Modeling Nickel-Silicidation using Physics-Informed Machine Learning

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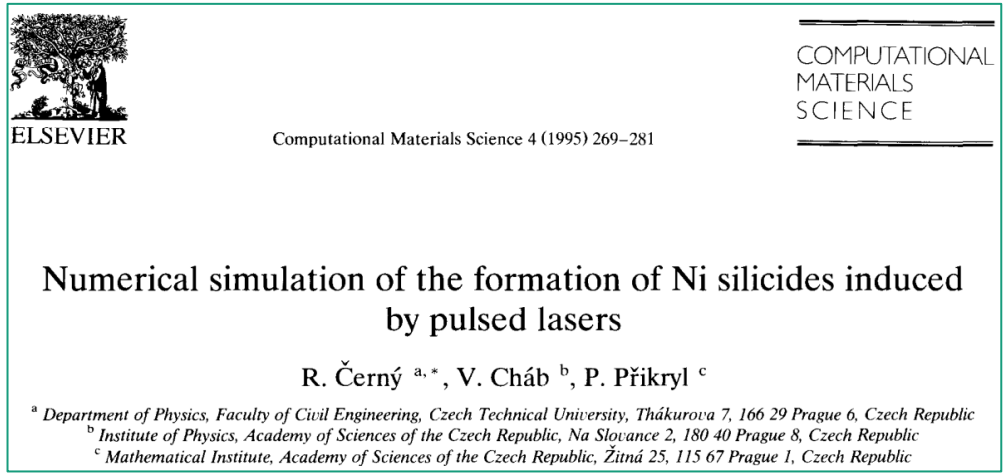
Problem motivation

- **Ohmic contact formation** fundamentally important for semiconductor technology (no contacts, no useful devices).
- Poorly understood, especially for novel materials such as silicon carbide.
- Contact quality highly **sensitive to**, e.g., **annealing temperature** and **duration.**
- Consider **nickel silicidation in silicon** as a **first step** towards proper silicidation models in silicon carbide.
- Analyse process by studying suitable nickel silicidation model and its solutions.

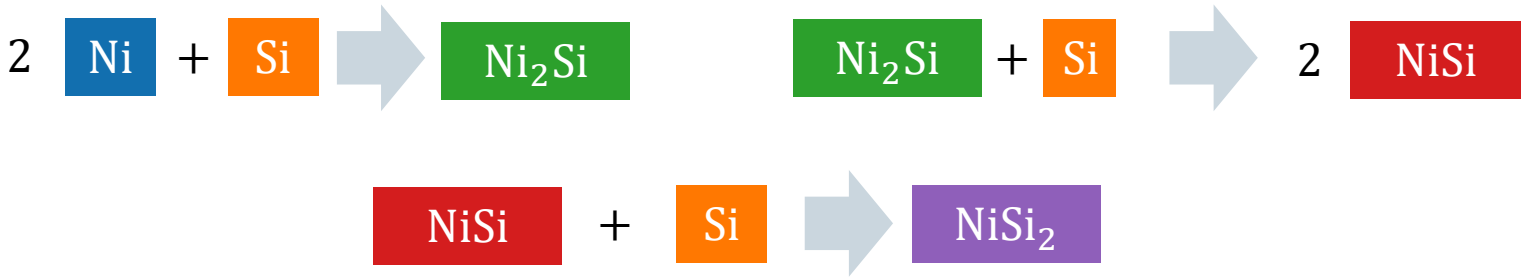
Nickel-Silicidation model

Chemical reactions and diffusion constants

- Continuum model for Nickel-Silicidation adapted from Černý et al.



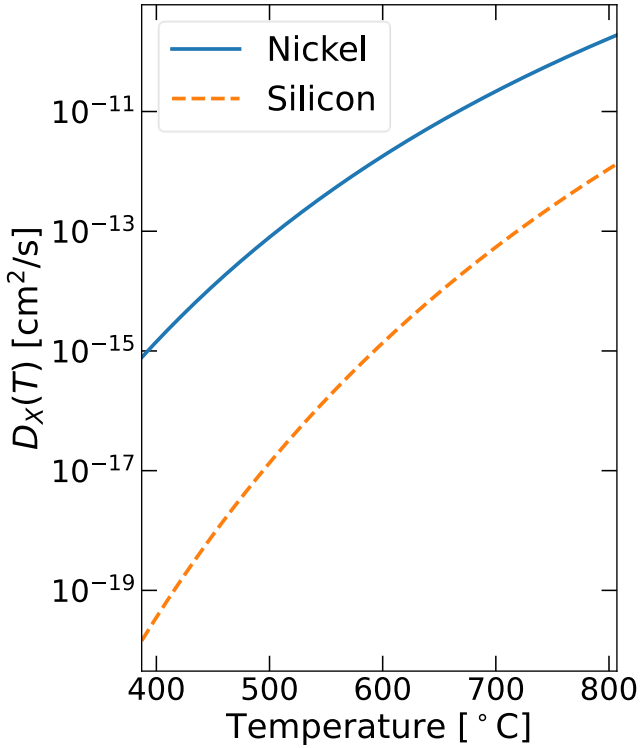
- Three implemented reactions:



- Diffusion of Ni and Si given by temperature dependent effective diffusion constants

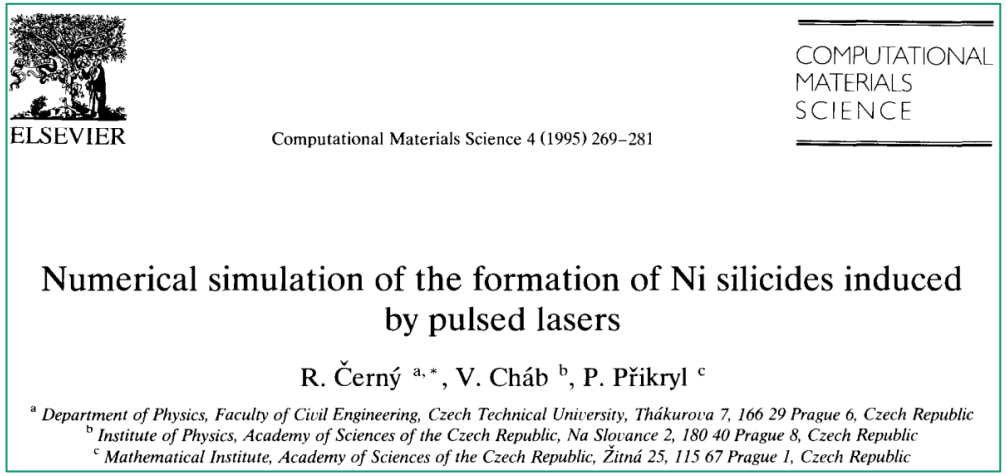
$$D_X(T) = D_{X,0} \exp(-\frac{E_X}{k_B T})$$

- Activation energy E_X and pre-factor $D_{X,0}$ were taken from literature sources.



