

Multi-Phase-Field Modelling of Thin Film Silicidation



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INTRODUCTION

Forming low-resistance ohmic **contacts** on wide-band-gap semiconductors (**SiC**, **GaN**) remains a key industrial challenge. Standard TCAD **silicidation** models use reaction-diffusion equations, which struggle with complex, multi-grain interface morphologies — critical for SiC, where **Graphite-clusters** form during annealing. Their role in contact formation remains unclear and has not been modeled numerically.

METHOD

The **Multi-Phase-Field (MPF)** model uses **Grand Potential Energy** Formulation described by N possible phases and K chemical species, [1]

$$\Omega[\phi, \mu] = \int (\omega_{int}(\phi) + \omega_{bulk}(\phi, \mu)) dV.$$

Their consecutive evolution equations can be monitored by **Allen-Cahn** and **Cahn-Hilliard equations**, given by

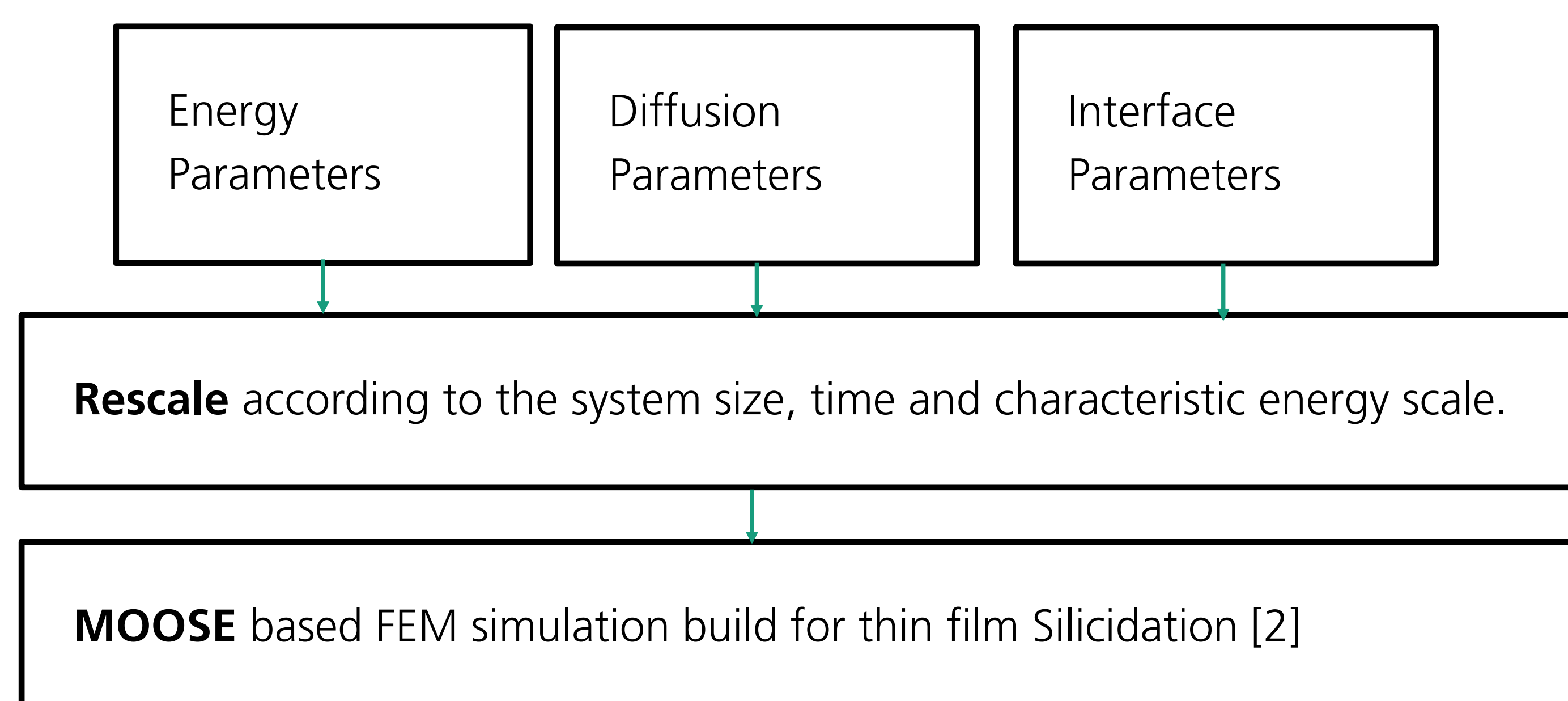
$$\dot{\phi}_\alpha = -L \frac{\delta \Omega}{\delta \phi_\alpha},$$

