

Multi-Phase-Field Modeling of Thin-Film Silicidation

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Abstract—We present a new model for the simulation of the evolution of thin silicide layers during high-temperature annealing in semiconductor processing based on the multi-phase-field method. Simulation results are shown for sequential layer growth in a one-dimensional nickel-silicon system, including the silicides Ni_2Si and NiSi . We further present, for a two-dimensional nickel-silicon-carbide system, the results of the carbon cluster growth during the annealing process. The results are presented together with experimental measurements on focused ion beam cuts with selected rapid thermal process recipes.

Index Terms—silicidation, phase-field model, simulation, focused ion beam.

I. INTRODUCTION

Developing and optimizing processes for the accurate formation of electrical contacts on semiconducting substrates remains a challenging task at the industrial level. For wide-band-gap materials such as silicon carbide (SiC) or gallium nitride (GaN), achieving reliable, low-resistance ohmic contacts is a crucial challenge and an ongoing research topic. Currently available TCAD models for silicidation are mostly based on reaction-diffusion equations [1], [2], often in conjunction with an interface-tracking algorithm such as the level-set method. Even though such approaches involve elaborate mathematical methods, they often struggle with complex, evolving interface shapes and the presence of multiple grains of the same phase. However, these are crucial aspects for modeling silicidation in some wide-band-gap semiconductors, such as SiC. During high-temperature annealing for the formation of electrical

contacts on an SiC substrate, carbon clusters are forming in the growing silicide layer [3]. While this is a well-known fact, the role of carbon clusters in the contact formation process is still unclear [4] and, to the authors' knowledge, has not yet been investigated numerically.

We explore the use of multi-phase-field (MPF) methods for the simulation of silicidation processes. Because the MPF method is based on thermodynamic potentials, it provides an intuitive, physics-based way to model solid-state reactions involving multiple phases. Representing chemical phases via phase-fields removes the need for an explicit tracking of their interfaces, thus enabling the simulation of multiple grains with potentially complex morphologies and their effect on the overall structural evolution. MPF models are highly versatile and can be applied to different material combinations employing the thermodynamic parameters from the corresponding phase diagram. Additionally, because MPF models are well-established in a variety of material science applications, additional aspects such as the influence of mechanical stress, volume expansion and grain-boundary diffusion can be included, drawing from a vast basis of existing research [5]. Despite the mentioned strengths of MPF models, to the authors' knowledge, they have not yet been applied to thin-film silicidation in the context of semiconductor process simulations.

II. GENERAL MODEL

In our MPF model, each chemical species A is represented by its relative concentration c_A , whereas each chemical phase α is tracked by a phase-field ϕ_α with ϕ_α close to 1

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and 0 in the presence and absence of phase α , respectively. We collect the phase-fields and the independent concentrations in the respective spacetime-dependent vectors $\phi(\mathbf{x}, t)$ and $\mathbf{c}(\mathbf{x}, t)$. Following the formalism in [6], we employ the grand potential functional

$$\Omega[\phi, \mu] = \int (\omega_{\text{int}}(\phi) + \omega_{\text{bulk}}(\phi, \mu)) dV, \quad (1)$$

to generate the dynamics of the phase-fields. Here, $\mu(\mathbf{x}, t)$ is the vector of chemical potentials of the affected species. The explicit dependencies on temperature and pressure are suppressed in our notation for brevity.

The first term on the right-hand side (rhs) of eq. (1)

$$\omega_{\text{int}}(\phi) = \sum_{\alpha} \left[\frac{\kappa}{2} |\nabla \phi_{\alpha}|^2 + \varepsilon \left(\frac{\phi_{\alpha}^4}{4} - \frac{\phi_{\alpha}^2}{2} + \sum_{\beta \neq \alpha} \gamma_{\alpha\beta} \phi_{\alpha}^2 \phi_{\beta}^2 \right) \right]$$

contains the local contribution of interfaces between different phases α to the total energy. Here, κ , ε and $\gamma_{\alpha\beta}$ are constants whose values determine the width and energy of interfaces between different phases. The bulk term

$$\omega_{\text{bulk}}(\phi, \mu) = \sum_{\alpha} h_{\alpha}(\phi) \omega_{\alpha}(\mu)$$

gets contributions from each phase α via the weighting functions $h_{\alpha}(\phi) = \phi_{\alpha}^2 / \sum_{\beta} \phi_{\beta}^2$. The grand potential density contribution ω_{α} from phase α is related to the corresponding Gibbs free energy density g_{α} through a Legendre transform:

$$\omega_{\alpha}(\mu) = g_{\alpha}(\mathbf{c}(\mu)) - \sum_A c_A(\mu_A) \mu_A.$$

The Gibbs free energy can be directly extracted from phase diagrams and is needed as an input for our calculation. To simplify calculations, we employ a parabolic approximation for the Gibbs free energy of each phase, resulting in a simple analytical expression for $\omega_{\alpha}(\mu)$ and for the concentration of species A in phase α , $c_A^{\alpha} = -\frac{\partial \omega_{\alpha}}{\partial \mu_A}$.