Nickel-Silicidation model (2)

Reaction-diffusion system



- Concentration functions solve **reaction-diffusion PDE system**:

$$\frac{\partial C_{\mathrm{Ni}}}{\partial t} = \nabla \cdot (D_{\mathrm{Ni}} \nabla C_{\mathrm{Ni}}) - 2k_1 \left(\frac{C_{\mathrm{Ni}}}{C_{0,\mathrm{Ni}}}\right)^2 C_{\mathrm{Si}},$$

$$\frac{\partial C_{\mathrm{Si}}}{\partial t} = \nabla \cdot (D_{\mathrm{Si}} \nabla C_{\mathrm{Si}}) - k_1 \left(\frac{C_{\mathrm{Ni}}}{C_{0,\mathrm{Ni}}}\right)^2 C_{\mathrm{Si}} - k_2 \left(\frac{C_{\mathrm{Ni_2Si}}}{C_{0,\mathrm{Ni_2Si}}}\right) C_{\mathrm{Si}} - k_3 \left(\frac{C_{\mathrm{NiSi}}}{C_{0,\mathrm{NiSi}}}\right) C_{\mathrm{Si}},$$

$$\frac{\partial C_{\mathrm{Ni_2Si}}}{\partial t} = k_1 \left(\frac{C_{\mathrm{Ni}}}{C_{0,\mathrm{Ni}}}\right)^2 C_{\mathrm{Si}} - k_2 \left(\frac{C_{\mathrm{Ni_2Si}}}{C_{0,\mathrm{Ni_2Si}}}\right) C_{\mathrm{Si}},$$

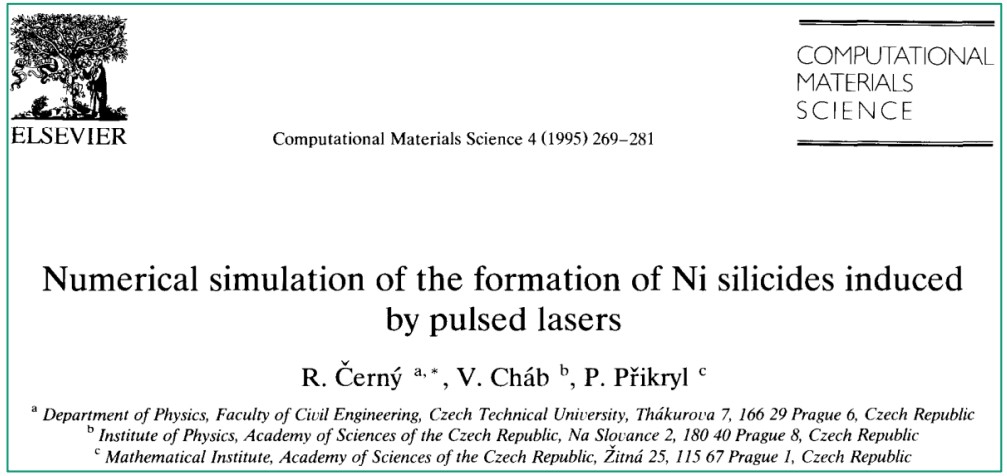
$$\frac{\partial C_{\mathrm{NiSi}}}{\partial t} = 2k_2 \left(\frac{C_{\mathrm{Ni_2Si}}}{C_{0,\mathrm{Ni_2Si}}}\right) C_{\mathrm{Si}} - k_3 \left(\frac{C_{\mathrm{NiSi}}}{C_{0,\mathrm{NiSi}}}\right) C_{\mathrm{Si}},$$

$$\frac{\partial C_{\mathrm{NiSi_2}}}{\partial t} = k_3 \left(\frac{C_{\mathrm{NiSi}}}{C_{0,\mathrm{NiSi}}}\right) C_{\mathrm{Si}},$$

where $C_{0,X}$ denotes the equilibrium configuration of phase X.

Nickel-Silicidation model (3)

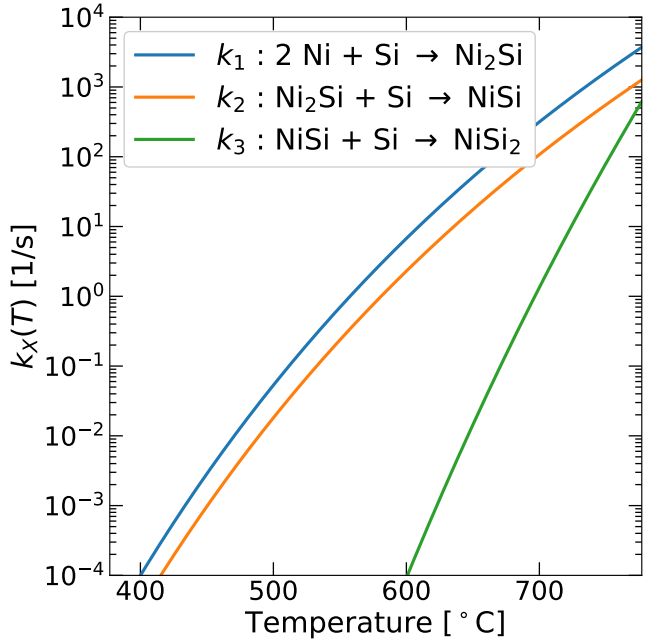
Reaction rates and boundary conditions



- **Reaction rates**
  - We assume that reactions are diffusion-limited, such that

$$k_i \propto 4\pi\, r_i\, D_{\mathrm{Si}}(T)\, \kappa(T; T_{i,c}).$$

  - Here, r_i is the capture radius of the chemical reaction ($\sim 1 - 10$ Å).
  - Each reaction happens only above a critical temperature $T_{i,c}$.
    - This is encoded in the cutoff function $\kappa(T; T_{i,c})$.



- **Boundary and initial conditions**
  - Reflecting boundaries → modeled via vanishing Neumann boundary conditions.
  - Initial conditions: $C_{\mathrm{Ni}}(x, 0) = C_{0,\mathrm{Ni}}$ within the Ni layer and $C_{\mathrm{Si}}(x, 0) = C_{0,\mathrm{Si}}$ within the Si domain.