$$\dot{c}_A(\mu_A, \phi) = \nabla \cdot (M_A \nabla \mu_A).$$

The **diffusion parameters** for different phases, are assumed as Arrhenius type:

$$D_i = A_i \exp\left(-\frac{Q_i}{k_B T}\right) \text{ cm}^2 \text{ s}^{-1}.$$

SIMULATION APPROACH – TEMPERATURE DEPENDENCE



DISCUSSION

- Key parameters governing dynamics are the **diffusion constants**, **phase-field mobility**, and **Gibbs free energies**. While free energies are well-characterized via phase diagrams, diffusion constants (especially **grain-boundary diffusion**) remain uncertain and were not separately modeled.
- Future work includes explicit **cluster modeling**, individual grain representation, **volume expansion** effects, and calibration against additional phases (**NiSi**, **NiSi₂**) and experimental techniques (e.g., **XRD**) to better capture non-homogeneous silicide thickness and cluster localization.
- Characterization of **diffusion-** or **interface-controlled growth** of the different silicides

RESULTS

- One-dimensional MPF simulation for an **Ni-Si interface**
- Physics-informed neural network** is trained to yield fast predictions [3]

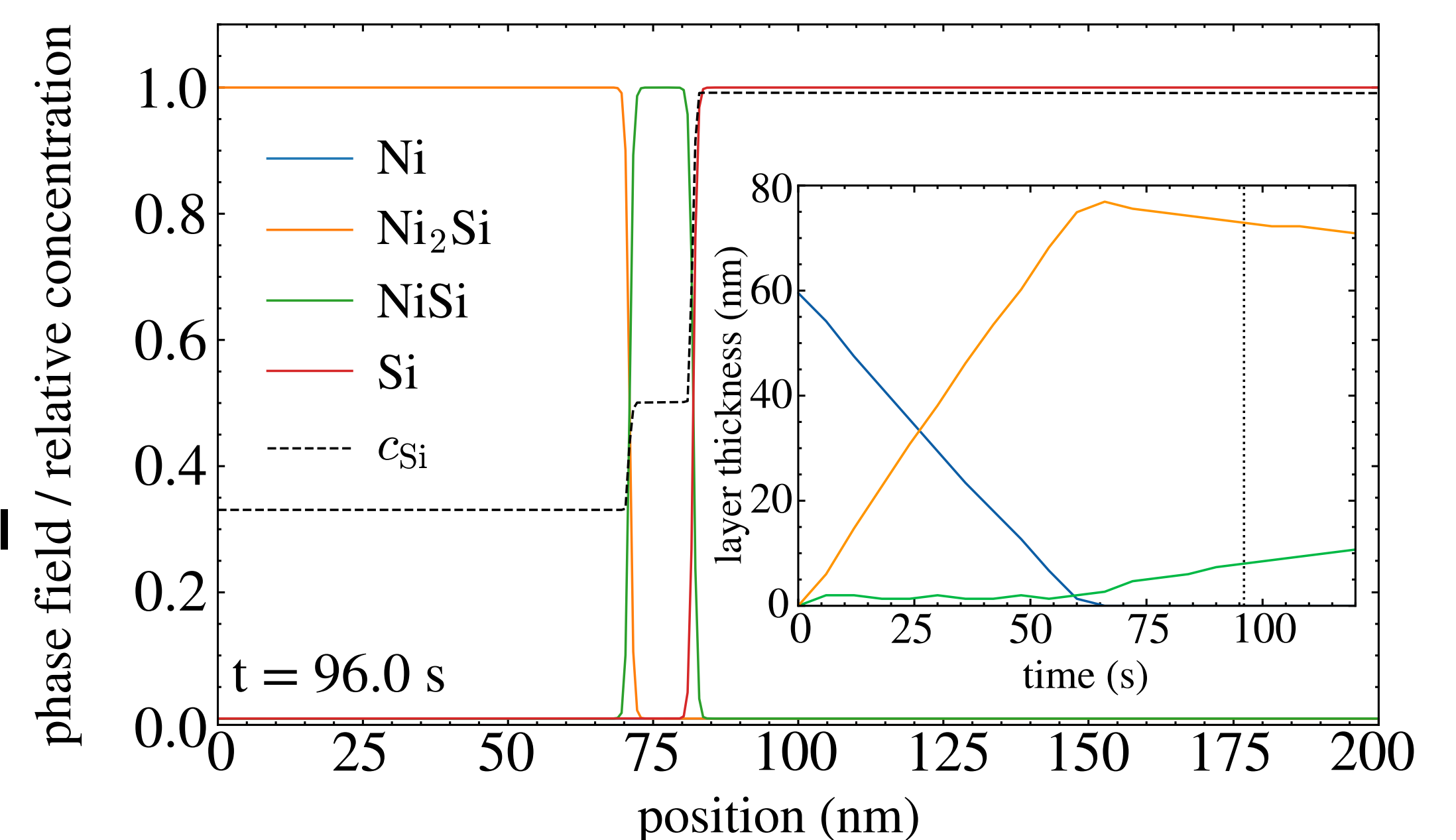


Fig.1: Snapshot of the phase-field distribution at 96s growth time. Inset: Time development of the thickness