Based on the grand potential functional, the time evolution of each phase-field ϕ_{α} is given by

$$\dot{\phi}_{\alpha} = -L \frac{\delta \Omega}{\delta \phi_{\alpha}}, \quad (2)$$

where the functional derivative on the rhs can be evaluated analytically. Here, L is the phase-field mobility which is related to the interface velocity [7]. The phase-field dynamics described by eq. (2) are coupled to the chemical potential vector μ , which is itself evolving due to the diffusion of chemical species. Each independent concentration c_A is described by

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

which is implicitly coupled to the phase-field evolution due to the dependence of c_A on ϕ [8]. Here, M_A is the mobility coefficient for species A , which is directly connected to the respective diffusion constant through $D_A = M_A \frac{\partial \mu_A}{\partial c_A}$. Note that the diffusion constant for each species A depends on the underlying phase α .

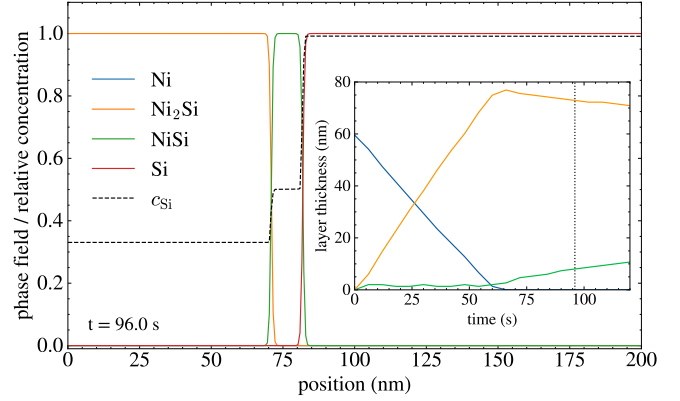


Fig. 1. Snapshot of the phase-field distribution after the complete depletion of the nickel layer (main plot) and simulated evolution of the thicknesses of different layers (inset).

III. EXPERIMENTS

For a comparison of the SiC simulation with experimental data, samples were fabricated using 4H-SiC substrate wafers. A 60 nm Ni–Al (2.6 at.% Al) film was deposited on both sides of the wafers by sputter deposition. For each side, an in-situ argon plasma etch was performed immediately prior to metallization to remove the native oxide layer from the SiC surface. Each wafer was then cleaved into four pieces to enable processing under varying conditions. Rapid thermal processing (RTP) was carried out in a carbon susceptor box under a nitrogen atmosphere for 120 s, with the residual oxygen level maintained below 20 ppm throughout the process. The temperature was varied in the range of 1173 K to 1373 K, which corresponds to typical values for SiC contact annealing. After processing, the layers are measured by performing focused ion beam (FIB) cuts and scanning electron microscopy (SEM), providing the data shown below in Fig. 4. Additionally, X-ray diffraction (XRD) measurements were performed to determine the chemical phases present in the silicide layer.

IV. RESULTS

We present two exemplary results, namely (IV-A) the sequential growth of Ni_2Si and NiSi during nickel silicidation of silicon and (IV-B) the formation of carbon clusters during the nickel silicidation of SiC. The temperature-dependent Gibbs free energies of all phases are extracted from [9]. All simulation results are obtained using the Multi-Physics Object Oriented Simulation Environment (MOOSE) [10].

A. Sequential layer growth in Ni-Si

The silicide growth of thin metallic layers exhibits a qualitatively different behavior compared to bulk metals. In the thin-film case, silicide layers form sequentially, starting with the most metal-rich layer and building up silicon-rich layers only once the metal layer is fully consumed [11].

In Fig. 1, we show that our model is able to reproduce sequential layer growth. At first, the dynamics of the system

