

# Nickel Silicide Growth Model: Coupling of Diffusion with Level Set Methods

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**Abstract**—Nickel silicide is being used as a Local-Interconnect (LI) and source-drain contact material in current CMOS technology. For scaling technologies it has become extremely important to reduce the parasitic resistances from Schottky contacts and LI. Modeling and predicting the silicide shapes has become necessary in order to estimate the transport through device accurately. This paper discuss the NiSi growth models implemented in Florida Object Oriented Process Simulator ( FLOOPS). Level set methods (LSM) coupled with Deal Grove’s kinetic model has been used for modeling and growth of NiSi. Focus in this work remains on implementing the above numerical techniques and obtaining the solutions by coupling LSM with the diffusion solver of the simulator. Dopant segregation capabilities are also demonstrated using chemical potential approach. These techniques can be easily used for advance technologies and special structures such as FinFET’s, Nano-Wires (Silicon), etc.

**Keywords**—nickel silicide, level set, simulations, diffusion, segregation.

## I. INTRODUCTION

Silicides are an essential part of modern technologies and they are used for contact and interconnects for many of the novel devices such as nanowires and FinFET’s. Both electrical and metallurgical properties of silicides are equally important for parasitic resistance control. Nickel Silicide is one of the best choices of material for current integrated circuits due to low thermal budget, low resistivity and ease of formation with silicon. Silicide formation is a thermally activated process with activation energy in the range of 1.4-1.6 eV for NiSi Phase [1]–[3].

Based on the growth kinetics from several studies [1]–[3] it is known that two phases of nickel silicide form sequentially. First Ni<sub>2</sub>Si phase is formed by totally consuming the nickel at temperatures around 300°C and then subsequent annealing at higher temperature (400-700°C) causes the phase transformation to NiSi phase. The Di-Nickel Silicide phase has a parabolic dependence on time, However the Mono-Silicide NiSi phase transformation occurs linearly with time. This Ni-Si system is considered to be a linear-parabolic system of growth taking diffusion and linear reaction rate into account as shown by Nemouchi *et al* [4] [5] . This is very similar to Deal-Grove’s model of silicon oxidation where oxide growth is linear and parabolic with time [6]. To better understand the interface shapes and properties of silicide growth and dopant segregation respectively we have coupled the Level

Set Methods with Deal-Grove’s Model to develop a complete numerical model to track the boundaries of silicide as well as to estimate the interfacial dopant concentrations.

## II. NUMERICAL TECHNIQUES AND MODEL

### A. Level Set Methods

Level Set Methods (LSM) are numerical techniques to track any evolving interface in two or three dimensions (2D/3D) [7]. It was developed by Sethian and Osher for propagating interfaces such as Flames, Oceanic waves, Material Boundaries, etc. There are many advantages of using LSM over variety of numerical algorithms such as marker/string method, cell-based method, etc. It does not break down in propagating sharp corners, also works for multi-dimensional problem of merging two disjoint interfaces and breaking interfaces naturally. LSM solves for the initial value partial differential equation. Numerical computations are performed on a fixed cartesian grid under eulerian settings. These techniques use hyperbolic conservation laws in conjunction with Hamilton-Jacobi formulation to obtain the solution for the advection equation.

The mathematical idea behind LSM is that it embeds the initial front information into a higher-dimensional function know as Level Set function  $\phi$ . It is defined all over the grid as a signed distance from the initial front or interface, positive in the direction of propagation and negative in the opposite direction. It solves the ordinary differential equation 1 and the interface at any point of time is given by zero level set  $\phi(x, y, z, t) = 0$ .

$$\phi_t(x, y, z, t) + F|\nabla\phi(x, y, z, t)| = 0 \quad (1)$$

where  $F$  is the propagation velocity dependent on diffusion coefficient, concentration, reaction rate, etc. Like level set velocity is also embedded into a higher dimensional function known as the *Extension Velocity* that is defined not only for the initial front ( $\phi = 0$ ) but for all the level set functions in the grid. Converting a problem into one order higher dimension could be computationally expensive to overcome but fast marching methods [7] allow this to be implemented efficiently. We have used dual level sets to tackle the nickel silicide growth modeling *Level1* representing the nickel diffusion and reaction

with the silicon and *Level2* to take care of the volumetric expansion of silicide.

