. J. Butcher, Phys. Rev. B **73**, 035401 (2006).

Cap Layer Current Leakage Modeling at RT



What p-cap doping and thickness are needed to minimize current leakage through the cap at RT?

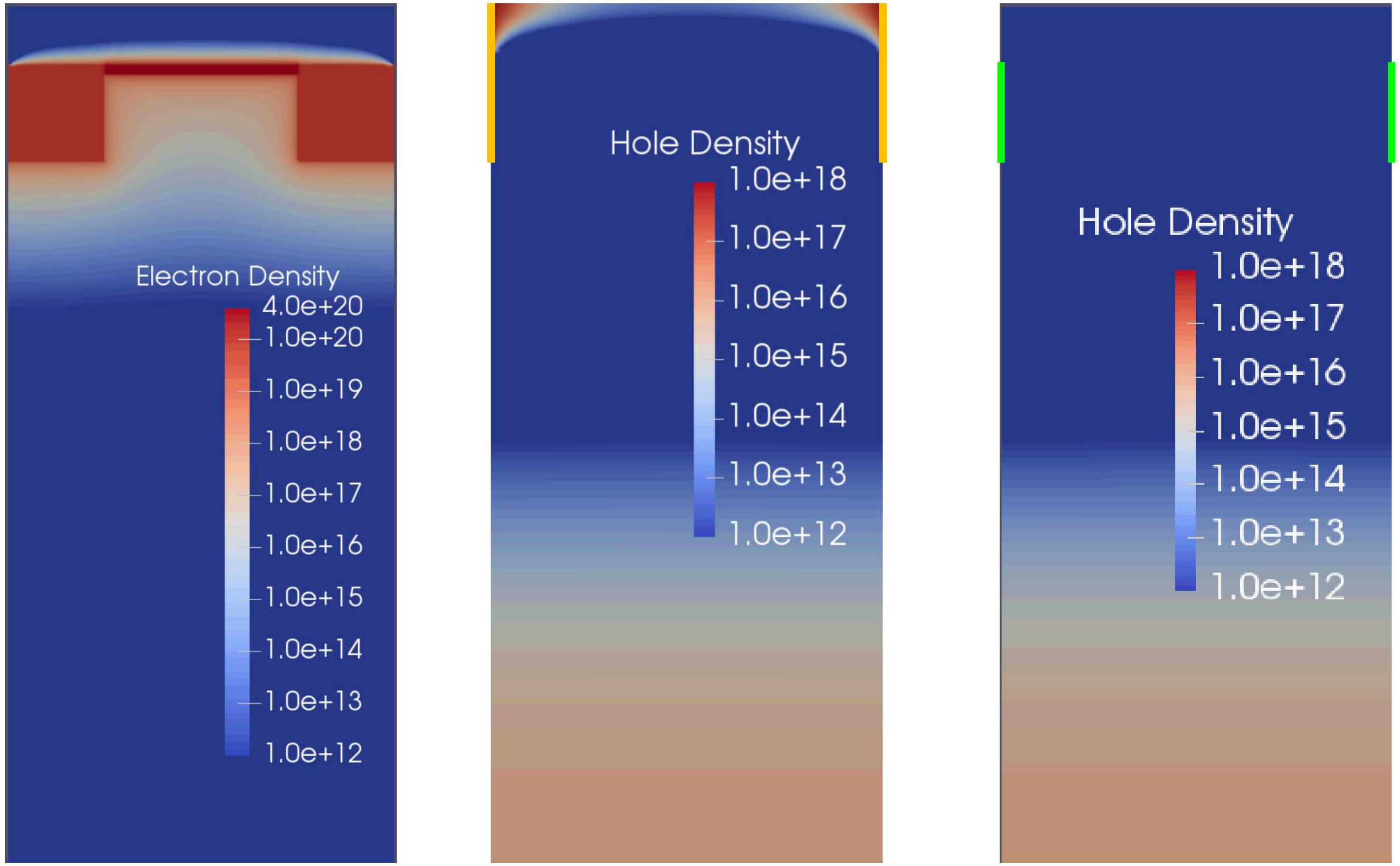
- Doping and thickness in the p-type cap layer are varied
- Current leakage is computed as the current difference between contacting (red lines) and not contacting (green lines) the cap layer
- Simulations were done using **Charon**

(charon.sandia.gov)

Carrier Density for Cap Doping=10^{18} & Thickness=30 nm

Cap contact included

No cap contact



Holes are fully depleted from the cap

negligible leakage

Using the PN junction depletion approximation:

$$W = \sqrt{\frac{2\varepsilon(N_d + N_a)V_{bi}}{qN_dN_a}}$$

we obtain $\boldsymbol{W_p = 37.75\ \mathrm{nm}}$, comparable to the cap thickness

