Modeling and Simulation of Dopant Segregation at NiSi/Si Interface Using Chemical Potential Approach

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***Abstract*—The effect of silicidation induced dopant segregation on Schottky Barrier Height (SBH) of a metallic source/drain junction has been a significant factor in governing transport and contact resistance of MOSFET devices. This paper focuses on numerical method for modeling and simulation of dopant segregation implemented in Florida Object Oriented Process Simulator (FLOOPS). Chemical potential approach is used to model the segregation of Arsenic (As) during the growth of Nickel Silicide (NiSi) on a 2D planar structure. Level set methods also implemented in FLOOPS helped us predict the silicide shapes accurately. We have coupled the silicide growth models with chemical potential based segregation equations to predict the dopant profiles during growth. We also did verify our results by using the accurate pre and post silicide dopant profiles from the existing SIMS data for various temperatures. Moreover these models can be used for any species based on their diffusion, segregation and transport coefficients in each material.**

***Index Terms*—nickel silicide, level set, simulations, diffusion, segregation.**

I. Introduction

Recently there has been a renewed interest in controlled dopant segregation at the silicide source/drain junction to modulate the Schottky Barrier Height as the device size is shrinking continuously [1], [2]. In order to lower the parasitic resistance at the metal semiconductor junction it has become important to reduce the SBH using segregation techniques, that ultimately helps in band bending and increased tunneling probability through the schottky barrier. Also dipole generated within 1-2nm due to dopants can also help in lowering the barrier height. This is advantageous as using the pre-existing impurity a highly doped silicon layer can be created at the interface without any special temperature annealing treatment.

Segregation or redistribution of dopants at silicon interface during nickel silicide growth has been observed in several articles [3]–[6]. Dopants like arsenic gets snow plowed into silicon due to its higher diffusivity and segregation coefficient. Several different species are also reported to reduce the SBH and parasitic resistance at the source/drain contacts for bulk, SOI and FinFET devices [7]. It is seen that segregation reduces SBH as well as transmission but transport is more favorable because it is exponentially dependent on SBH [8]. In this work we have implemented a numerical model based on thermodynamic chemical potential to model the dopant segregation that can be used for any given species based on various physical parameters.

II. Numerical Method and Modeling

A. Chemical Potential

Chemical potential (μ) measures the tendency of particles to diffuse as a function of position [9]. It measures the rate of change of a thermodynamic function per particle and for individual species. In simple words chemical potential of a species in the mixture can be defined as the partial derivative of the free energy (G) with respect to change in concentration (C) of that species. In case of an ideal semiconductor chemical potential is in the middle of the band gap and is known as the Fermi Level. A general representation of chemical potential is a partial differential of Gibbs free energy G(x) with respect to the concentration and is given by Eq.1, it is directly proportional to the log of normalized concentration of the species. Where k_B is the Boltzman constant, T is temperature of the system and C is the concentration of particles.

$$\mu(x) = \frac{\partial G(x)}{\partial n(x)} = \frac{1}{2} k_B T \ln C(x) \tag{1}$$

This quantity is quiet useful in order to tackle the segregation-diffusion problem as is present in our system of NiSi/Si interface and diffusing Arsenic impurity. Based on the chemical potential on both sides of the interface μ_A and μ_B (as shown in Fig.1), differential equations are solved to calculate the segregating profile.

B. Numerical Model for Segregation

To develop a numerical model we assume that the difference in Chemical Potential (CP) between two materials is the driving force behind dopant segregation(refer to fig.1). Also the particles will continue to segregate until chemical potentials reach an equilibrium, to represent segregation a simple flux equation can be used.

$$F_{ab} = h * (C_a - \frac{C_b}{m_{ab}}) \tag{2}$$

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Where h is the transport coefficient, C_a and C_b concentration in each material and m_{ab} is the segregation coefficient. The segregation driving force on a particle is given by gradient of its chemical potential $-\frac{\partial \mu(x)}{\partial x}$. Finally a flux equation Eq.3 is established based on CP to determine the particle movement with growth.

