Full device scale atomistic kinetic lattice Monte-Carlo simulation of metal-induced lateral crystalization process

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***Abstract*— In order to have a high-quality crystallinity for boosting the device performance, the metal-induced lateral crystallization (MILC), using Ni becomes a critical process in semiconductor industries. Simulating full process has difficulties because of scale difference between nanometer-scale atomistic process and micrometer-scale device. In this study, we first present full device scale simulation of MILC process, using efficient atomistic kinetic lattice Monte Carlo simulation. Balance between thermodynamics and kinetics reveals that the crystallization rate is dominated by the energetically stable interfaces. Moreover, we found the dynamic instability of the MILC process, which could potentially fail the device fabrication in a few micrometer scale.**

Keywords*— *Metal-induced lateral crystallization (MILC), kinetic Monte Carlo (KMC), Nickel Silicide

I. INTRODUCTION

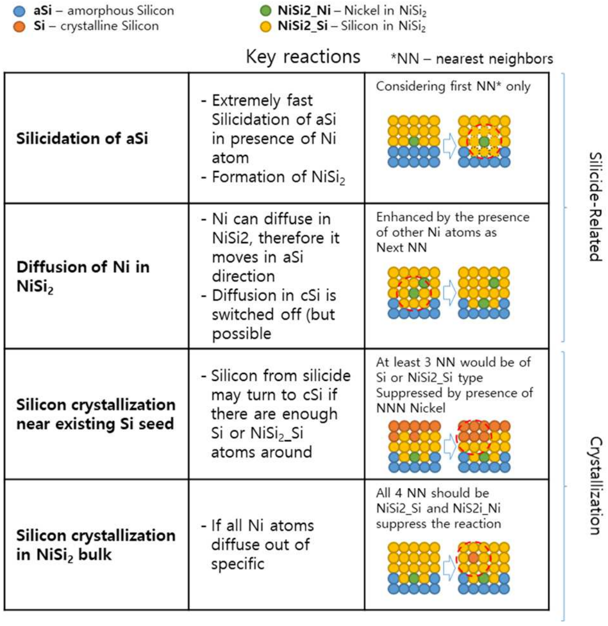
In modern flash memory technology, highly-integrated three dimensionally stacked transistors are connected through a vertical silicon channel. These channel lines are initially deposited as an amorphous silicon phase, and then annealed at high temperatures to crystalline into poly silicon. Recently, as stack height becomes higher, it becomes necessary to achieve higher crystallinity of the silicon channel. Metal-induced lateral crystallization (MILC) is a promising technology to make a silicon channel as a single crystal [1]. Once Nickel is deposited on the amorphous silicon, silicidation process creates $NiSi_2$ layer. Nickel silicide further propagates in the amorphous silicon, while leaving the single crystalline phase behind.

In this study, for the first time, we have simulated full device scale process of the MILC, in a fully atomistic manner. A kinetic lattice Monte Carlo (KMC) method is employed to simulate atomistic reactions inside the silicide. By using KMC method we could simulate a few micrometer scale process within a reasonable computational time.

II. ATOMISTIC KMC METHODOLOGY

For efficient simulation of kinetic behavior of each atom in a system, we've applied KMC method to simulate MILC process. KMC only considers positional changes of each device atom while ignoring unnecessary vibrational events. Hence, we can simulate atomistic behaviors in a full device scale [2].

Since KMC is inherently an empirical method, we should define the corresponding atomistic reactions a priori to the simulation. We have made KMC reaction events according to



Silicidation of aSi	- Extremely fast Silicidation of aSi in presence of Ni atom - Formation of $NiSi_2$	Considering first NN* only
Diffusion of Ni in $NiSi_2$	- Ni can diffuse in NiSi2, therefore it moves in aSi direction - Diffusion in cSi is switched off (but possible	Enhanced by the presence of other Ni atoms as Next NN
Silicon crystallization near existing Si seed	- Silicon from silicide may turn to cSi if there are enough Si or $NiSi_2$_Si atoms around	At least 3 NN would be of Si or NiSi2_Si type Suppressed by presence of NNN Nickel
Silicon crystallization in $NiSi_2$ bulk	- If all Ni atoms diffuse out of specific	All 4 NN should be NiSi2_Si and NiS2i_Ni suppress the reaction

Fig 1. All atomistic reactions are illustrated in the table. We have considered reactions inside the silicide and the interface crystallization/silicidation reactions, all in atomistic manner.