Flat setting

Initial condition

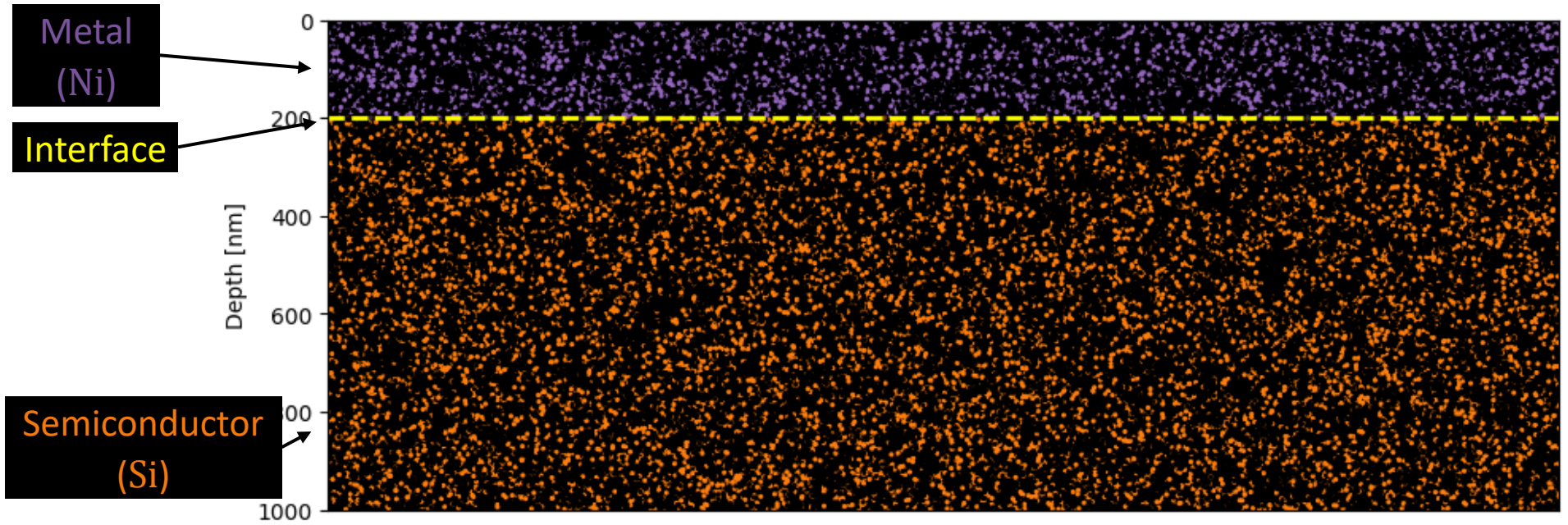
Image: Fraunhofer IISB

Consider the following setting:

- Flat initial Ni-Si interface. → Model silicidation far away from edges of deposited Ni layer.

→ Simulate RTP

- Thickness of Ni layer: 200 nm. Depth of Si domain: 800 nm.



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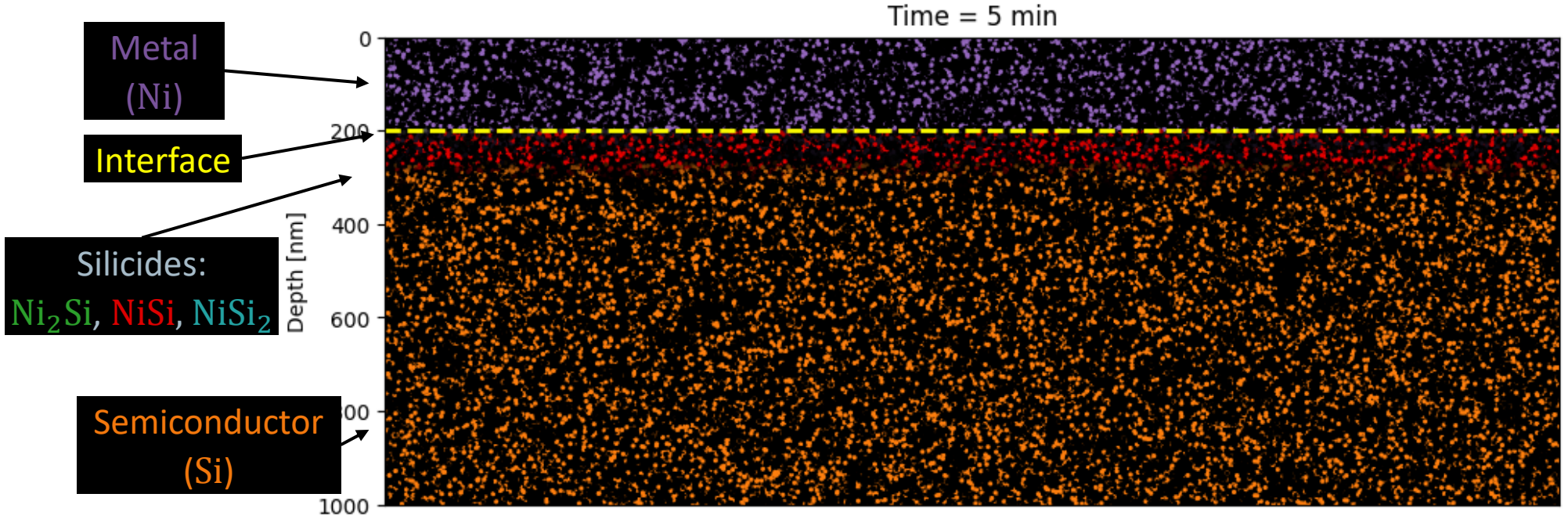
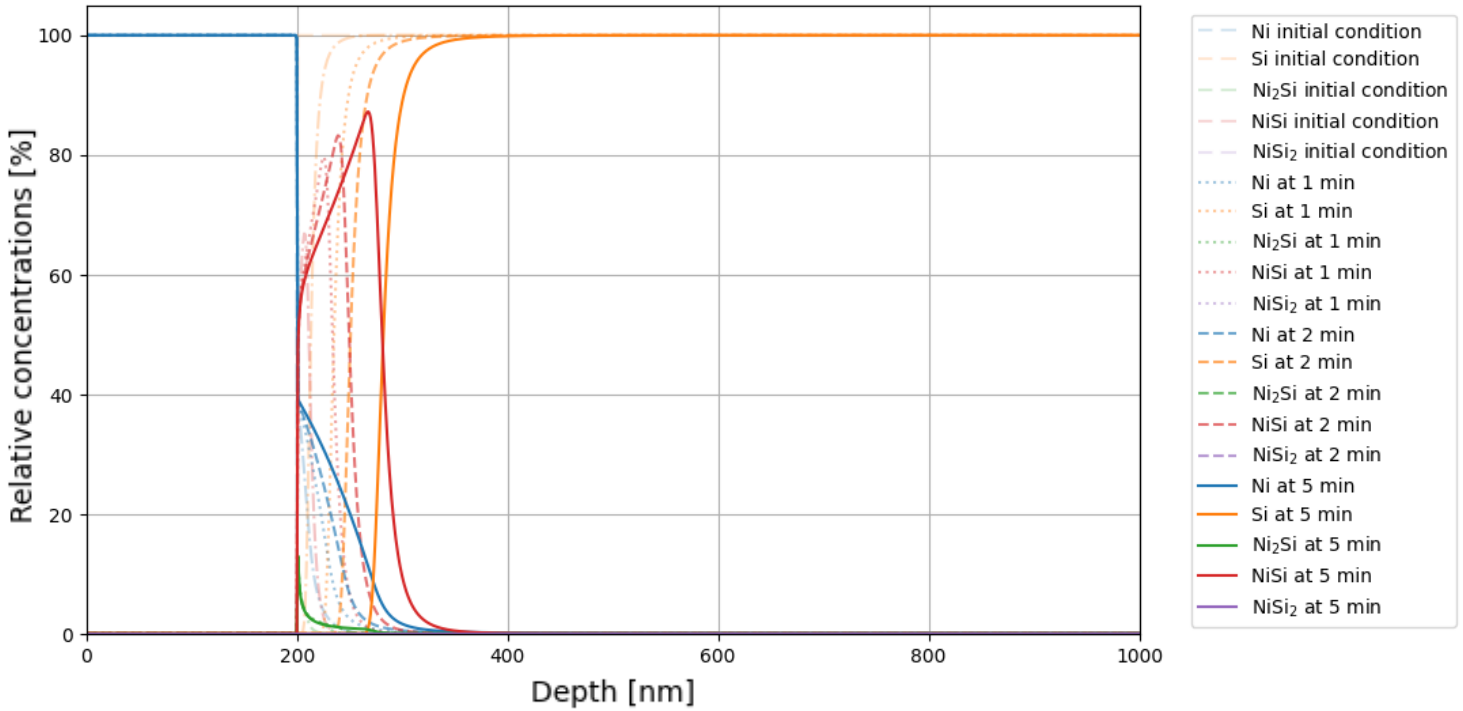