$$J(x) = D * C * \nabla(\Theta(x)) \quad (3)$$

Where D is diffusivity, C is the concentration of impurity and Θ is directly based on chemical potential. A time dependent Partial Differential Equation (PDE) Eq 4 is solved numerically on a 2D grid to obtain the dopant concentrations at each time step of growth. This model has been coupled with previously demonstrated diffusion and growth models of silicide using Level Set Methods [10]. Then for each discrete time step of growth segregation equation is also solved concurrently.

$$\frac{\partial C(x,t)}{\partial t} - D * C(x) * \nabla(\Theta(x)) = 0 \quad (4)$$

Where $D = D_1 :: D_2 :: h$ is dependent on As diffusivity in materials NiSi (D_1), Silicon (D_2) and transport coefficient h at NiSi/Si crossing interface using Level set function. $\Theta = log(C(x)) + K(Level < 0)$ where K is the segregation coefficient between silicide and silicon. Based on sign of K and interface information (Level) we can simulate either snowplowing or depletion of impurity atoms (refer to [10] for Level). This kind of formulation has been used by *Tan et al* for diffusion-segregation problem of point-defects [11]. Using appropriate constants we simulated the growth and snowplowing effect of nickel silicide. Above PDE's are implemented as an Alagator script in FLOOPS [12].

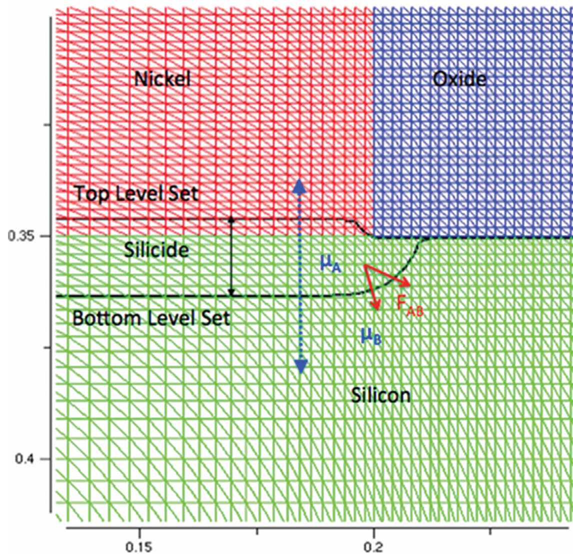

Fig. 1. Level Sets showing silicide growth with segregation flux from silicide to silicon.

III. Results and Discussion

Simulations were performed for 20nm of silicide growth at various temperatures and using eulerian type grid settings with spacing of 2nm. A concentration dependent term was added to diffusivity and transport coefficient used was also high enough to maintain continuity.We have used the SIMS (Secondary Ion Mass Spectroscopy) data from *Hoummada et al* as a benchmark to verify our results [5]. Initial As profile in silicon as shown in Fig.2 was digitized and used as an input to our simulations.

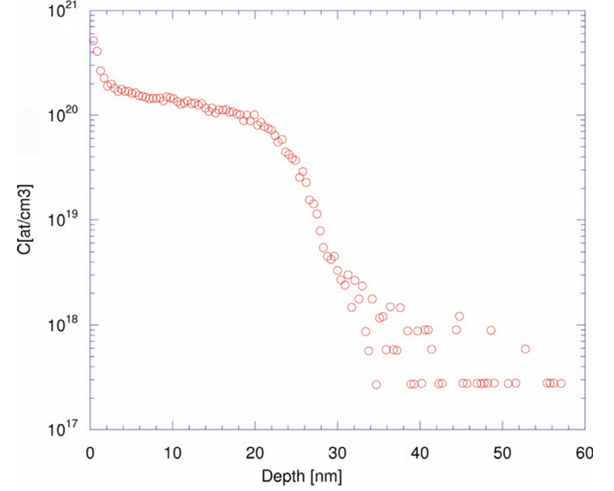

Fig. 2. Doping profile of Arsenic in silicon before silicidation. [5]