### B. Deal Grove's Model

The kinetic's of silicon oxidation is accurately defined using the Deal Grove's model [6]. It uses the physico-chemical constants of the system and is based on the flux balance equations. Three fluxes used to completely model the growth are given below:

- The transport flux of diffusing species from bulk of the gas to the outer surface of oxide
- Diffusion flux of species through the oxide to the silicon
- And finally, the reaction flux between oxygen and silicon

Using the flux for each transport and reaction a linear-parabolic growth model equation is derived. Two limiting cases as we know diffusion controlled(parabolic) and reaction limiting (linear) growth are governed by the equation 2.

$$\frac{dx}{dt} = \frac{\frac{kC}{N}}{1 + \frac{k}{h} + \frac{kx}{D_{eff}}} \quad (2)$$

Where thickness ( $x$ ) of growth is estimated based on the diffusion ( $D_{eff}$ ) and transport coefficient ( $h$ ), reaction rate constant ( $k$ ) and concentration of oxidants ( $C$ ). It has been shown that the nickel-silicon system is very similar to oxidation growth [4] [5]. So we have solved for these fluxes numerically all over the two-dimensional grid and used the nickel concentrations and appropriate constants to simulate the silicide growth. This allows inclusion of limited source and spreading corner effects on the complex simulation shapes.

### C. Coupling of LSM with Diffusion: Model

Coupling of Deal Grove's diffusion model with level set is the basis of our numerical formulation to model and simulate the silicide growth. We know that nickel is the main diffusing species for  $NiSi$  formation and it behaves like an oxidation system. As shown in the flow chart (Fig.1) firstly level sets are initialized based on the nickel-silicon interface. Positive in the nickel and negative in silicon for *Level1* and vice versa for *Level2*. Level set equations are solved based on the initial silicide growth velocity for a very small time step  $\delta t$ . Then deal grove's flux equations are solved in Nickel, Silicide and Silicon to obtain the concentration values of nickel in the bulk and at each material boundaries. Appropriate diffusion coefficient and reaction rate constants has been chosen based on available data [8] [9] .

Level set updates are calculated, Bottom level set *Level1* (silicide growth) is updated based on the nickel concentration, nickel-silicon reaction rate and unit cell volume of  $NiSi$ . Top level set *Level2* (volumetric expansion ) is updated based on the amount of nickel leaving (estimated using a four point flux in a rectangular grid) and the difference between unit cell volume of nickel and silicide. To maintain the integrity of our model it is necessary that the level set never out runs diffusion. Finally a check is performed and to control that diffusion time steps are kept much smaller than level set update time steps

so that there are multiple or at-least one diffusion step before a final level set update is done to minimize the errors.

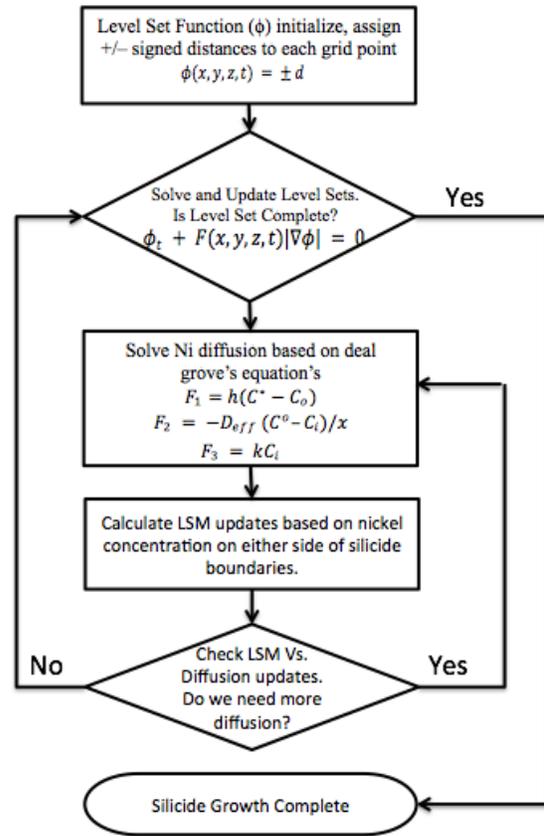


Fig. 1. Flow chart showing step by step simulation sequence and coupling of both Level Set Method with Deal Grove's Model.

### D. Chemical Potential Approach for Dopant Segregation

It is shown in several studies that the dopants present in silicon tends to segregate at the silicide-silicon boundary during the growth [12] [13]. It is really important to understand the interfacial properties such as dopant concentration to estimate the lowering of schottky barrier height at the contacts. One of the main goal of our simulation is to correctly predict these segregation profiles. In order to do that we have used a thermodynamics approach of chemical potential.