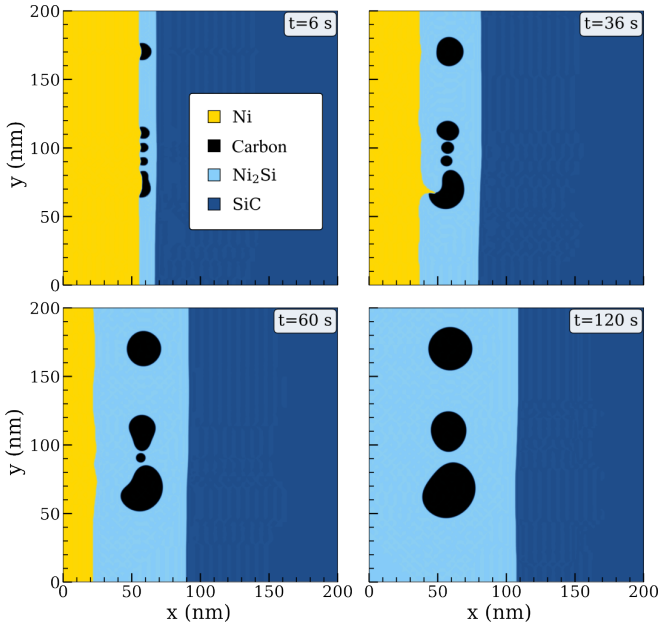


Fig. 2. Simulated growth of carbon clusters (black regions) during nickel silicidation of SiC (darkblue). Nickel is shown in yellow and Ni₂Si in lightblue.

favors the nickel-rich silicide phase of Ni₂Si. The corresponding layer exhibits rapid initial growth, consuming the diffusive metallic Ni layer. The model then allows the NiSi phase to grow once the Ni layer is fully depleted. This behavior is mainly controlled by the diffusion constants in the various material layers, which are difficult to determine and are treated as free, temperature-dependent parameters in our model. Note that NiSi grows even though the Gibbs free energy of Ni₂Si is lower than that of NiSi, highlighting the fact that the thermodynamic parameters of the silicides are not the dominant factors in the growth of the layer. As with other models describing layer growth, the phase-field method does not allow for the dynamical creation of new phases, only for the growth of existing ones. Therefore, all phases that are to be simulated need to be included in the initial conditions.

B. Carbon clusters in SiC

In this example, we illustrate the application of MPF models to ternary systems, in our case Ni-SiC, where we are able to track the development of carbon clusters during a high-temperature silicidation process. Since XRD measurements showed the sole presence of the Ni₂Si phase in our processed samples we modeled the silicide layer by this phase alone. Fig. 2 shows the simulated time evolution of carbon clusters within the growing silicide region. As the initially thin Ni₂Si layer at the Ni/SiC interface starts growing and depleting SiC, the leftover carbon diffuses through the silicide layers and precipitates to localized clusters. Note that the seeds of the clusters are included in the initial conditions of the simulation, i.e., we do not explicitly model the stochastic nucleation of new grains. Nevertheless, the model captures the essential

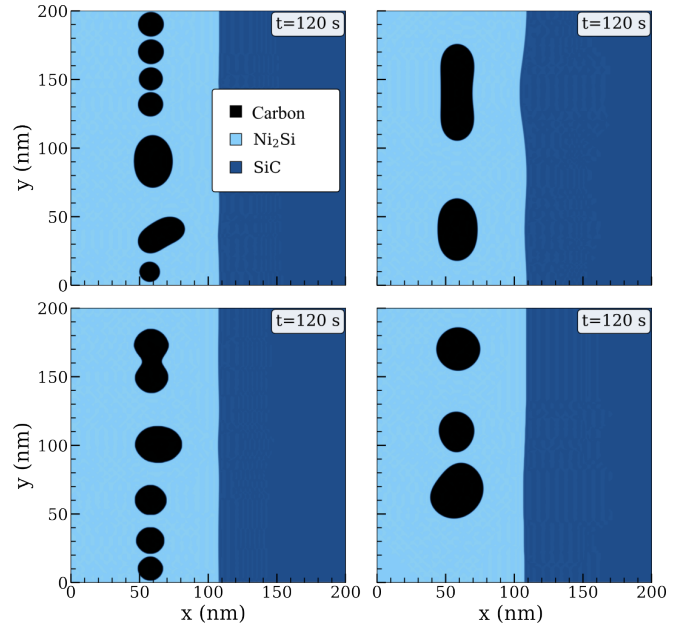


Fig. 3. Development of different origins and shapes of combined carbon clusters (black) during nickel silicidation of SiC (darkblue) after an RTP time of 120 s. The nickel fully vanished while Ni₂Si is shown in lightblue.