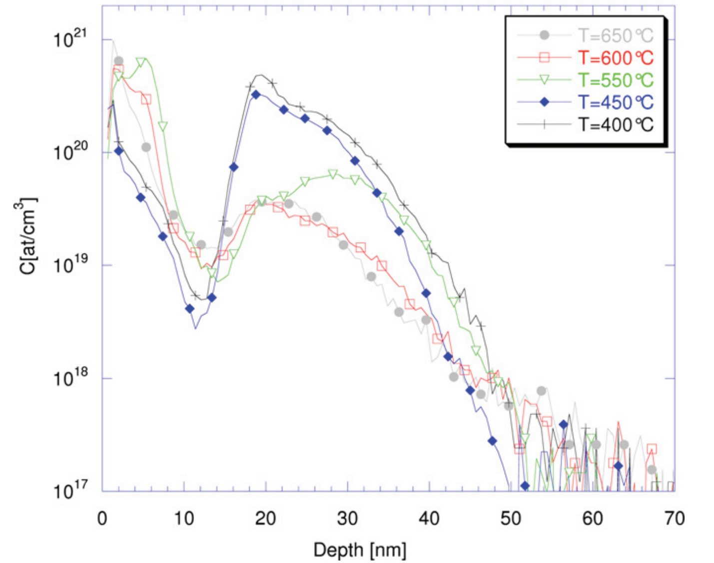

Fig. 3. Arsenic profiles after 20nm silicide growth at various temperature showing accumulation at the interface and surface. [5]

Figure 3 is the profile of As after silicide growth as a function of depth at various RTP (Rapid Thermal Processing) temperature. We can clearly observe that redistribution of arsenic in 20nm NiSi layer is towards the accumulation

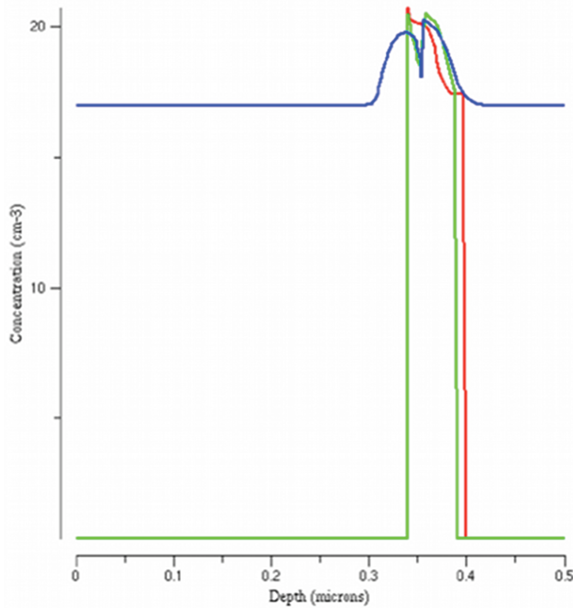

Fig. 4. Arsenic segregation simulation results with background doping of 1e17/cm-3.