Carrier Density for Cap Doping=10^{19} & Thickness=30 nm

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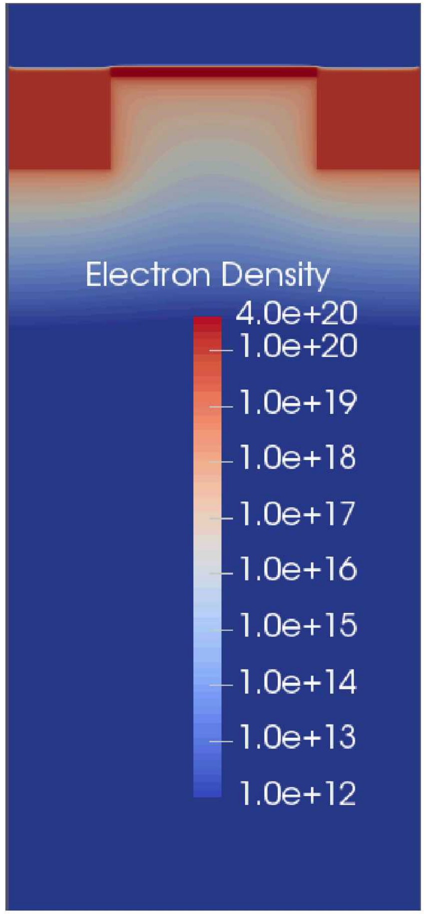
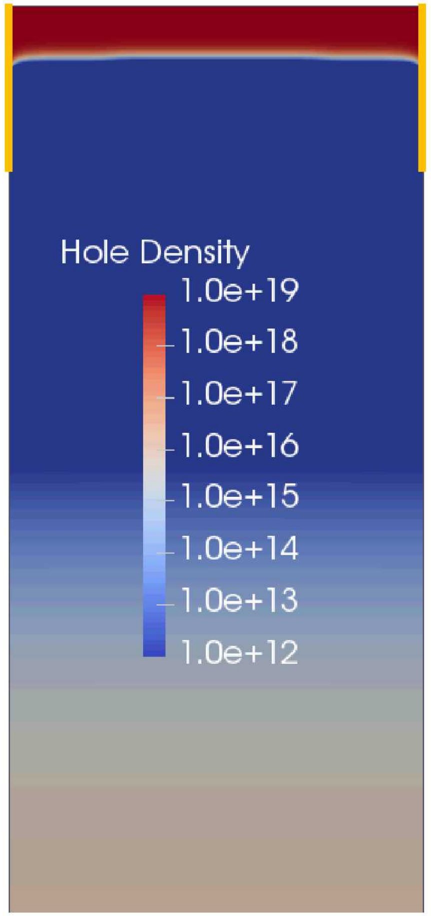
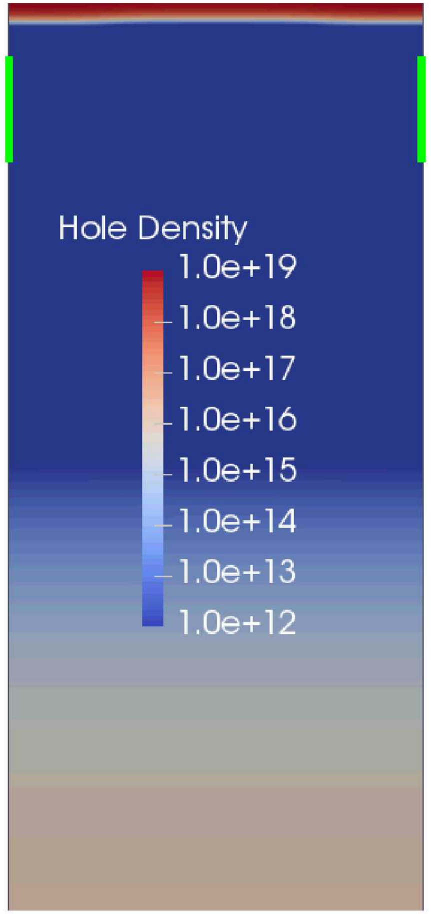
More confined compared to (A)



Cap contact included



No cap contact



Substantial holes reside in the cap
(cap doping = 10^{19} cm^{-3},
cap thickness = 30 nm),