physics of cluster coarsening and evolution driven by diffusion and energy minimization. The growth rate of the silicide layer is determined by multiple parameters, most notably the diffusion constant $D_{\text{Ni}}^{(\text{Ni}_2\text{Si})}$ of nickel (the mobile partner in this reaction) in the silicide layer and the phase-field mobility L . To a lesser extent, the growth rate also depends on the interface energy parameters ε and κ , which were chosen to obtain an interface width of 10 nm and an interface energy between SiC and Ni₂Si of 1.5 J/m². Since carbon clusters form as a byproduct in the silicidation, their growth rate follows a trend that correlates with that of the silicide layer. During their growth, clusters obtain various shapes due to merging with neighboring grains. In Fig. 3, we compare simulations starting with various initial positions for the carbon cluster seeds after an annealing time of 120 s. The choice of the initial conditions was based on experimentally revealed distinct dark regions in the FIB cuts within the silicide layer, which we identify as carbon inclusions (see Fig. 4). The simulated interfaces reproduce the key features observed experimentally: a continuous Ni₂Si layer with embedded carbon clusters of comparable size, spatial distribution and morphology. Both experiment and simulation show that the clusters reside predominantly inside the created silicide interface, consistent with the expectation that carbon is released at the reaction front and has limited mobility. Our findings demonstrate that carbon clusters tend to agglomerate into larger clusters, a trend that is observed both experimentally and in the MPF model.

It is known from experiments that electrical properties of contacts on SiC depend on whether the contact is located on the C- or on the Si-side of the wafer. This can likely be traced back to the differing interface energies, which are naturally

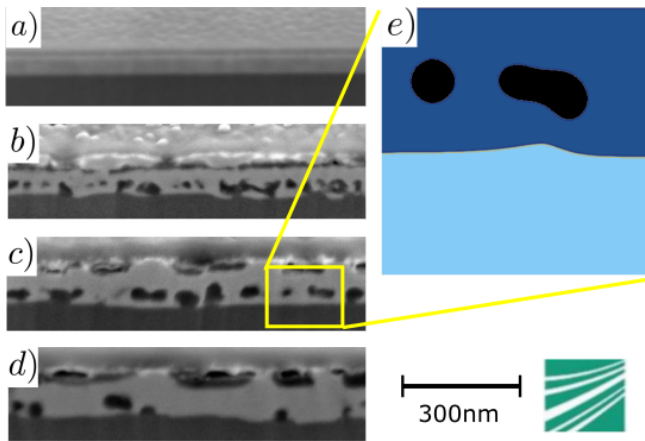


Fig. 4. Experimental FIB cuts after 120 s at different RTP annealing temperatures [b) $T = 1173$ K, c) $T = 1273$ K, d) $T = 1373$ K], where a) is a reference cut presenting the nickel thickness of 60 nm. e) An exemplary simulation adjusted to match the experimental FIB cut in c).

part of the MPF model and can be adapted according to the configuration. Further refinement of the model can be done in multiple ways. Since MPF models are firmly rooted on sound, physical principles, additional aspects such as explicitly implementing the nucleation of new carbon clusters, modeling the silicide layer by individual grains and including volume expansion during the phase transition can be readily included and will be explored in future work.

V. CONCLUSION

A multi-phase-field (MPF) model for the evolution of silicide layers with different numbers of phases and non-trivial grain structures was presented. A detailed description of the model was provided, since it differs considerably from more established methods like diffusion-reaction systems. While we focused on nickel silicidation of silicon and silicon carbide substrates, the MPF model can be applied to arbitrary metal-semiconductor systems.

In a simple one-dimensional example for nickel silicidation of a silicon substrate, we illustrated that the MPF model can reproduce sequential layer growth, a growth regime which is usually observed in thin-film silicidation [11]. We have shown an exemplary layer distribution, as well as the corresponding layer growth in time.

The second example concerns the growth and shape evolution of carbon clusters during the nickel silicidation of silicon carbide. Qualitatively, the MPF model reproduces experimental data obtained from FIB cuts of processed silicide layers. Starting from different initial seed positions for the carbon clusters, we obtain a wide variety of grain morphologies. The general evolution of the carbon clusters starts from several localized grains, evolving in time to combine into bigger clusters of different shapes. The exact shape of a cluster strongly depends on the localization. For example, the shape of the cluster differs close to an interface or within the bulk of the silicide.

In general, the main factors determining the system's dynamical evolution are the diffusion constants, the phase-fields mobility and the Gibbs free energies of the individual phases. While the latter are extracted from equilibrium phase diagrams and are well-known, diffusion constants are difficult to measure and carry a lot of uncertainty within the literature. For example, we did not describe grain-boundary diffusion, which happens orders of magnitude faster than diffusion through the bulk by a separate diffusion process.

Furthermore, for the two-dimensional situation, a more detailed calibration to the experimental results is desired. This includes both temperature and time evolutions. One example is the increase of the cluster size as well as their tendency of being localized at the top or bottom of the silicide. We expect that this potentially leads to the non-homogeneous thickness of the silicide, see Fig. 4 a)–d).

While the simulations in this work have a strong focus on the creation of Ni_2Si , additional phases, such as NiSi and NiSi_2 , strongly modify the size of the silicide. Those phases arise naturally at high annealing temperatures, such that one can improve the MPF model by further calibrations on other experiments such as XRD.

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