Ab initio calculation of mobility degradation caused by Si-vacancies in SiC/SiO_2 channels

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Introduction

- 4H-SiC for power semiconductor devices
- High density of electrically active defects at the interface
- Consequences:
  - High specific ON-state resistance
  - Instability of the threshold voltage
  - **Lower channel mobility compared to bulk**

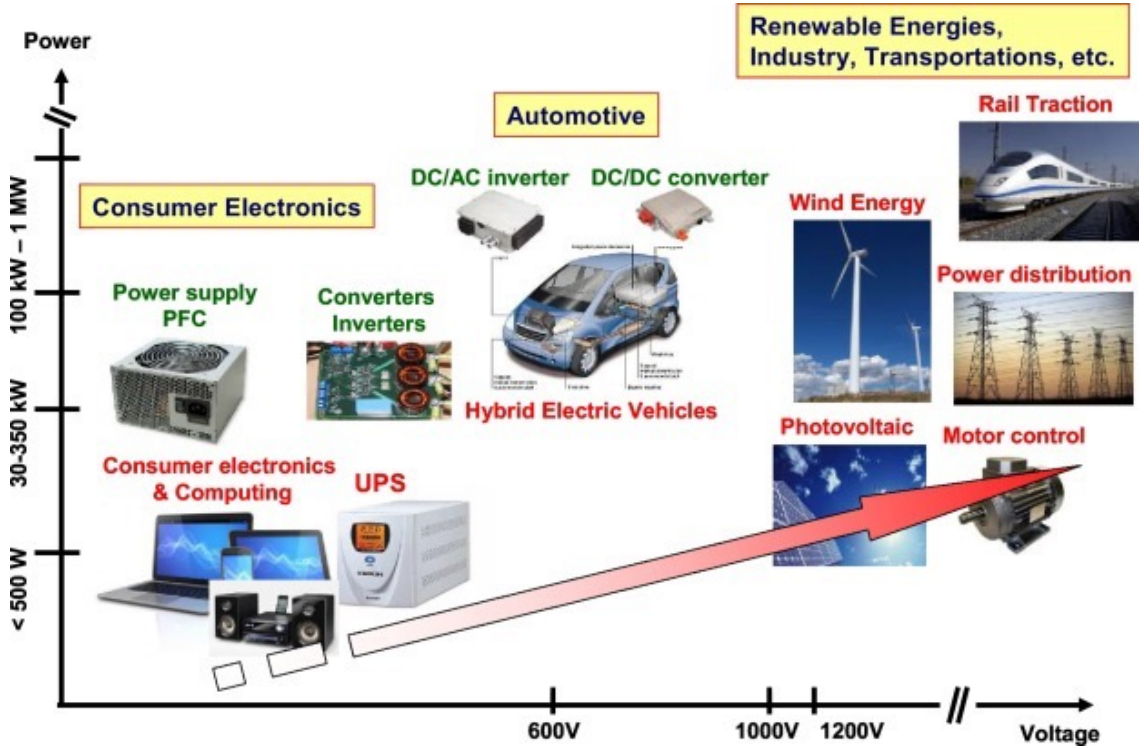
Material comparison

Quantity	4H-SiC	Si
Band gap [eV]	3.26	1.1
Critical breakdown field [MV/cm]	2.4	0.3
Thermal conductivity [W/cm*K]	4.5	1.5

Typical mobility values

	Mobility [$cm^2/(Vs)$]
Bulk 4H-SiC	1000
4H-SiC/SiO_2 channel	80-85

From: K.Tachiki et al. (2021)



From: F. Roccaforte et al. (2018)

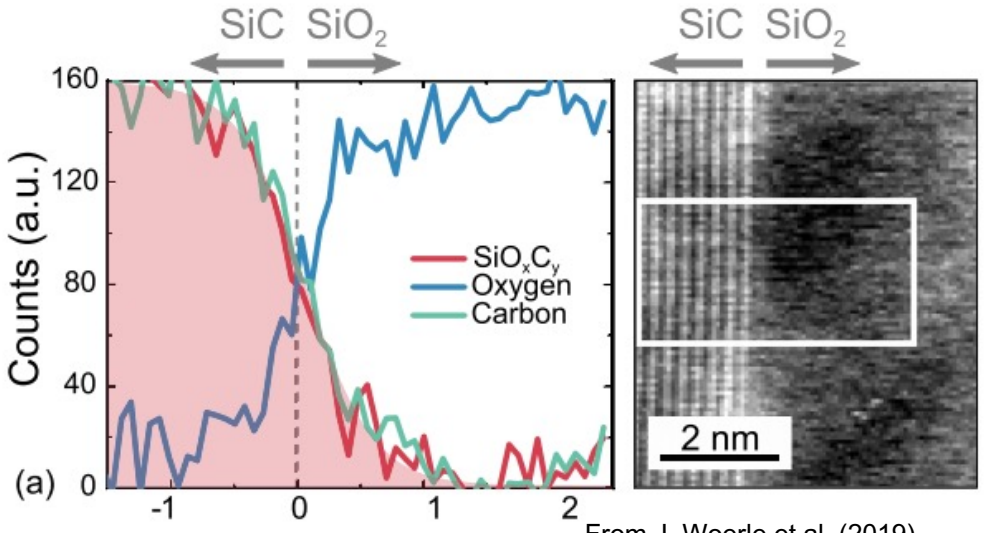
Outline

1. 4H-SiC for power semiconductor and SiC/SiO_2 channels
2. Background
3. Creating SiC/SiO_2 interface structures
4. Calculating Mobility Degradation
5. Conclusion

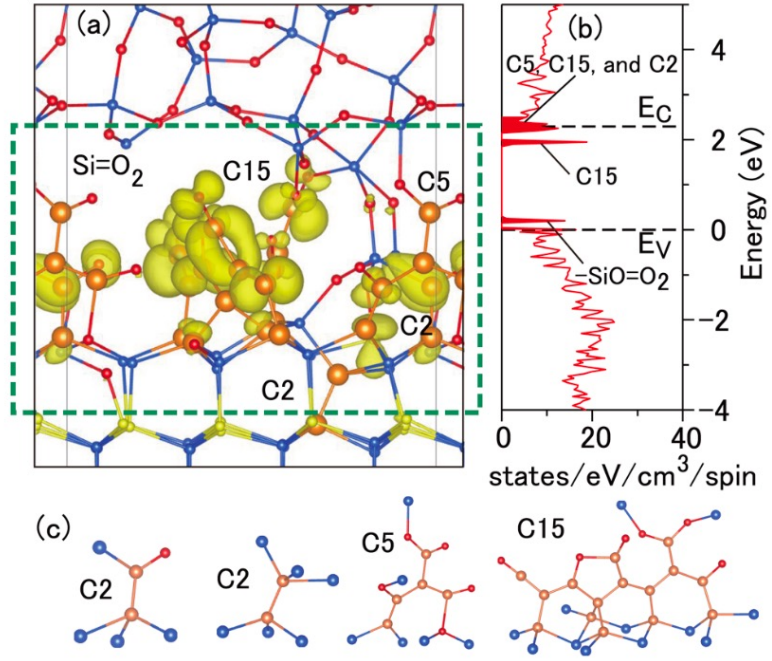
Background

- Mobility degradation is attributed to defects at the SiC/SiO_2 interface.
- **Experimental:** E.g., EELS-Spectroscopy, microscopy (STEM), mobility measurements, etc.
- **Computational:** Mostly DFT studies
- Proposed near-interface traps:
  - Si interstitials
  - C-clusters
  - O vacancies
  - Si vacancies
- **Still open question:** Exact nature of the defect and their influence on mobility