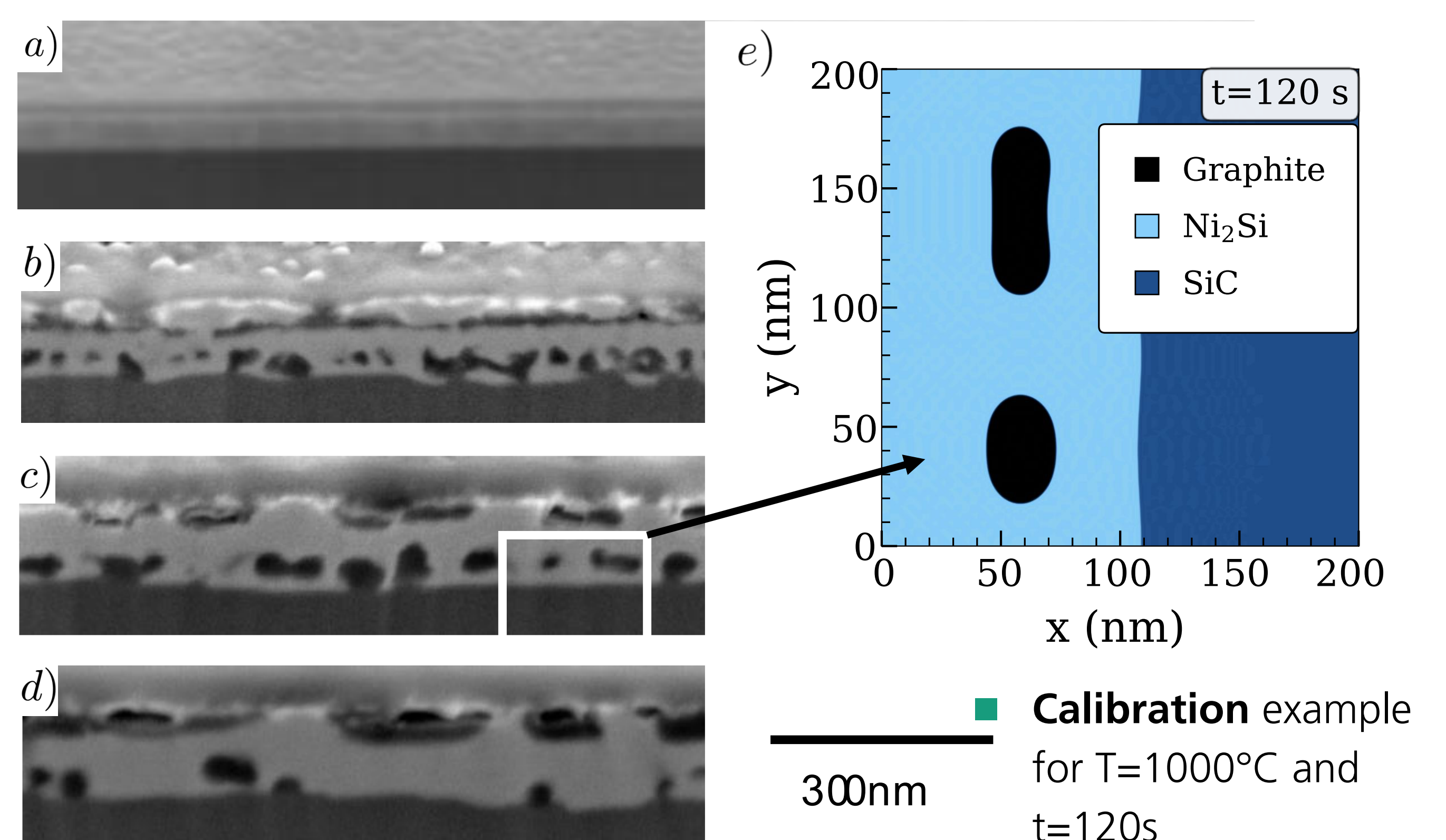


Fig.2: Focused Ion Beam-Cuts after Rapid Thermal Processing at different temperatures vs. simulation