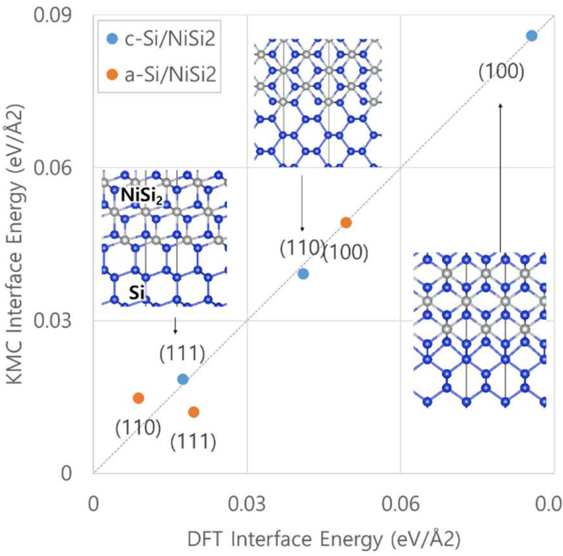


Fig 2. Binding energy calibration result of the KMC model. The DFT interface energy and the interface energies from the KMC bond counting model agrees well.

the previously reported atomistic reaction pathways [3]. The corresponding reactions are illustrated in the Fig. 1. Compared to atomistic methods such as DFT or molecular dynamics, the advantage of KMC is that it only considers initial and final configurations, and considers the transition kinetics by efficient reaction rates. In this way, we can only simulate the configuration changes, without computing vibrating atoms, which do not change the bond configuration. This enables KMC to simulate the real device structure in a real process time. For each KMC reaction, the rate is calibrated so that the stable MILC can occur through a μm scale.

In order to describe the crystallographic feature of the MILC process, we adopted the bond-counting model in the KMC simulation. It is well reported that for the during the crystalline epitaxial growth, each orientation has distinct crystalline rate. This growth kinetics determines the final shape of the epitaxial crystal. This final shape follows the thermodynamic property of surfaces (or interfaces). It is energetically favorable to have smaller area of high energy surfaces/interfaces. It can be achievable when the higher energy surface has faster growth rates. Then the fast growing surface leaves behind the slow growing surfaces on its boundary, and finally the whole structure is covered by the low energy surfaces. It is reported that the silicon bond-counting model can successfully describe the epitaxial shape on the silicon growth [4]. Within this model, each bond has an effective binding energy for the additional atom attachment. The KMC growth rate is then calculated by the Arrhenius relation of the binding energy. Therefore, the bond configuration with the high energy has the faster crystallization rate, and as a result, the surface with the higher energy has the faster growth rate. In that sense MILC process is somewhat similar to the epitaxial growth of the silicon. As the $NiSi_2$ layer proceed into the amorphous region, the remaining region becomes crystalline. In addition to this, the interface between two different materials in MILC is analogous to the surface of silicon in the epitaxial growth. By these reasons, we adopt the bond-counting model in the MILC process, which is defined on the auxiliary silicon lattice.

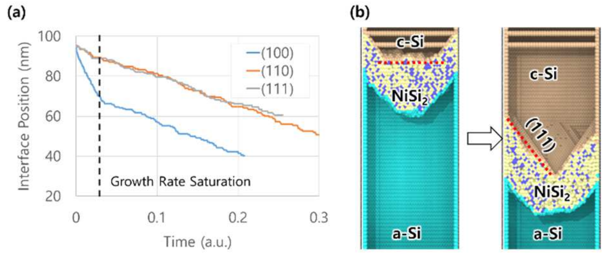


Fig 3. (a) Time dependent crystallization profile, on each key Si orientations. After certain time, all orientations shows same crystallization rate. (b) {111} Facet formation during the crystallization process. Because {111} facet is energetically most stable, and hence has the slowest reaction rate, regardless of the initial orientation, the interfaces tends to form {111} facets. Once faceting is completed, the rate saturates.

The KMC bond parameters are calibrated according to the interface properties from DFT calculations. In general, the interface has higher energy compared to its bulk structures because the bonds are broken on the interfaces. By counting the numbers and types of the broken bonds on the surfaces, we can map the surface energy onto corresponding bond energies. Analogous to this, we can consider the interface as the effective surface, and map the interface energy to corresponding effective broken bonds. In MILC, there are two interfaces: c-Si/$NiSi_2$ and a-Si/$NiSi_2$. On both interfaces, we calculated DFT interface energies, and mapped to the auxiliary silicon bond model. Fig. 2 shows good agreement between DFT interface energies, and the energy converted by the bond-counting model. We expect these energy values properly capture the crystalline behavior during MILC process.