Method used here: NEGF + DFT study of SiC/SiO_2 structures



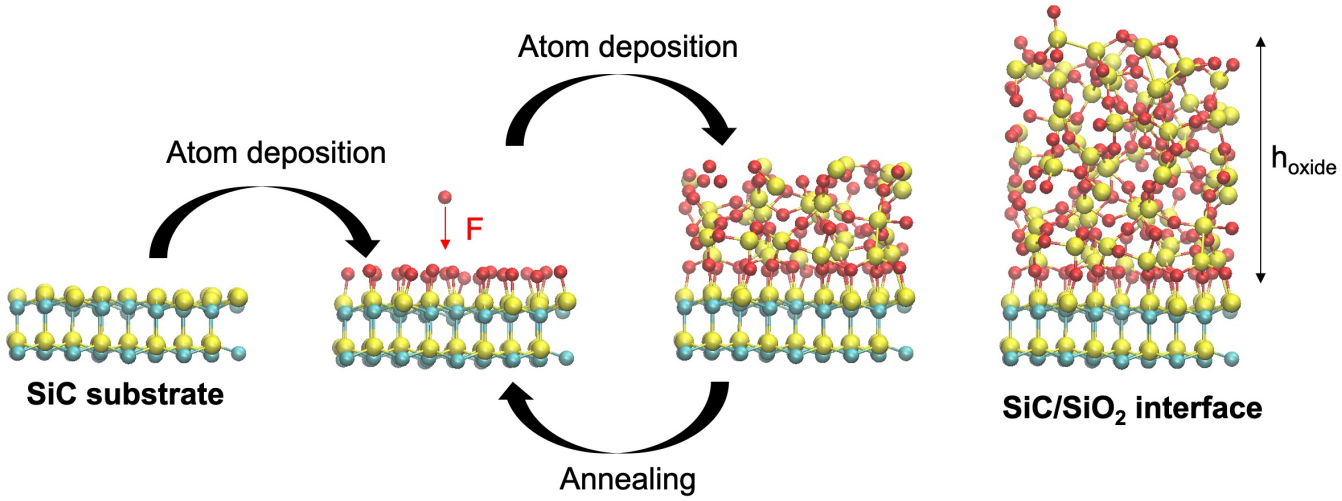
From J. Woerle et al. (2019)



From Y. Kagoyama et al. (2019)

Creating SiC/SiO_2 Interface Structures

- **Challenge:**
  - Create SiC/a-SiO_2 interface with as few defects as possible
- Use these structures to study selected defects
- **Solution:**
  - Layer-by-layer method



Layer-by-layer procedure

- Start with bulk SiC
- Calculate the number of O and Si atoms to get the pre-selected oxide density
- Repeat for n layers for desired height:
  - Randomly place either Si or O atoms within a minimal distance
  - Perform geometry optimization with force field F while applying a force to these atoms towards the SiC surface
- Annealing with force field
- Geometry optimization with DFT(B)

Important Parameters

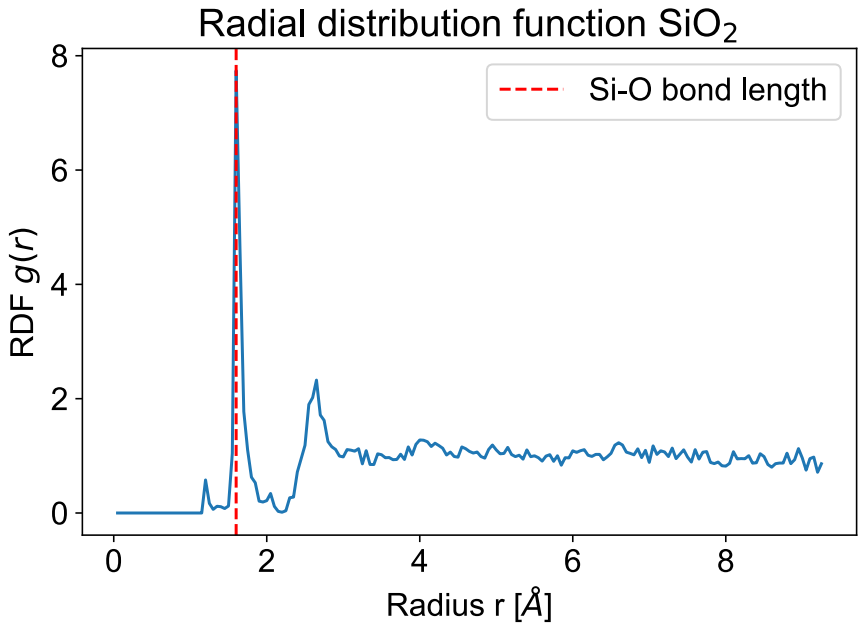
- Oxide density: $2.196*10^{-27}$ kg/Å^3
- Force field: ReaxFF by D.A. Newsome et al.
- External force F: 0.22 eV/Å