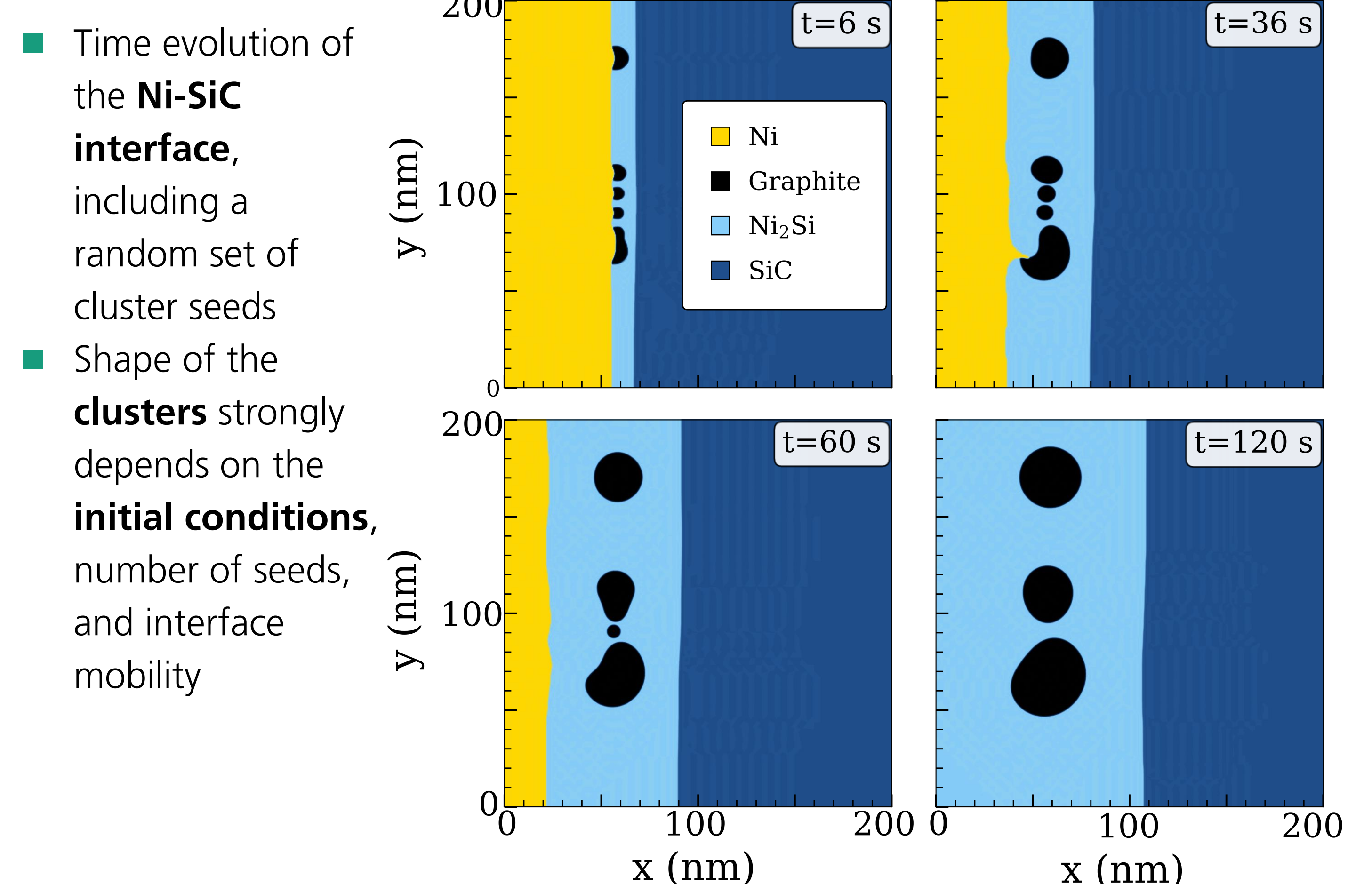


Fig.3: Time evolution of the phase fields including cluster growth

¹ L. K. Agesen, Y. Gao, D. Schwen, and K. Ahmed, "Grand-potential-based phase-field model for multiple phases, grains, and chemical components," *Phys. Rev. E*, vol. 98, no. 2, p. 023309, 2018.

² L. Harbour et al., "4.0 MOOSE: Enabling massively parallel multi-physics simulation," *SoftwareX*, vol. 31, p. 102264, 2025.

³ C. Straub, S. Mundinar, J. Klönn, C. Pixius, and A. Roskopf, "Modeling nickel-silicidation using physics-informed machine learning," in *2025 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*, pp. 1–4, IEEE, 2025

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