Flat setting
Evolution

- Consider the system for a maximum annealing time of $5\ \mathrm{min}$.
- Model this setting via 1D concentration functions.



Flat setting

Final concentrations

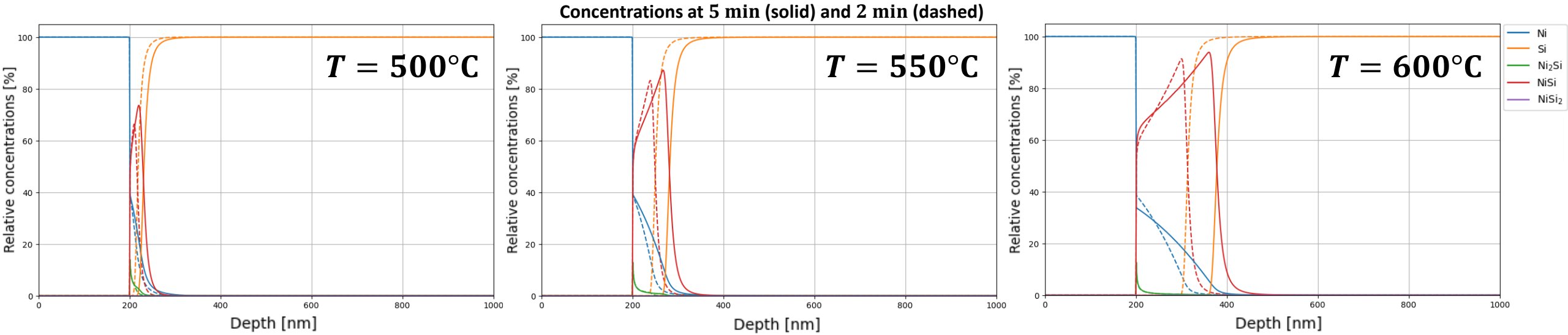
SYNOPSYS® Sentaurus Device
An Advanced Multidimensional (1D/2D/3D) Device Simulator

With Synopsys' Sentaurus (commercial FEM solver):
A single computation takes

- ~ 25 s for 1D simulation,
- ~ 4 min 30 s for 2D simulation.

- Main quantity of interest: Final concentrations.

- So far: Considered temperature $T = 550°C$. Different temperatures lead to different final concentrations.



➢ Application of physics-informed machine learning: Model that can directly compute the concentrations for general temperatures and annealing times, without needing to rerun simulations for new settings.