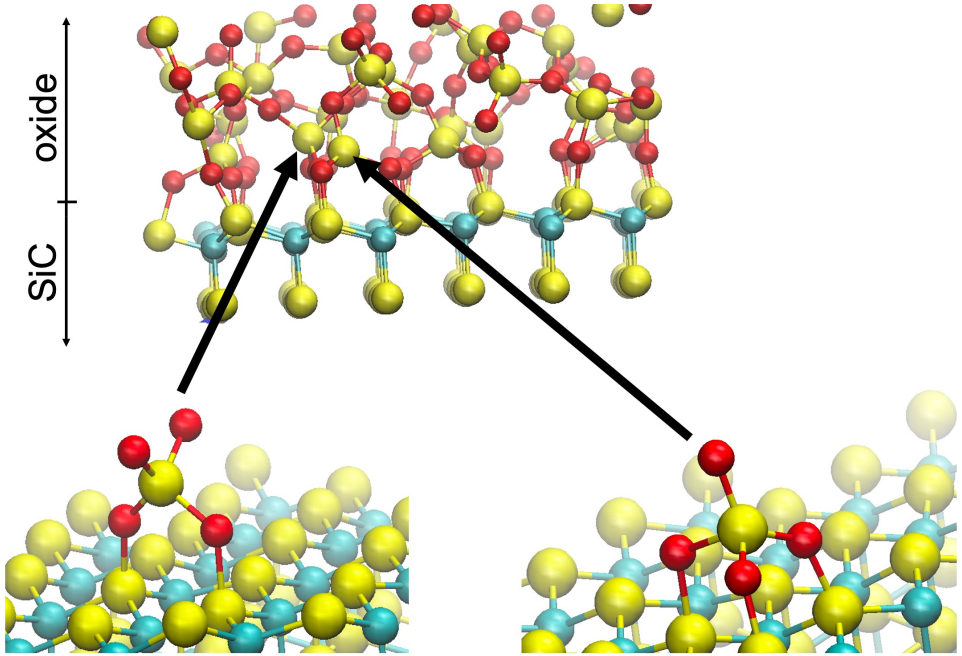
Creating SiC/SiO_2 Interface Structures

- **Pre-sort to avoid:**
  - Dangling bonds
  - Holes in the oxide
  - Hard-to-optimize structures

- **Observed features:**
  - (Almost) no dangling bonds
  - Amorphous SiO_2
  - Tetrahedral SiO_4 structure at the interface

- **Other design parameters:**
  - Unfix some of the SiC layers
  - Introduce defects during LbL process

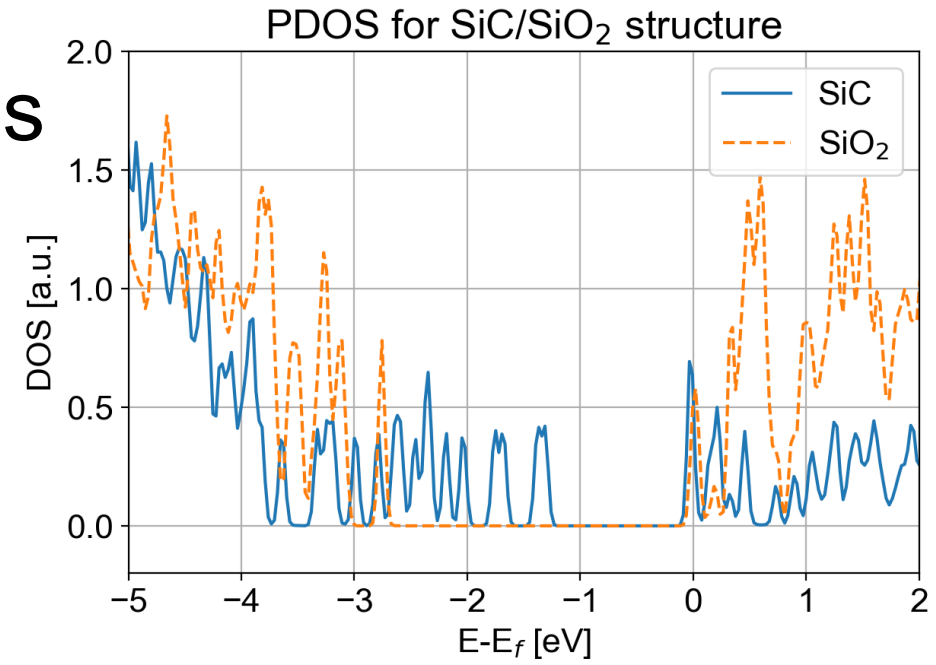


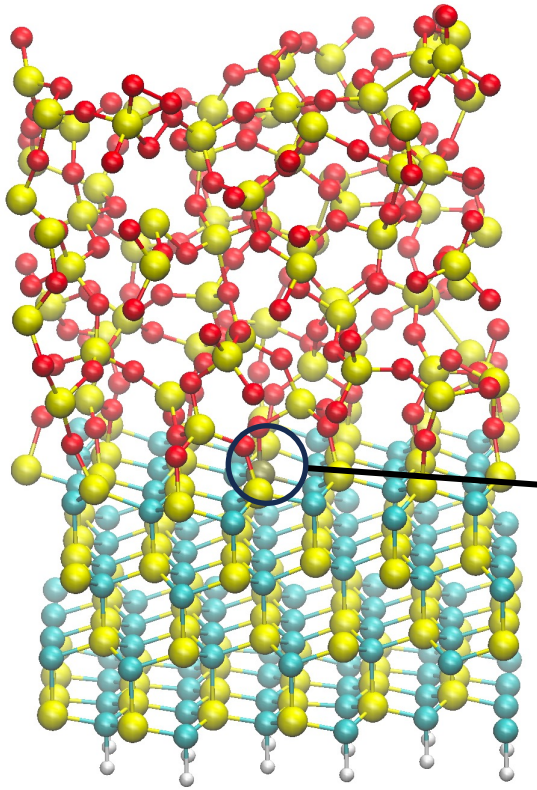


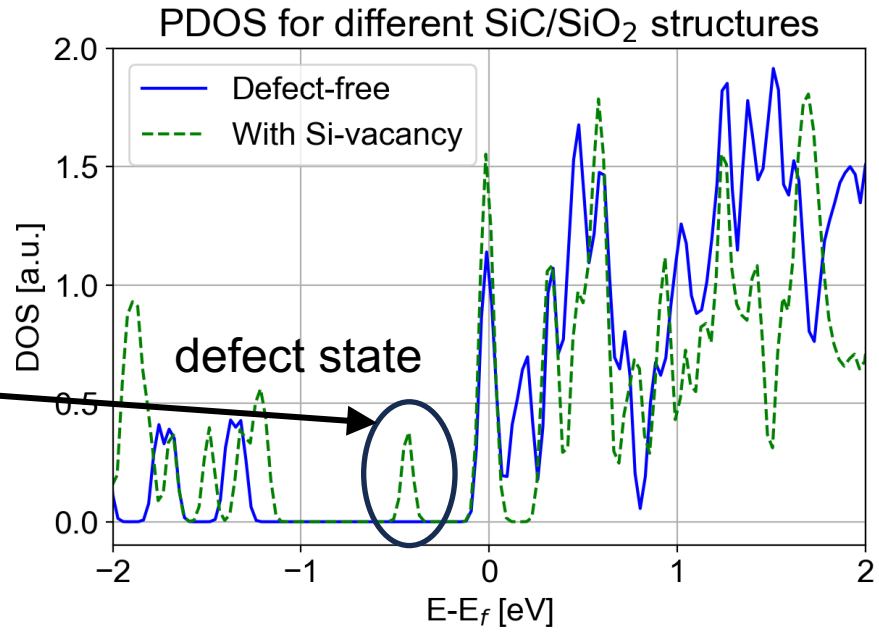
Creating SiC/SiO_2 Interface Structures

- Electronic structure (GGA)
  - Without defect
  - With defect (Si-vacancy)