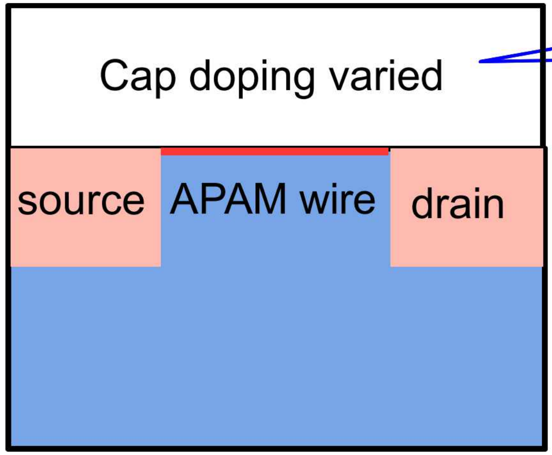
significant leakage

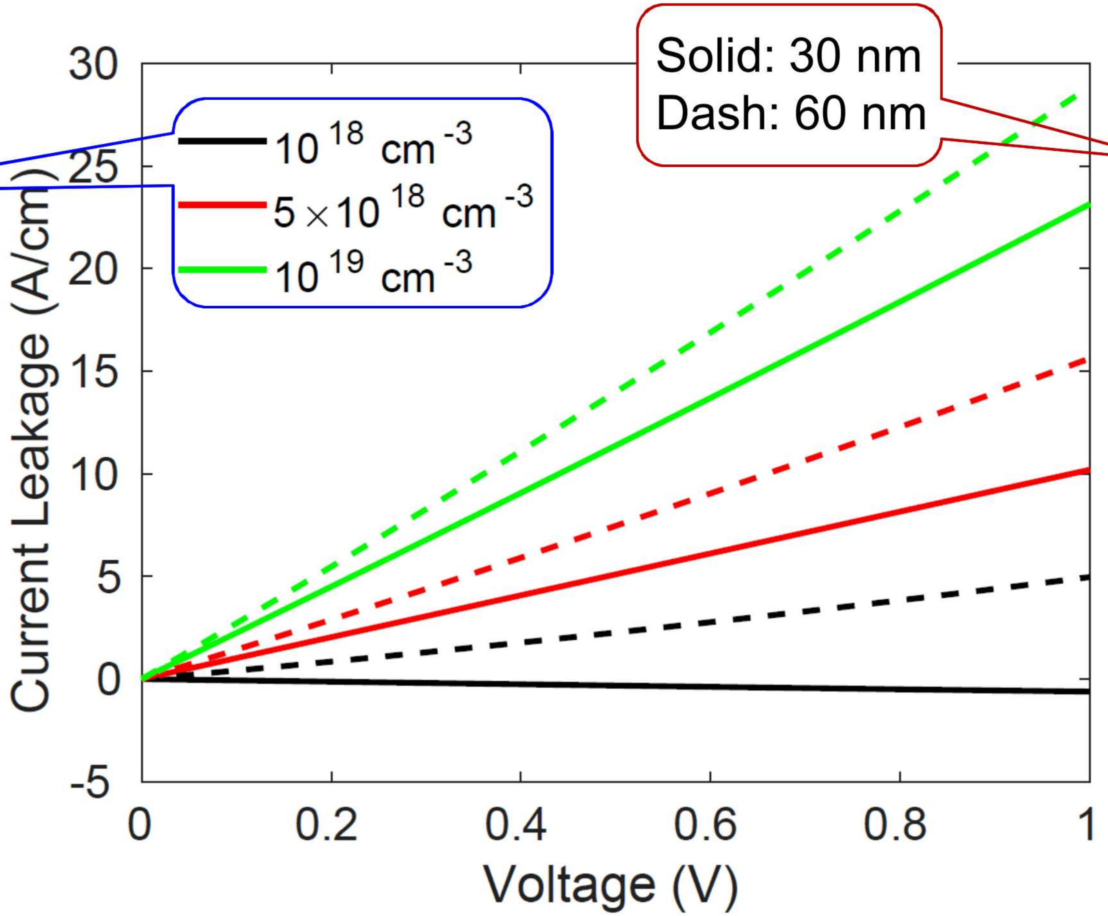
Using the PN junction depletion approximation:

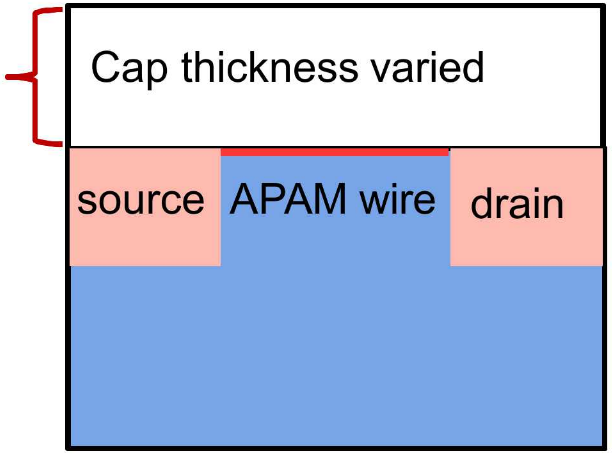
$$W = \sqrt{\frac{2\varepsilon(N_d + N_a)V_{bi}}{qN_dN_a}}$$

we obtain $\boldsymbol{W_p = 12.12\ \mathrm{nm}}$,
smaller than the cap thickness