A chemical potential  $\mu$  of a species is given by its tendency to change from one state to another lower energy state. This concept is very similar to the quasi fermi levels in a P-N junction, as two materials with different fermi levels are joined together diffusion of electron or holes takes place to balance the chemical potentials on each side. In our case of dopant segregation in silicide we have used this concept of  $\mu$  to simulate the segregation profiles after silicidation. We implemented this to be solved hand in hand with the diffusion and level set solution, as level set advances based on diffusion steps segregation takes place simultaneously. The chemical

potential of a species is assumed to be directly proportional to the log of its concentration Eq.3.

$$\mu \propto \frac{1}{2}k_B T \ln C \quad (3)$$

To model the snow plowing or segregation effect we have implemented the flux (from material A to B) Eq.4 into FLOOPS in terms of  $\mu$ .  $m_{AB}$  is the segregation coefficient between two materials.

$$F_{AB} = h(C_A - \frac{C_B}{m_{AB}}) \quad (4)$$

The equation is of the form

$$J = D * C * \nabla \mu \quad (5)$$

Where  $\mu$  is equal to  $\log C + K$  (related to  $m_{AB}$ ),  $C$  being the concentration of moving species and  $D$  is controlled by the diffusivity of the species in each material as well as transport rate  $h$  at the interface. The chemical potential is a useful quantity to represent the thermodynamics of a system in our case segregation of dopants. It takes care of the physical process involved accurately. Some preliminary results are presented in Fig.5

### III. SIMULATION RESULTS AND DISCUSSION

To simulate the silicide growth and check the models validity with the TEM (Transmission Electron Microscopy) data we used few structures including complete process simulation. A rectangular grid is used in FLOOPS to create the structures. Grid spacing is maintained at  $0.002\mu m$  near the simulation edges and is relaxed away from it to save the computation times. However, the level set grid is generated with uniform spacing of  $0.002\mu m$  to reduce any interpolation errors. Several structures are presented and the first one is similar to a Spacer-Source/Drain edge profile in a MOSFET (Metal-Oxide-Semiconductor Field-Effect Transistor).

As shown in the Fig.2 nickel (Red) is deposited on top of silicon (Green) and an oxide (Blue) layer is added to act as a spacer. Both zero level sets (Top and Bottom) are shown (black curves) after simulation is finished. Typically a thin layer of nickel is deposited and is completely consumed for silicide formation, but in our case nickel supply is maintained at high for the sake of growth simulations. Silicide formation under the spacer edge due to the limited supply of nickel is captured in this simulation model. This comes directly from our solution of the diffusion - reactions equations for Nickel based on Deal Grove behavior. Silicon consumption ratio has also been maintained,  $1^\circ A$  of nickel reacts with  $1.83^\circ A$  of silicon to form  $2.3^\circ A$  of nickel silicide [11]. Diffusion coupling with LSM is shown in Fig.3 each blue line represent level set update with multiple diffusion steps.

Second structure is a narrow poly gate with nickel deposited on top and oxide spacers on the sides. Simulation results as shown in Fig.4 is a mushroom dome kind of formation that matches well with the literature TEM data [10] We can clearly see that due to the large supply at the two edges

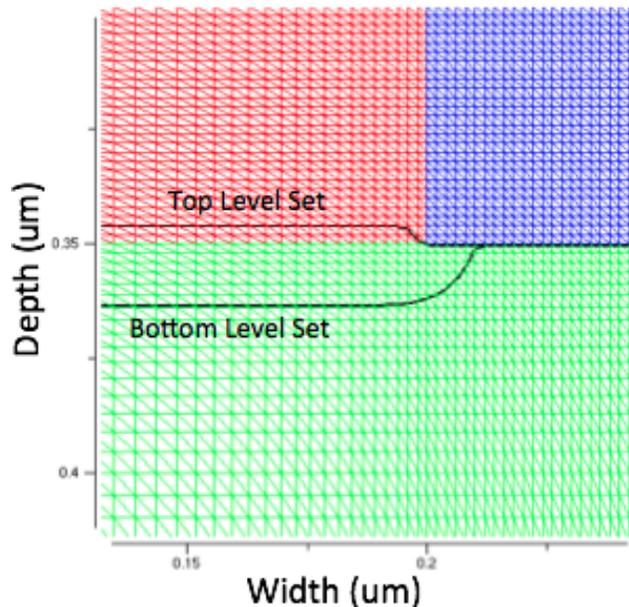


Fig. 2. 2D Silicide growth simulation results shown on FLOOPS grid with two zero level sets representing NiSi growth and volumetric expansion. Nickel(Red), Silicon(Green) and Oxide(Blue).