- Example: Si-vacancy at the SiC/SiO_2 interface



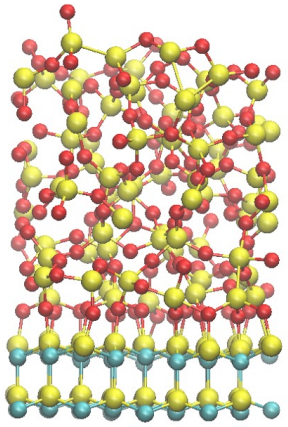




Calculating Mobility

- DFT + NEGF approach for transport
- H-/S-matrix:
  - DFT basis set: 3SP – GTH
- Approximation: Coherent transport, no electron-phonon interaction
- Mobility with dR/dL method: Expect linear increase of the resistance with device length

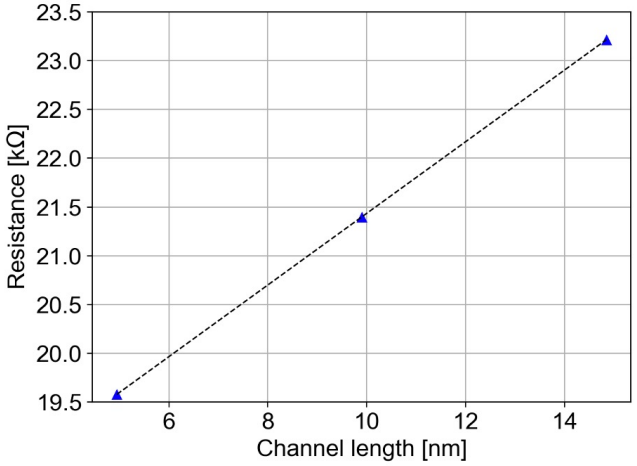
Layer-by-layer procedure



DFT

NEGF - Formalism

dR/dL - Method



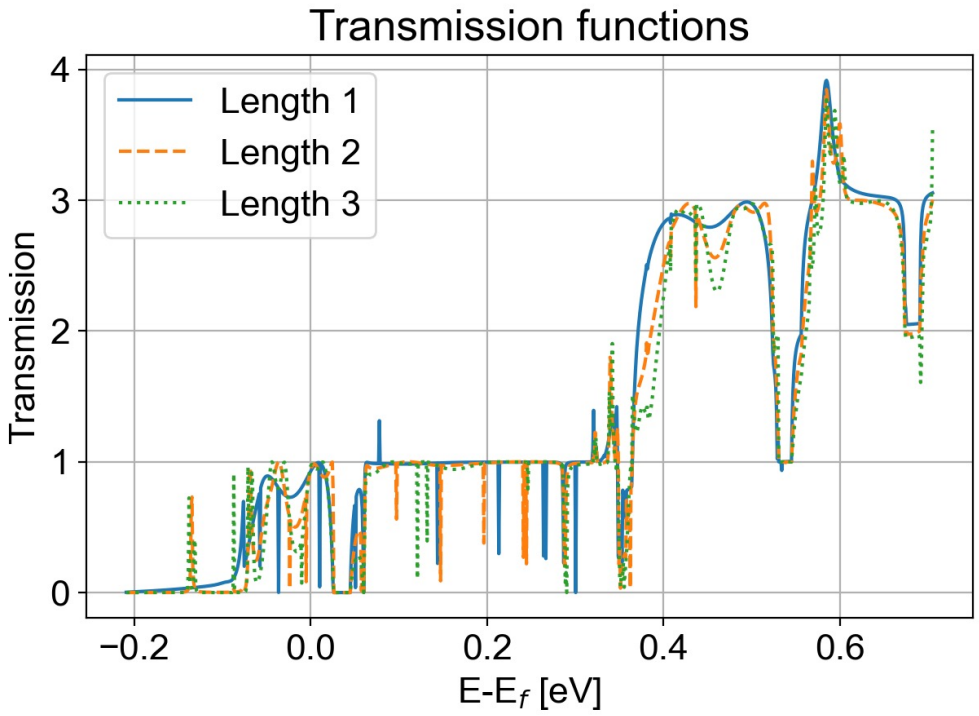
SiC/SiO_2 structure → H-, S-Matrix → Transmission T(E) → Mobility

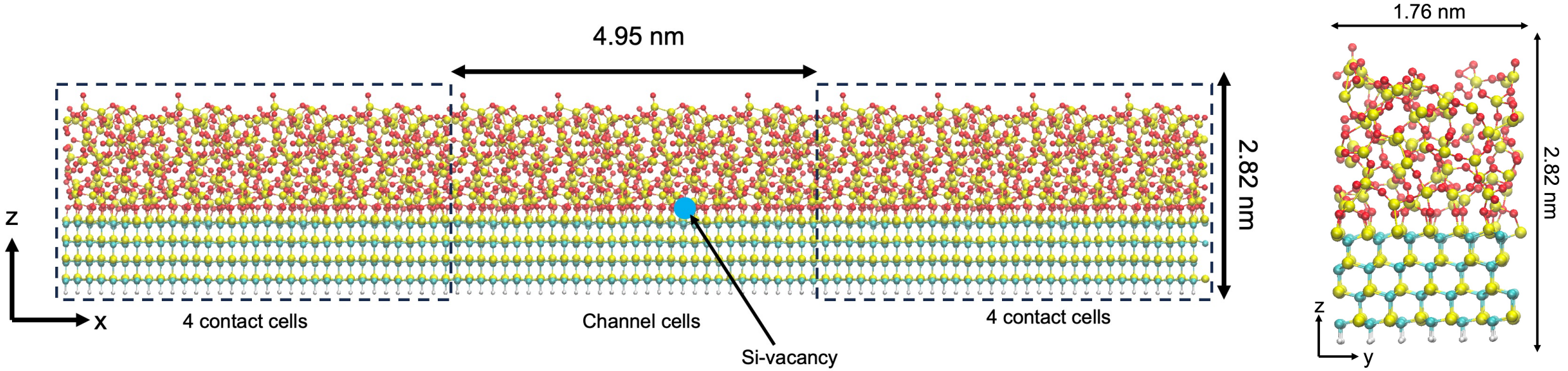
Calculating Mobility

dR/dL- method (K. Rim et al. 2002)

1. Construct unit cell with desired defect concentration
2. Repeat unit cell 1x, 2x, and 3x + add contacts
3. Compute the corresponding channel resistance R
4. Extract channel resistivity and mobility (~dR/dL)