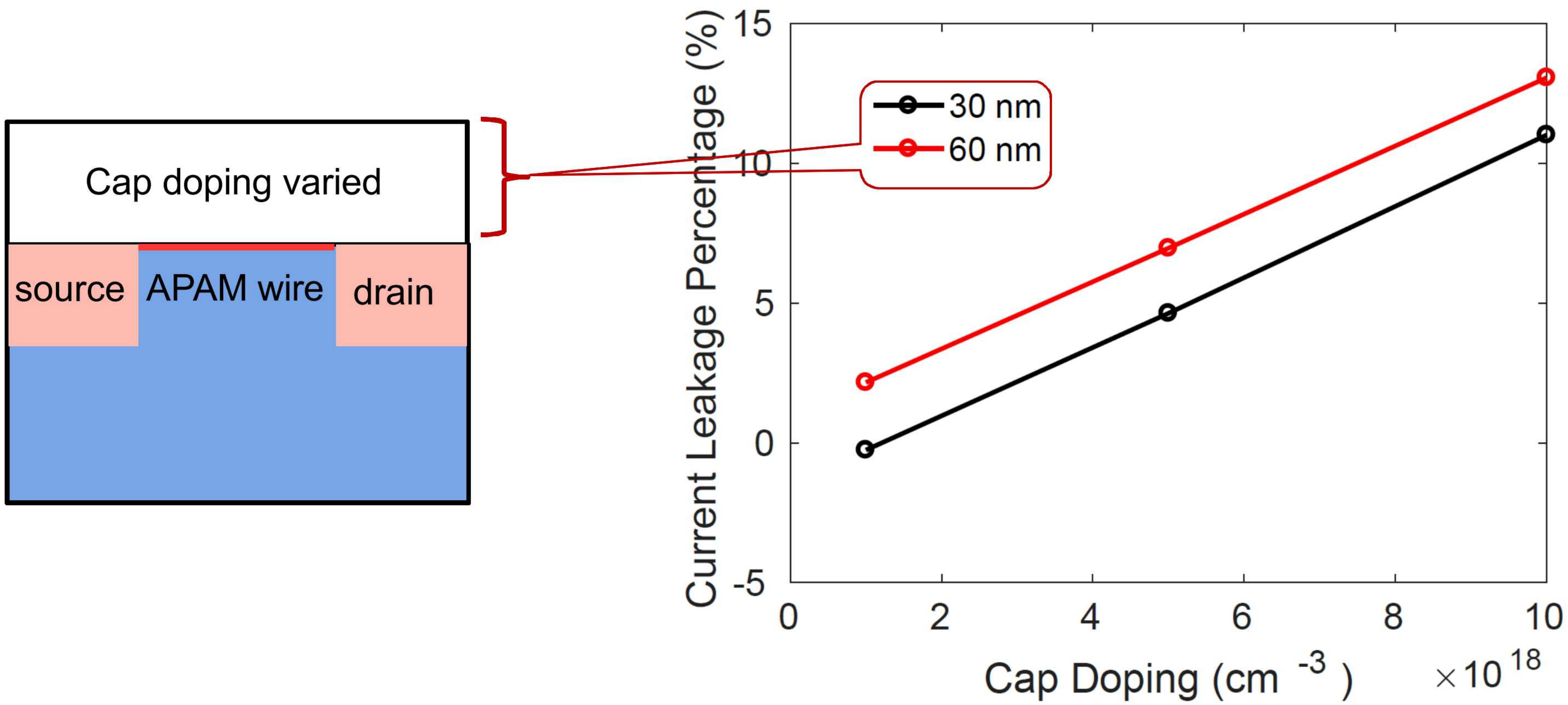
Cap Layer Control for Room Temperature Operation







Cap Layer Control for Room Temperature Operation



- Current leakage through the cap layer strongly depends on cap doping and thickness
- **Require cap doping and thickness engineering to achieve RT operation for APAM devices**

Summary

- Established the **usefulness of semiclassical device simulation** for realistic APAM devices

- Modeling results **provide direct guidance** on cap doping and thickness requirement to the experimental team **to design APAM device for RT operation**

Device for RT