Fig. 3. Level set function for several delta time step each blue lines represent  $\phi = 0$  at various point during LS update. Every curve is a result of diffusion updates for level sets.

amount of nickel diffusing through the poly edges is much more than the bulk causing more growth on the side walls resulting in the dome shape silicide formation. Inset in figure.3 again shows the level set progress for each time step coupled with diffusion. Both the structures display a good match for 2D silicide growth, thus this model can be used for shape matching simulations. These models can be easily extended to be used for silicide shape predictions on novel structures such as FinFET's, silicon Nano-Wires, etc.

Finally dopant segregation profiles are also simulated simultaneously with the growth and diffusion using the *Alagator* scripts. It is a scripting language used in FLOOPS to represent the partial differential equations. Of most relevance in this case, is the ability to use relational operators and if then else

constructs with the differential equation. This allows an easy comparison of which side of the level set interface. For our case diffusivity is implemented in a way ( $Level1 > 0.0$ )?D1:D2 this provide a different diffusivity on either side of the interface. It is also used to set the chemical potential difference that drives the segregation across the interface using the formulation .

It requires us to couple three different equations (similar to 1, 2 and 5) simultaneously for each time step. As nickel diffuses through silicide following Deal Groves models, level sets are updated after a certain time step and then the bottom zero level set ( $Level1$ ) data is used to segregate the dopants concurrently. As shown in Fig.5 is the dopant profile after silicide growth at three different locations blue curve represents the segregation at most silicide thickness, green being lesser and red curve for the least amount of silicide. Simulations are in good agreement with some of the observed SIMS profiles [12] [13].

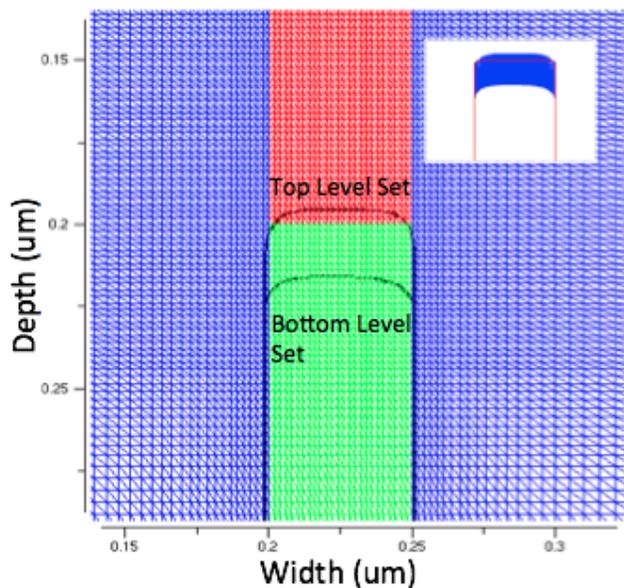


Fig. 4. Narrow poly gate simulation results with zero level sets shown in black. Inset shows the level set updates with multiple diffusion steps.

#### IV. CONCLUSION

In summary the 2D silicide growth models were implemented in FLOOPS using Level Set Methods and Deal Grove's models. Diffusion is successfully coupled with LSM. Good agreement is observed between simulated results and TEM data. This dual level set technique with accurate physics of the growth process can be used for simulating a wide variety of novel structures as well as numerous metal silicides schemes with minimal changes. These models can be easily transferred to a commercial TCAD simulator such as synopsys sentaurus process. Promising initial results are also shown for dopant segregation profile prediction.

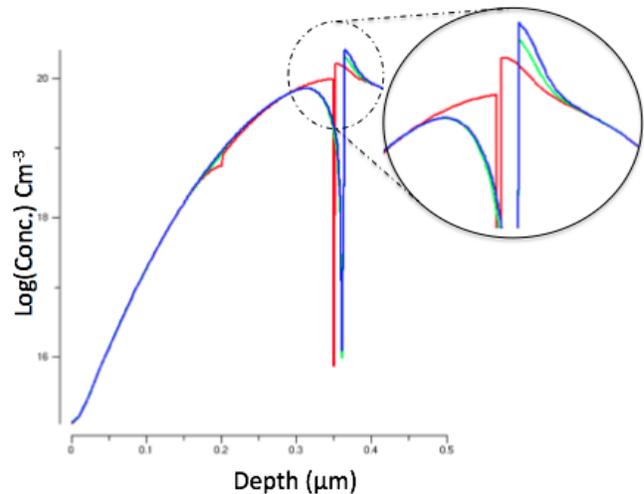


Fig. 5. Dopant segregation simulation for various depths, showing accumulation at the silicide-silicon interface.

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