- Defect density in the channel: $1.26*10^{14}$ cm^{-2}
- Charge density: $1.55*10^{14}$ cm^{-2}





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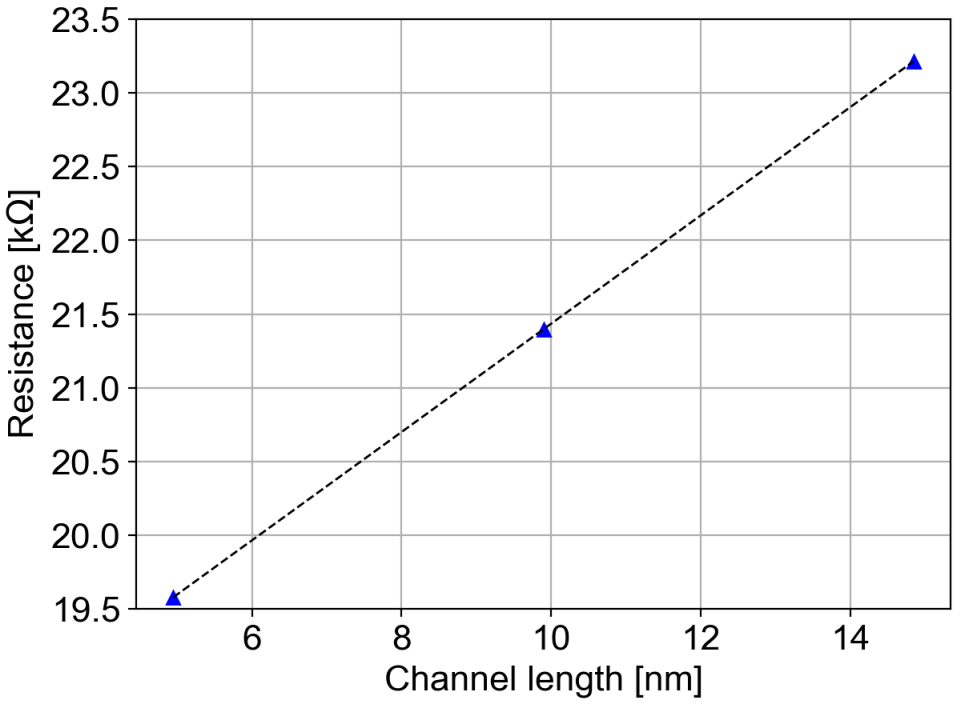
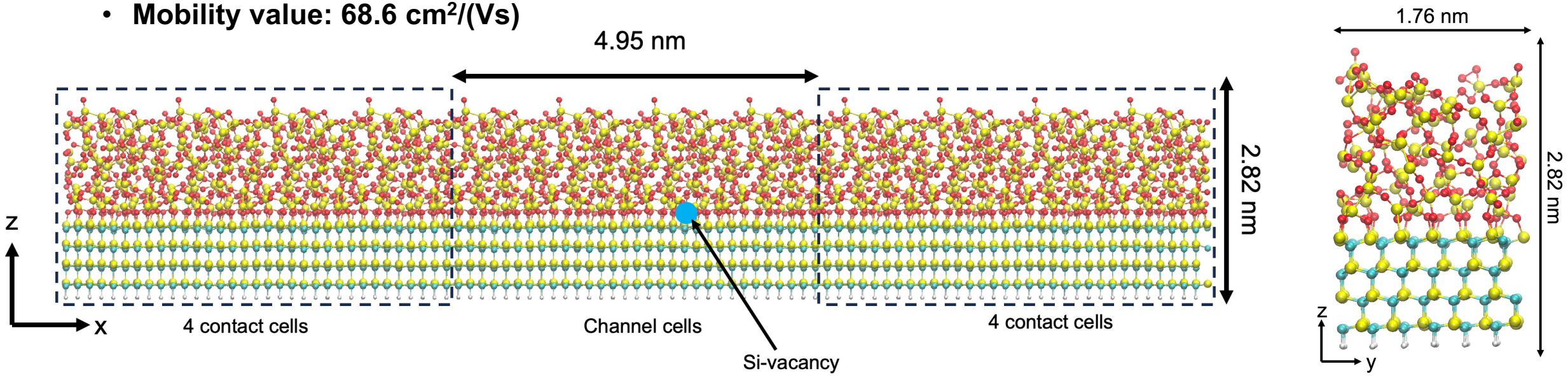
- Defect density in the channel: $1.26*10^{14}$ cm^{-2}
- Charge density: $1.55*10^{14}$ cm^{-2}
- **Mobility value: 68.6 $cm^2/(Vs)$**