ESPINN

Fraunhofer IISB

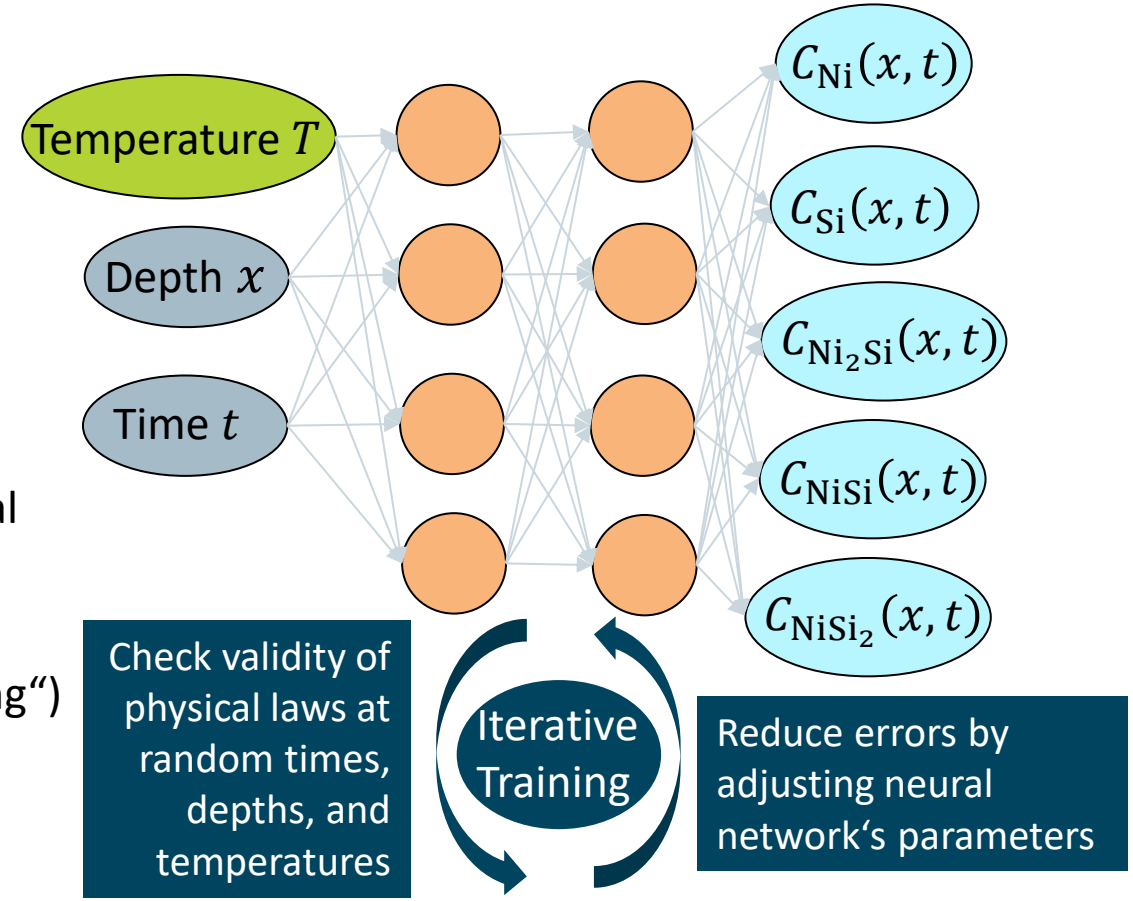
Physics-informed machine learning

Main ideas:

- Represent the solution of the silicidation process as a neural network.
- Optimize the neural network‘s internal parameters („training“) by minimizing the errors of the governing physical laws (PDEs, initial conditions, boundary conditions).

➢ No data needed for neural network training.

➢ Resulting model is a „**physics-informed neural operator**“ (**PINO**).



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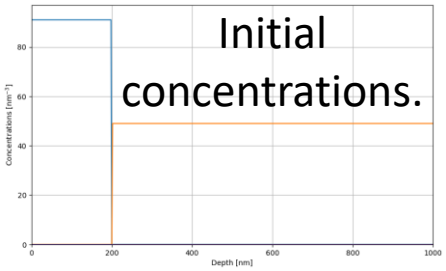

Reflecting boundaries.

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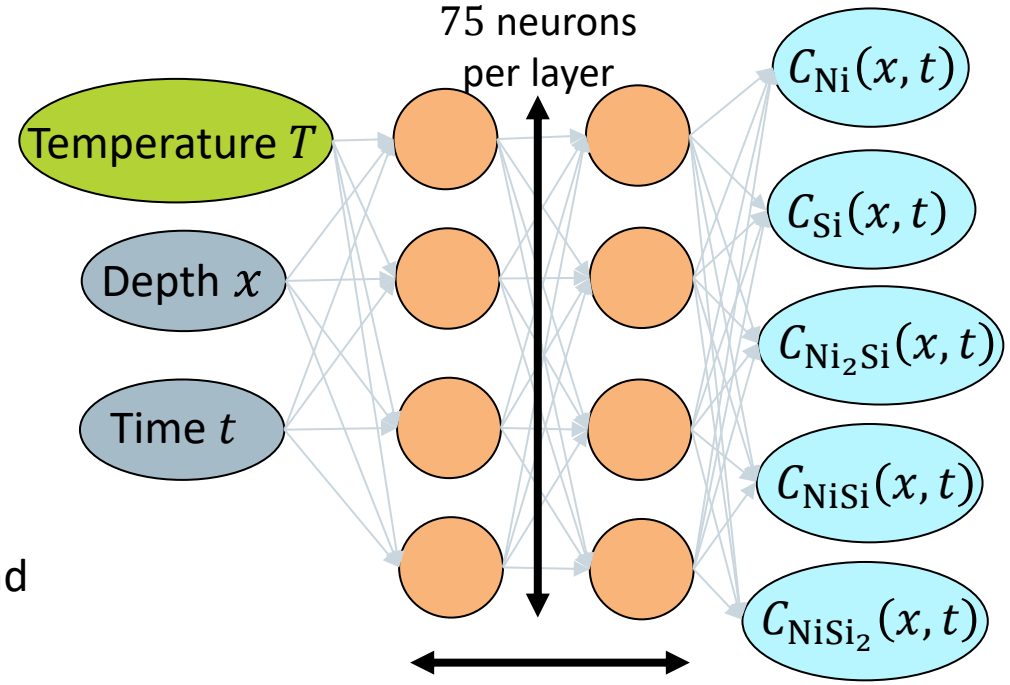
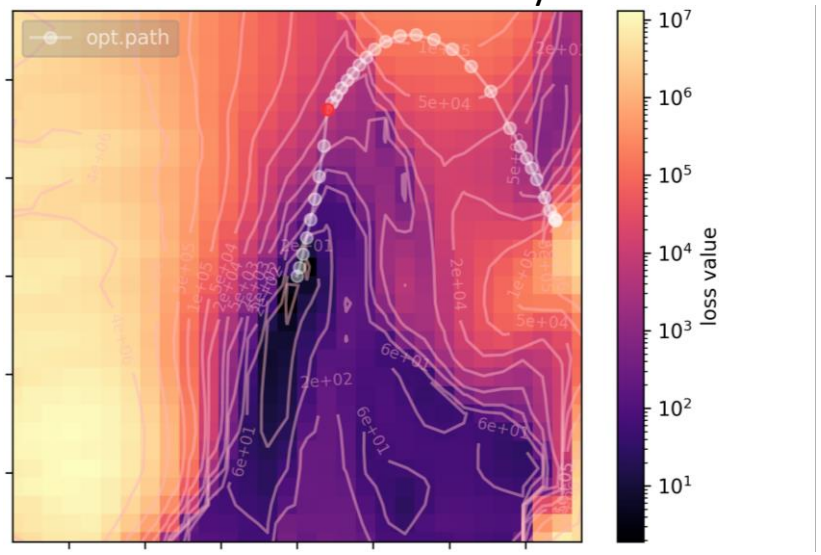
Physics-informed machine learning