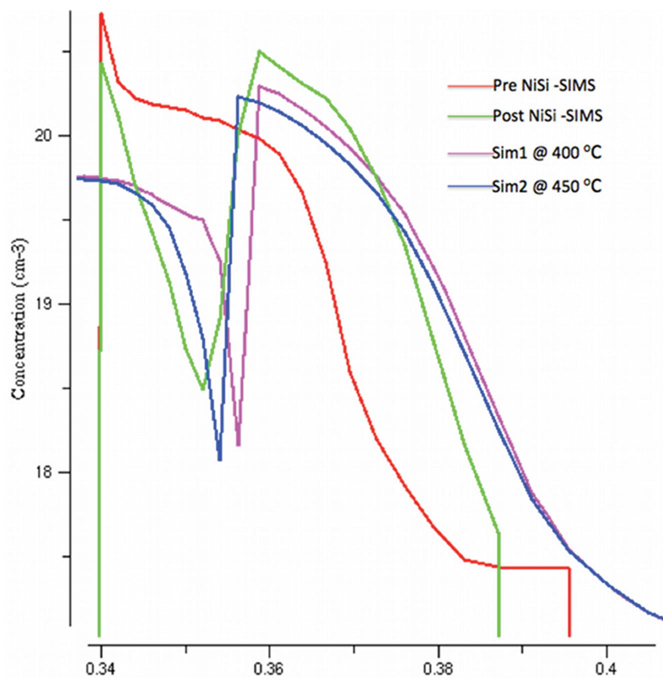

Fig. 5. Zoom in profile of arsenic segregation simulations at 400 and 450C. Red and green are Pre and Post SIMS data, pink and blue are simulated profiles.

at the surface and at the interface and increase of arsenic concentration is observed after silicidation.

Segregation simulation results for couple of temperatures are shown in Fig.4&5 along with the initial and final profile of dopants from SIMS analysis. A constant impurity profile of 1e17/cm^{-3} was used as a background for simulation purposes only. Red and green curve are the initial and post silicide growth impurity profile taken from SIMS, pink and blue are simulated profiles for 400 and 450°C respectively.

Both the shapes show a close match with the real data. It has also been observed that at a higher temperatures the accumulation peak is reduced which is clearly captured in our simulation profile as well (blue curve for 450°C). At further higher temperatures 500-700°C arsenic peak goes down substantially that can be explained by agglomeration of NiSi.

Simulation data at the surface show a lower peak as compared to real data, it can be accounted for due to the limitation of accurate SIMS measurement of dosage present at a few nanometer depth beneath the surface. Also another factor that could result in lower surface concentration is that our structures has open boundaries to let impurities diffuse on both side of the surface as observed in Fig.4.

Grid sensitivity is sometimes a concern when solving diffusion like equation on varying grid sizes. Segregation equation implemented were tested in 1D in order to estimate the errors. Results are shown in Fig.6 for varying grid size we can clearly see that bigger grid size leads to more error. Nevertheless, computation error is no worse than solving diffusion error solved on FLOOPS grid. Overall this model seems to be reliable for predicting the profiles and has been implemented in successfully.

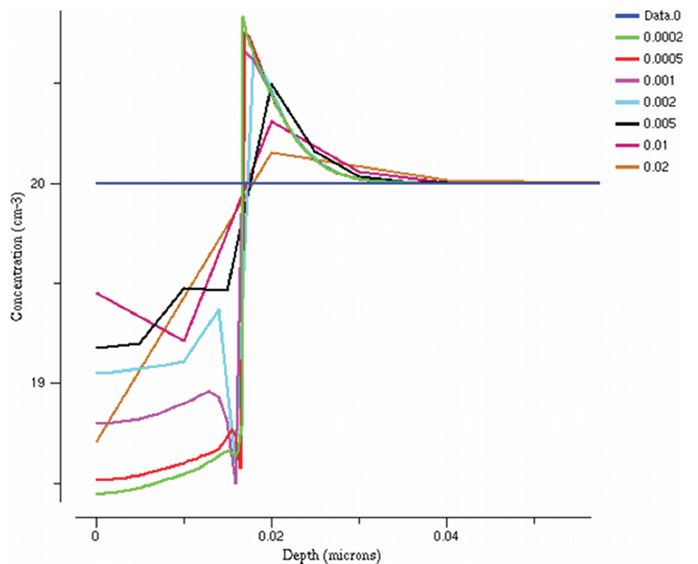

Fig. 6. Grid sensitivy simulation results showing increasing error with big grid size.

IV. Conclusion

2D modeling of dopant segregation using chemical potential approach was implemented in FLOOPS and coupled to the nickel silicide growth model using Level Set Method and Deal Groves model. Arsenic result show a good match with the SIMS data from several studies. This model can be used for various impurities. These models can be easily transferred to a commercial TCAD simulator such as synopsys sentaurus process.

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