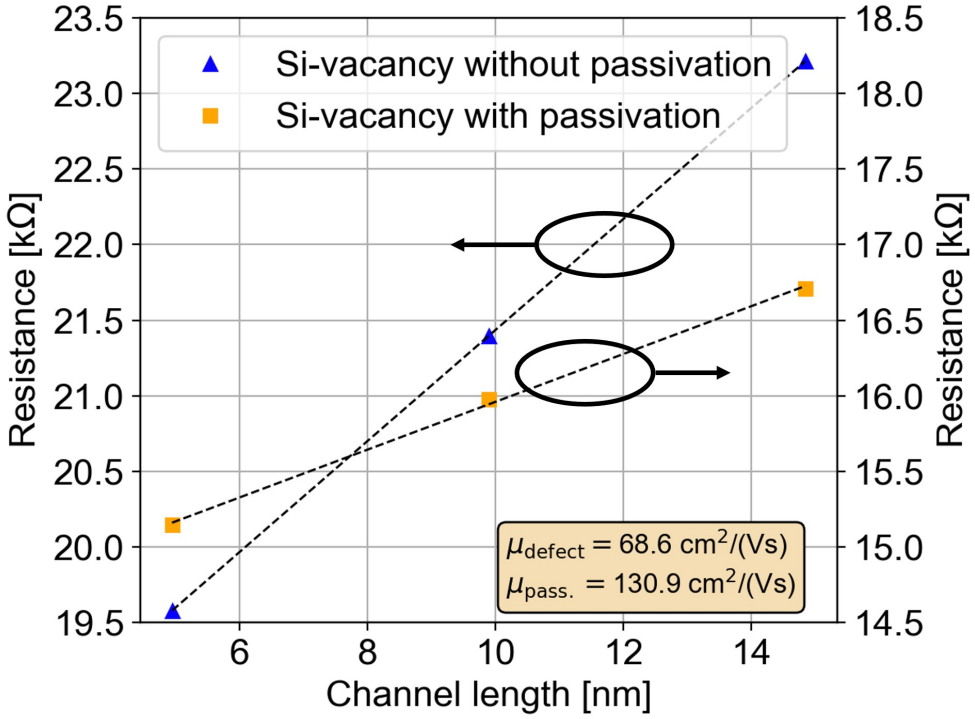


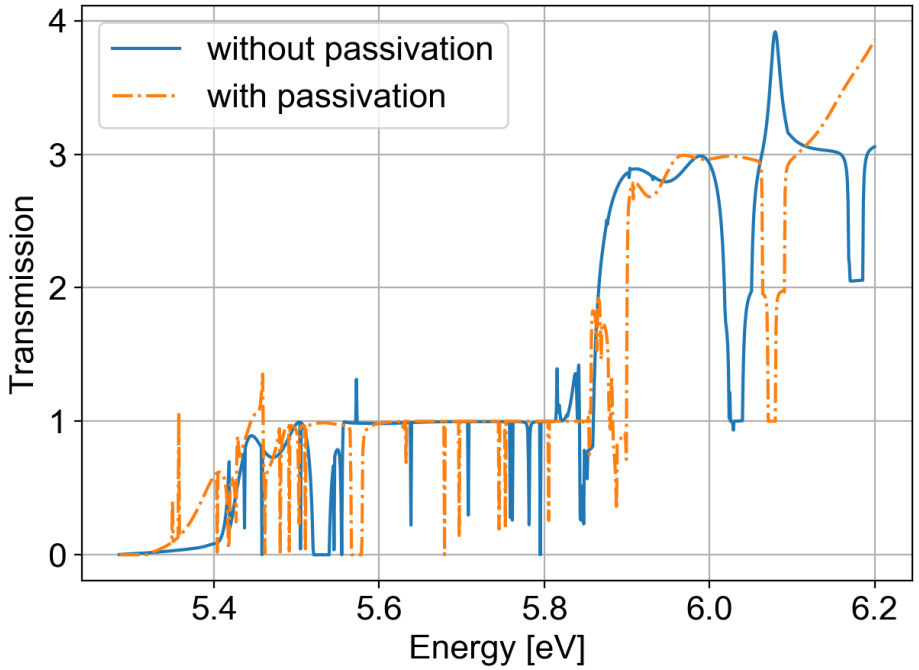


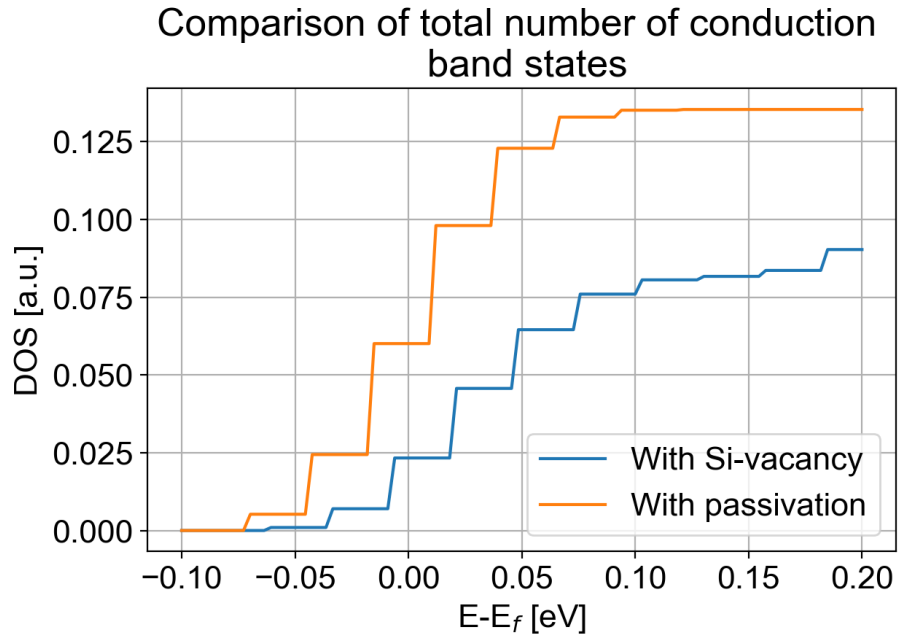
Nitrogen Passivation

- Goal: Increase mobility through nitrogen passivation
- Mobility enhancement thanks to increased transmission
  - Example: For short structure (4.95 nm)