Details

- **Neural network architecture:** MLP (multilayer perceptron / fully connected neural network) of size 3×75.
- **Training:** $\sim 60\,000$ iterations with combination of Adam and L-BFGS optimizers.
  → Training time: ~ 3 h on a GPU (NVIDIA A100).
- **Collocation points:** Semi-adaptive sampling during training based on residuals („RAS“).
- **Hard-constraining:** Several properties directly included into neural network structure: all outputs ≥ 0, upper bounds on concentrations, vanishing Neumann boundary conditions.
- **Implementation:** DeepXDE with backend PyTorch

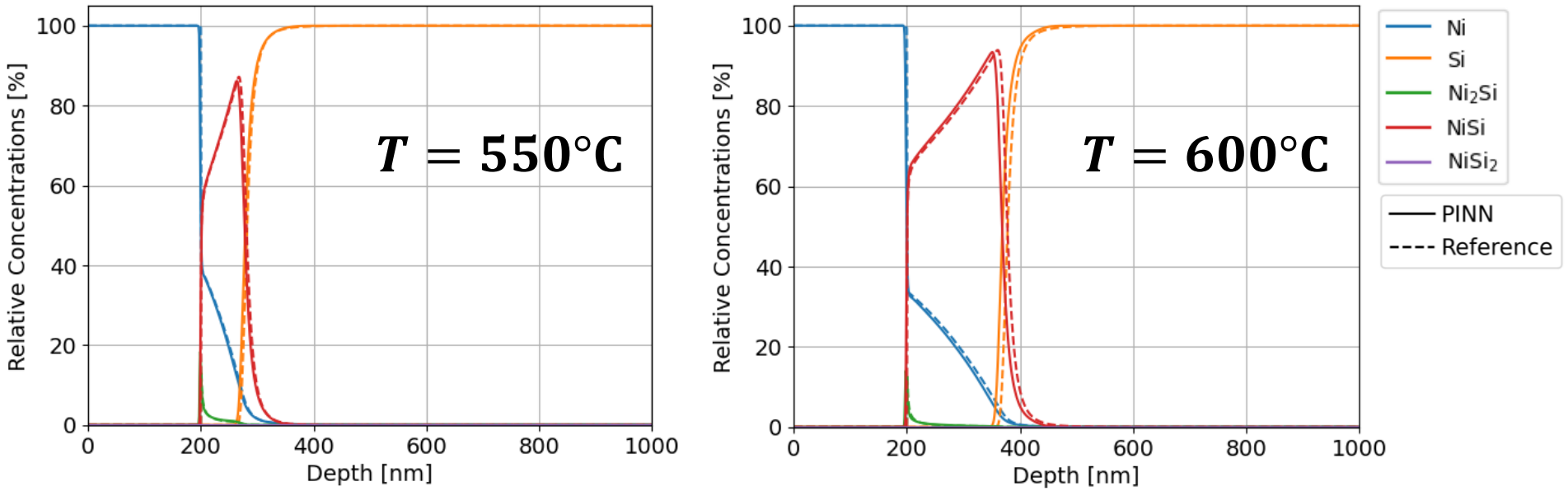




Results

Accuracy of PINO

Comparison of physics-informed neural operator with reference simulation at annealing time $t = 5\ \mathrm{min}$.



Similar accuracies for other temperatures:

Temperature	Error*
$T = 450°C$	2.54 %
$T = 500°C$	3.98 %
$T = 550°C$	3.96 %
$T = 600°C$	6.87 %
$T = 650°C$	8.76 %

* Relative L^2-distance to reference solution, averaged over components Ni, Si, and NiSi.

➢ PINO can accurately predict the silicidation of Ni in Si.

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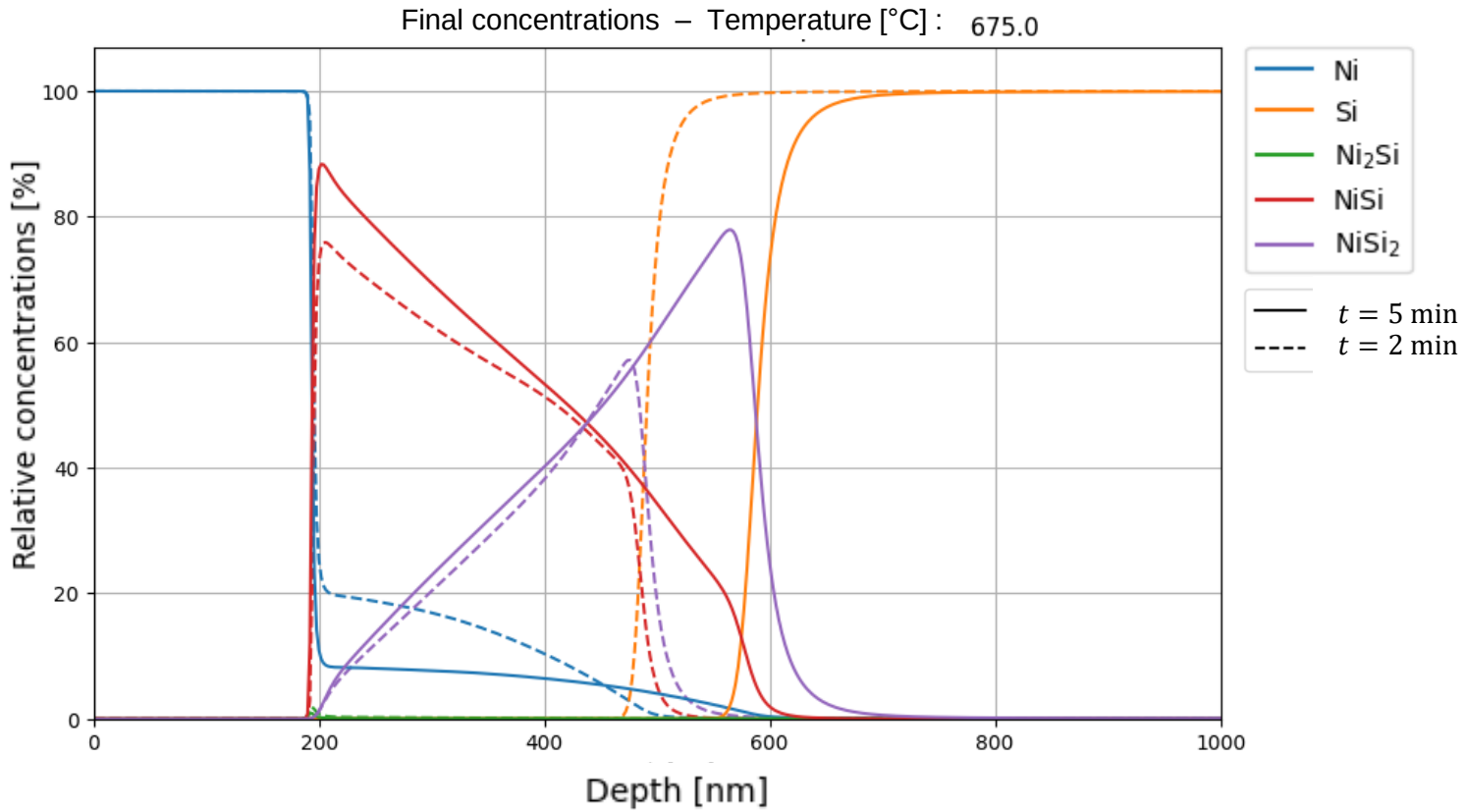
Results