- **Mobility value: 130.9 cm²/(Vs)**







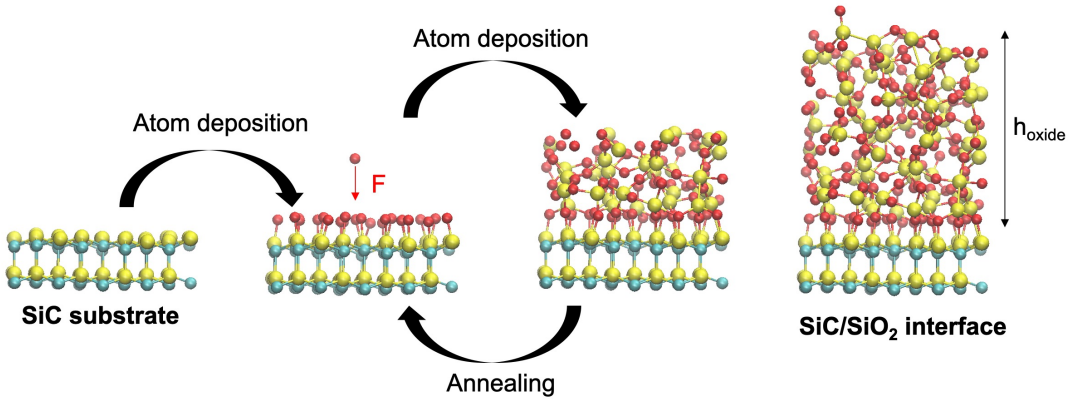
Conclusion

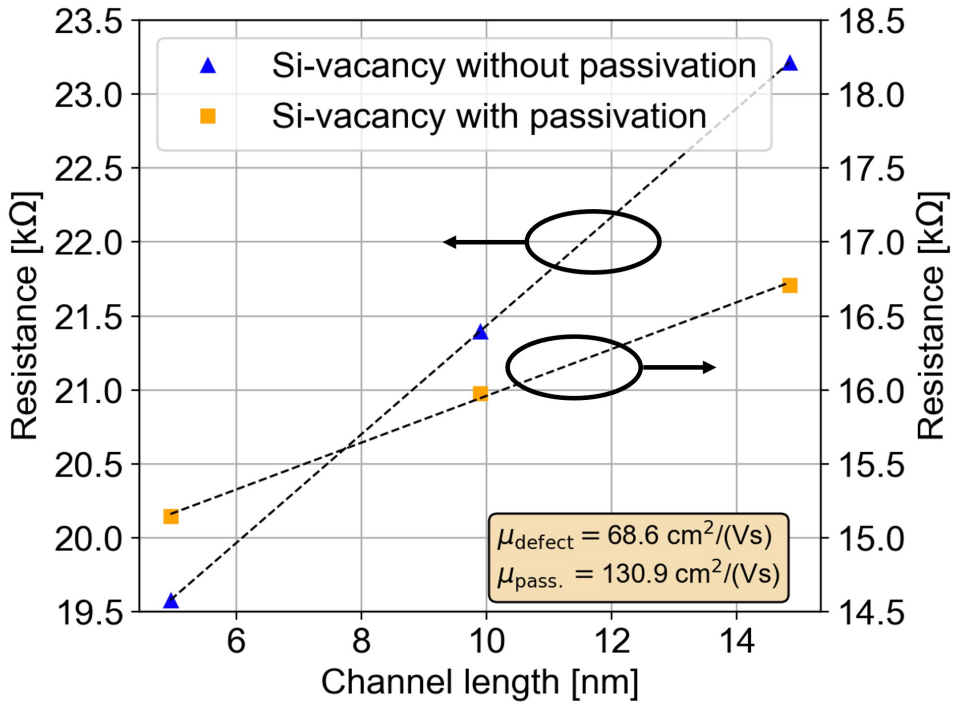
Summary

- Framework to study transport in SiC/SiO_2 structures with goal to increase mobility in power semiconductor devices
- Layer-by-layer approach: SiC/SiO_2 structure creation
- Mobility calculation for Si-vacancy (68.6 $cm^2/(Vs)$) with dR/dL method and N-passivation (130.9 $cm^2/(Vs)$)

Future research directions

- Compile a library of calculated mobility values for different charge states and other defect types like interstitials, carbon chains, etc.
- Investigate different passivation schemes to improve the mobility

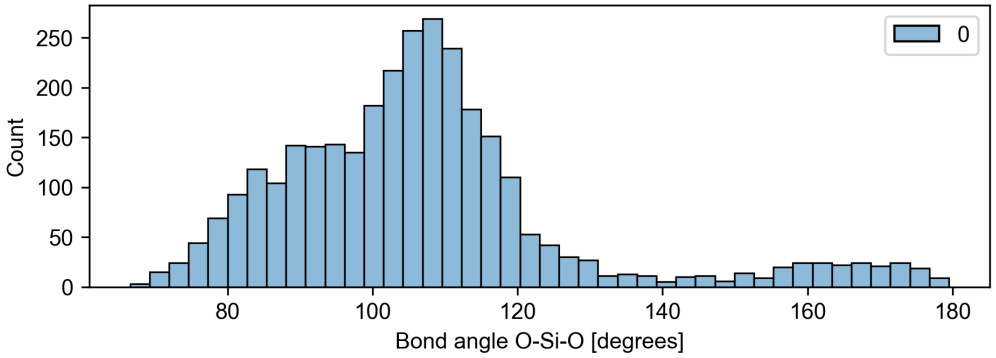


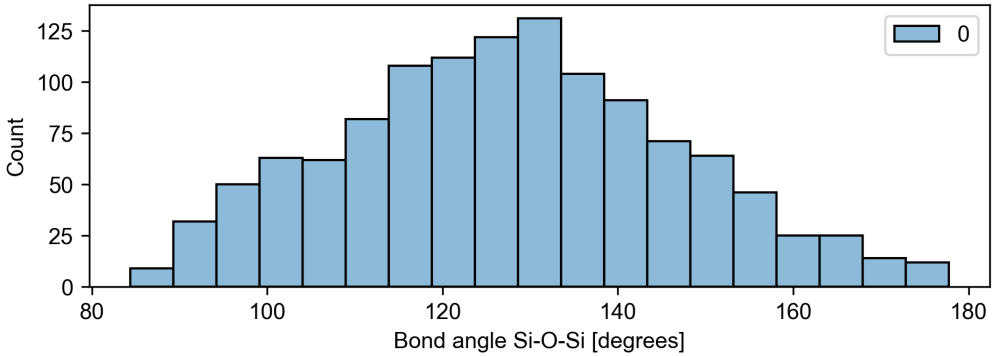


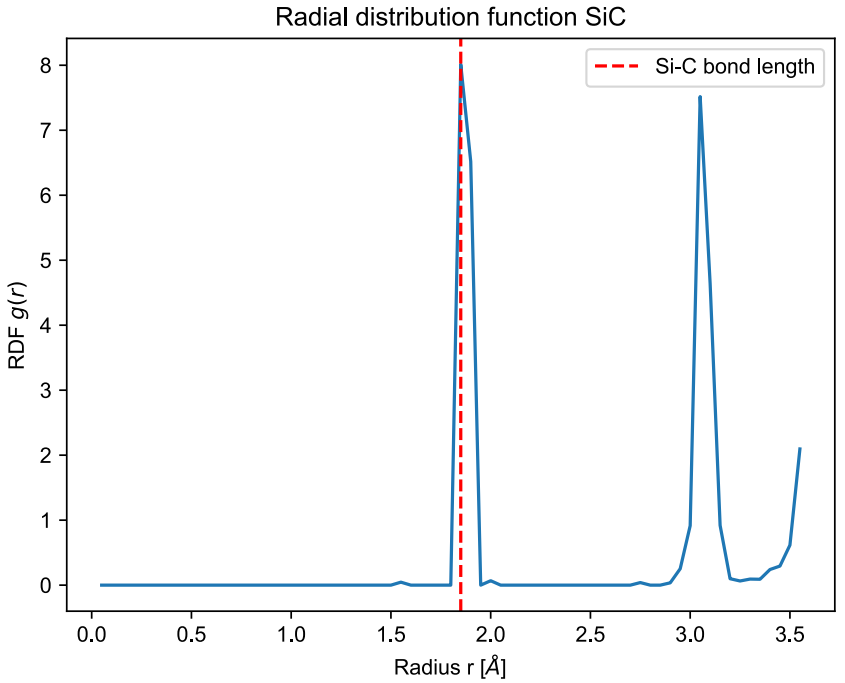
Thank you for your attention!

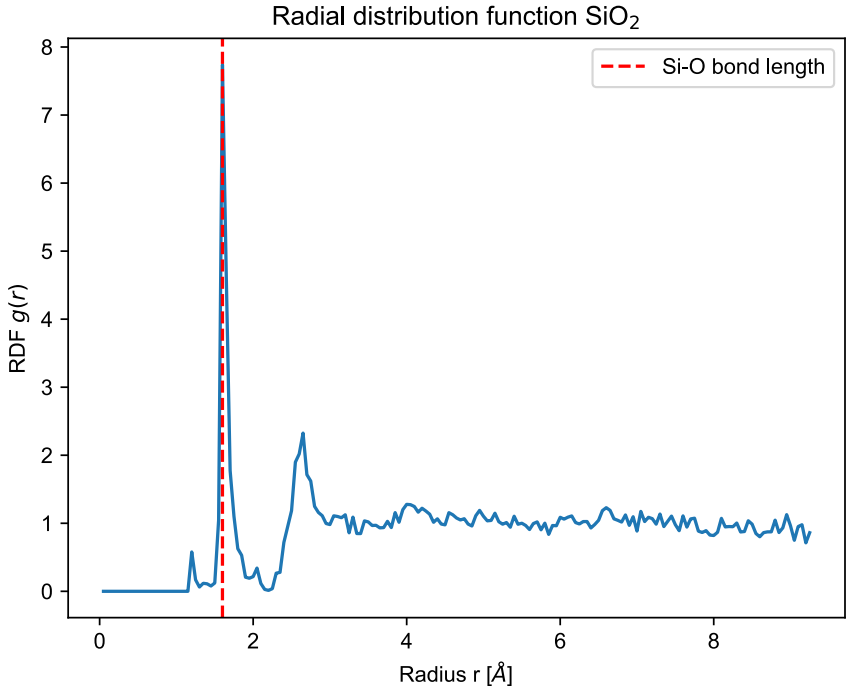
Oxide Quality

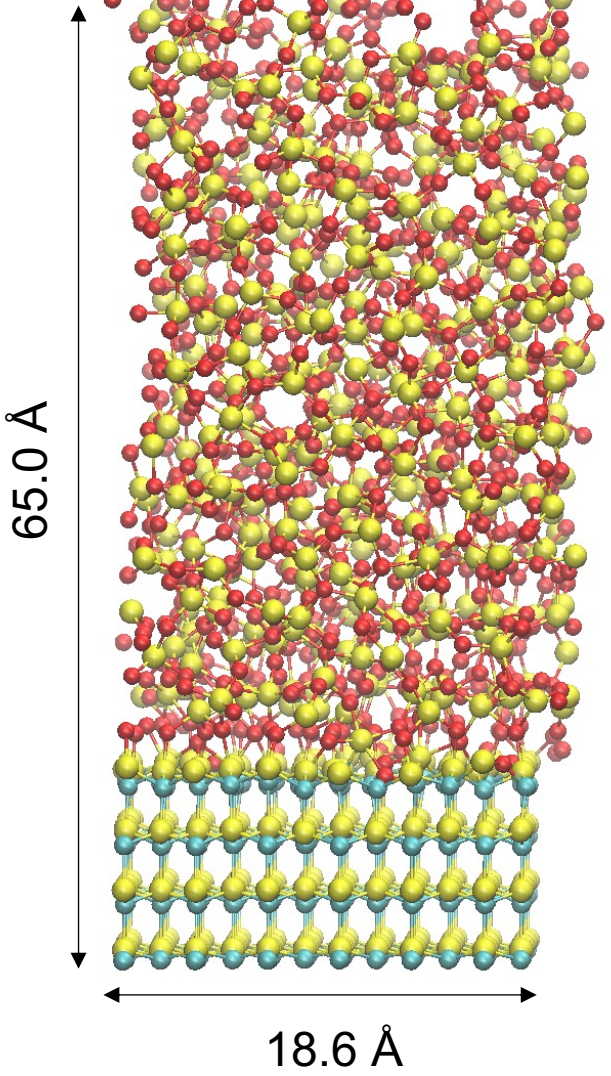
- SiC/SiO_2 structure analysis
  - Radial distribution function: amorphous oxide
  - Bond angle distribution





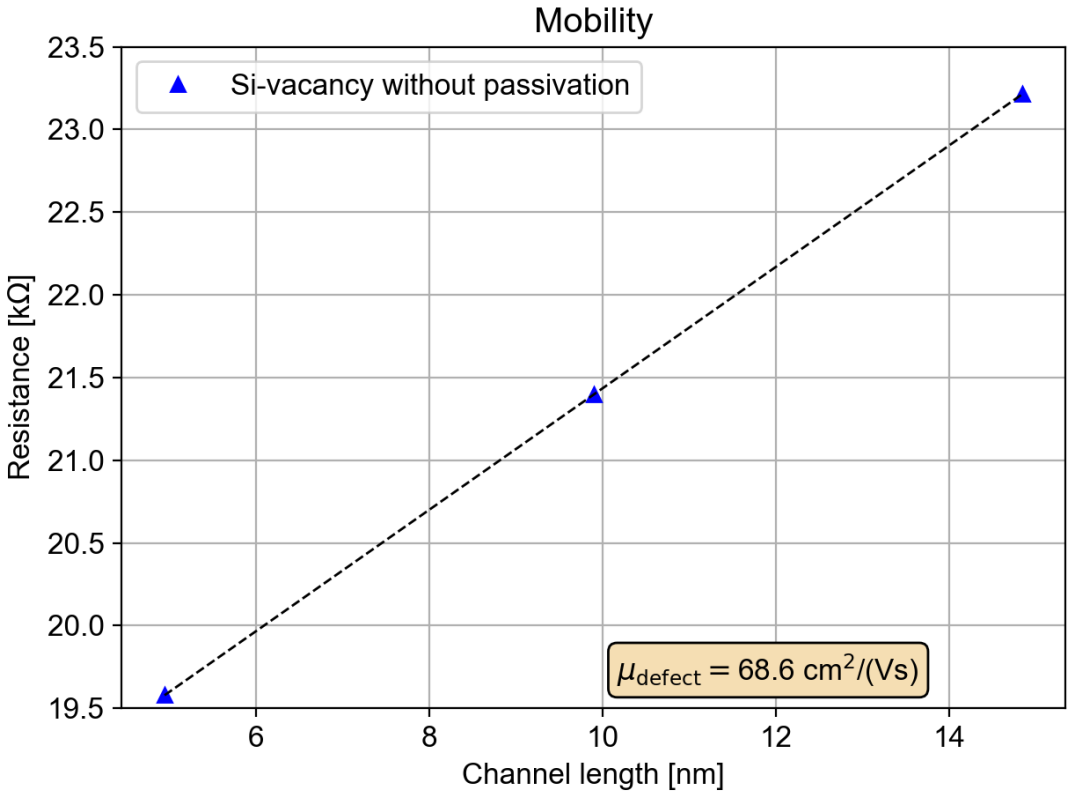






dR/dL - Method

- 3 systems with increasing length
- Inverse of the dR/dL is proportional to the mobility.



$$R(L) = \frac{\Delta V}{I_d}$$

$$\rho = \frac{dR}{dL}$$

$$\mu = \frac{1}{qn\rho}$$

Legend

R(L) = resistance
ΔV = bias difference
I_d= drain current

ρ = channel resistivity

n = charge density
q = elementary charge
μ = mobility

Bandstructures

More Backup Slides