General temperatures

Trained PINO can be evaluated for general temperatures and annealing times without retraining.



Computational costs to create animation:

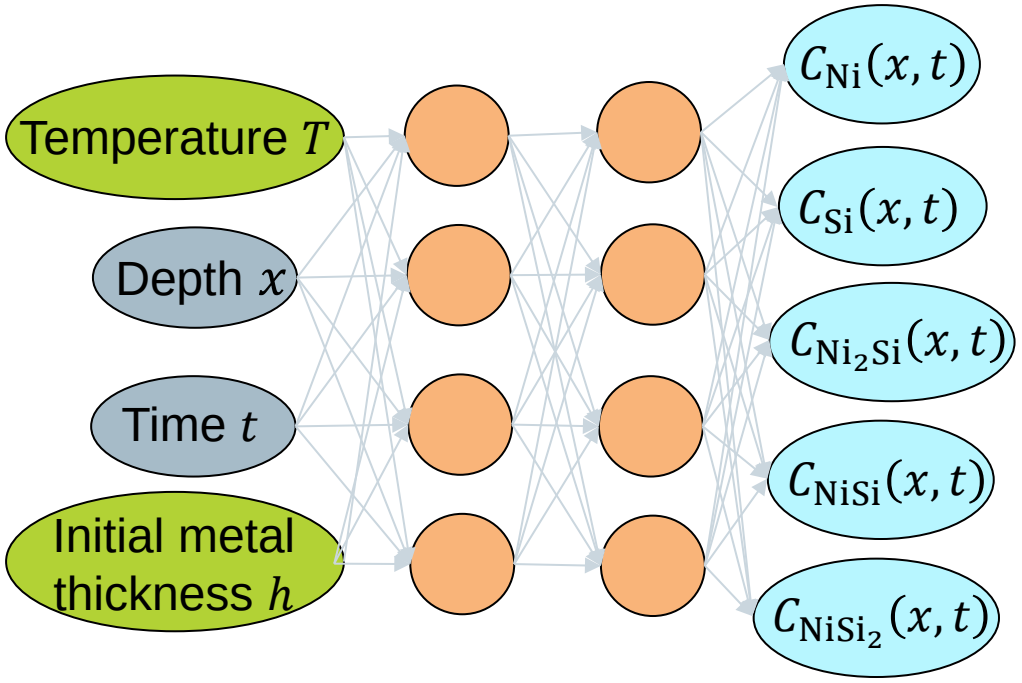
- Evaluation at 501 depth values (step size 2 nm) for 450 temperatures takes $\sim$ **53 ms** on a laptop.
- Sequential classical simulations for 450 temperatures take $\sim$ **3 h 5 min**.
  → Similar to model's training time.

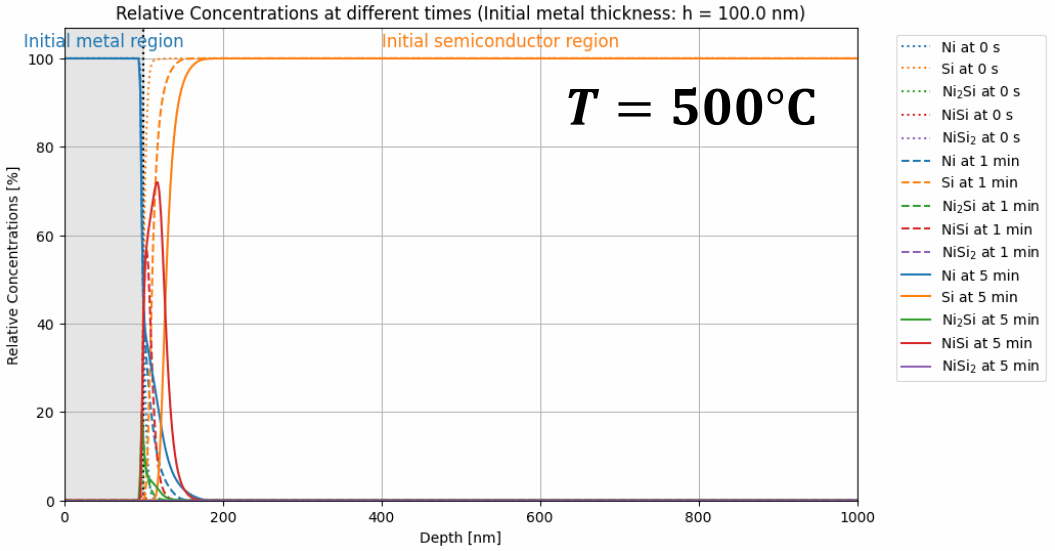
Outlook

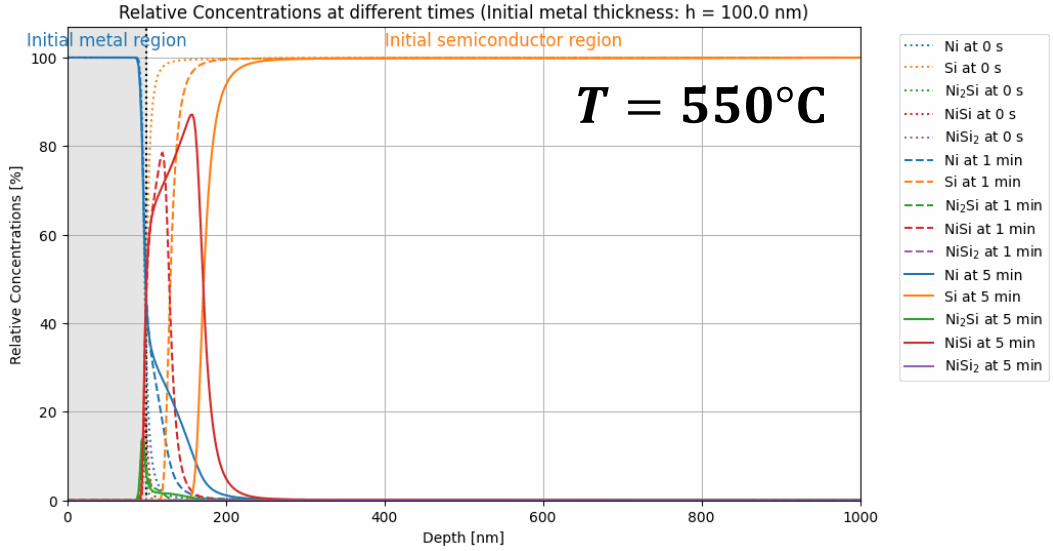
Further parameter dependencies

To offer fast optimization in parameters beyond temperature:
Extend parametric dependency of PINO.

- Also generalize over different initial geometries.
- In future: also allow time-dependent temperature profiles.







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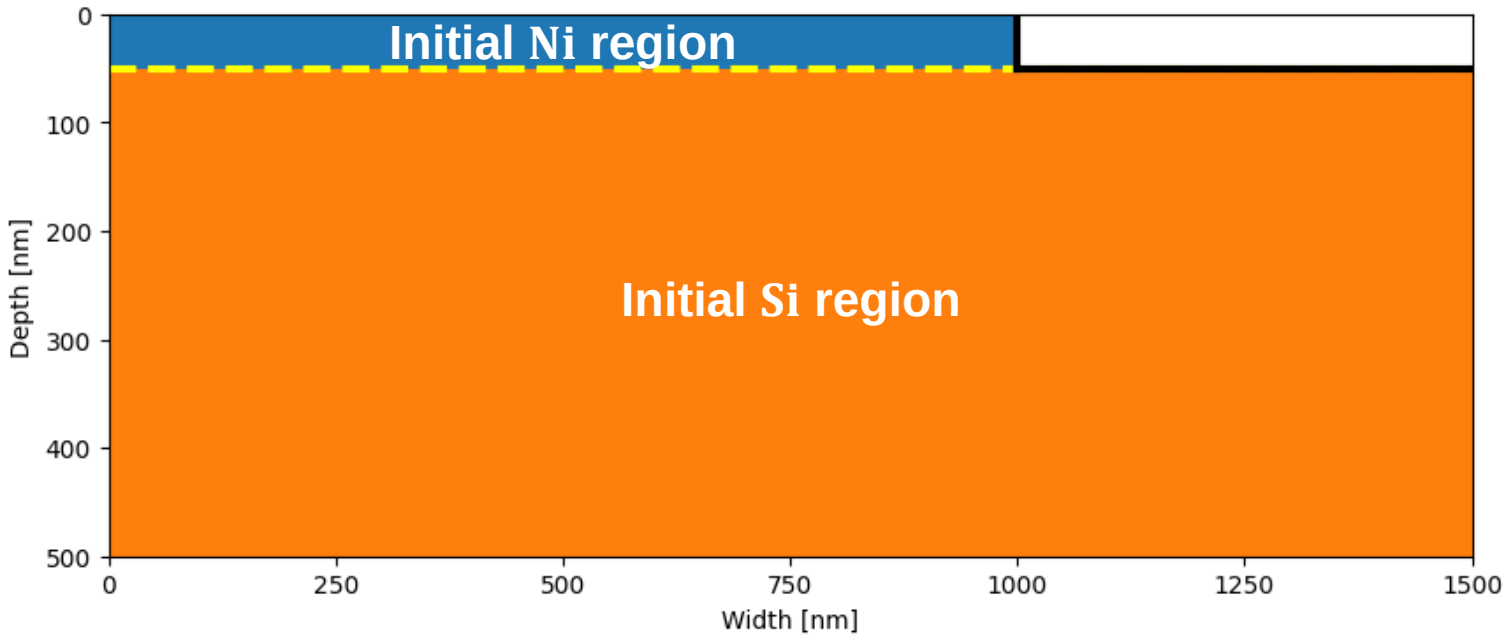
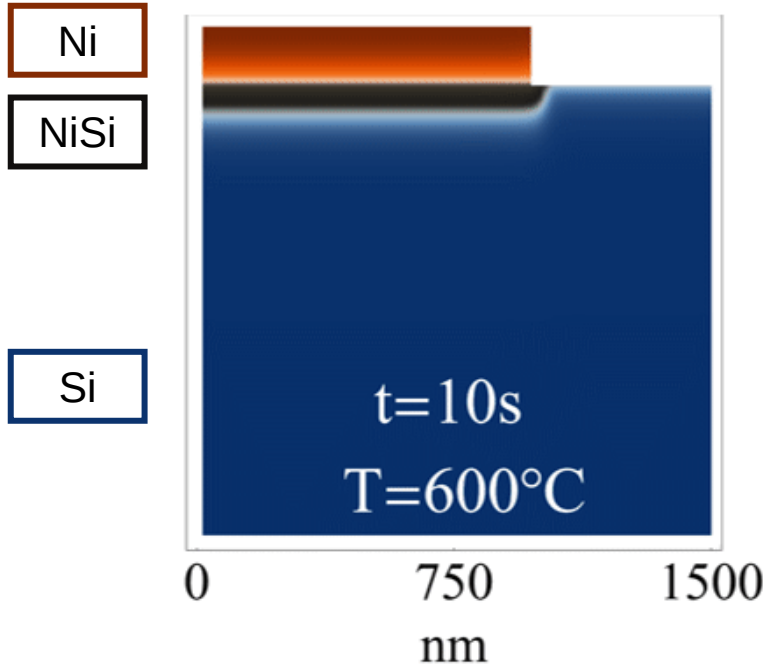
Outlook

- PINOs can be integrated in process control on edge devices.
- Extend PINO to 2D and 3D settings.





- Develop and calibrate model for Ni silicidation in SiC and train PINOs for it.

Contact

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