III. APPLICATION OF THE METHODOLOGY

First, we have tested crystallization rates depending on crystallographic orientations, and the result shows seemingly contradictory growth kinetics. In these tests parameters on microscopic reactions are carefully calibrated to realize stable crystallization growth on a few hundreds of nanometers. Fig. 3 (a) shows the crystallization position through process time, on 3 key directions: <100>, <110>, and <111>. Our KMC results shows that the final crystallization rate saturates to a constant value regardless of the grain orientation. It is well

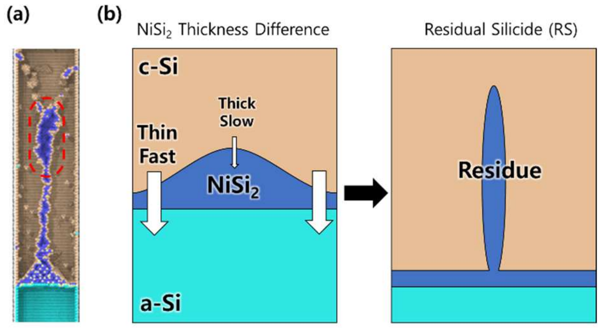


Fig 4. (a) A dynamic unstable crystallization of MILC process. A chunk of silicide is left behind the crystallization front. This reduces the total amount of Ni at the c-Si/$NiSi_2$/a-Si interface, and potentially stop the process. (b) Once stochastic randomness creates deviation of the thickness, due to the difference of the MILC rate, the slow thick region is left behind the crystallization front, forming a residual silicide.

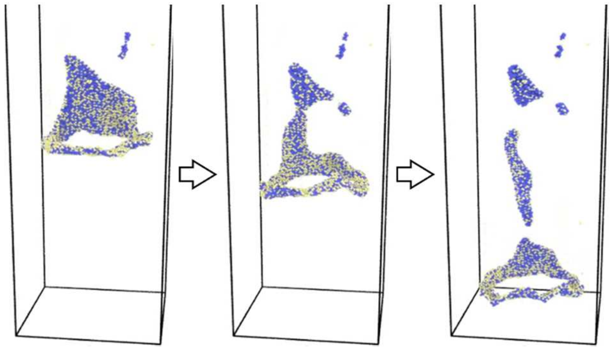


Fig 5. Residual silicide is forming from the dynamic instability of the $NiSi_2$ layer. For simplicity, only the $NiSi_2$ part is shown in the figure. A thicker part becomes slower, left behind the MILC reaction front. The MILC process exagerates the thickness deviation, and finally the thicker part completely surrounded by the crystalline silicon.

known that on the single crystal growth, the growth rates vary depending on the surface energy of the given orientation. In order to minimize the total surface energy, the crystal tends to form the smallest surface area for the largest energy surface. As we have shown in Fig. 2, the {100} interface has the highest energy on both c,a-Si/$NiSi_2$ systems. From these values, one might think that the <100> grain direction has the fasted MILC rate.

In order to clarify this mismatch, we have investigated detailed interface structures on early stages of the process. On Fig. 3(a), on early stage of the growth, the <100> direction has the fastest crystallization rate, which is due to higher energy of {100} interfaces. After some moments has passed, the rate becomes saturated. Fig. 3(b), shows the interface structures before and after the saturation. On the initial stage, as marked as red lines, there exists {100} facet, which has faster crystallization rate. In order to reduce this high energy facet, stable {111} facet starts to grow from the boundary of the structure, where there is no crystallization seed to grow crystalline silicon. As {111} grows from the boundary, it finally covers all crystallization interfaces. Once energetically stable {111} facet was formed on the interfaces, the growth kinetics is dominated by the {111} facet, and hence the final rate does not have dependency on the facet orientation. Though this saturation is purely geometric depending on the width of the structure, we expect that for real devices, with high-aspect ratio, this initial facet formation is negligible and all orientations might have the same crystallization rate.

We further investigated possible dynamic instabilities during the MILC process by changing the KMC reaction parameter values. Fig. 4 (a) shows an example of MILC failure. There exists long tail of $NiSi_2$ behind the reaction front at the amorphous silicon. As the process goes further, this tail will be completely surrounded by the crystalline silicon, and becomes a residue of the silicide, which would affect further crystallization reaction. This residue formation consumes the silicide and could possible stop the crystallization due to lack of the silicide.

One might guess that this instability is originated from the kinetic property of the process, because this residue can form even without introducing any external defect in the system. The KMC model is an intrinsically stochastic model, which inevitably has random noise during the system. This randomness could be a physical noise, because thermal process including diffusion is well known non deterministic process. If a process has any dynamic instabilities, that instability grows larger as time progresses.

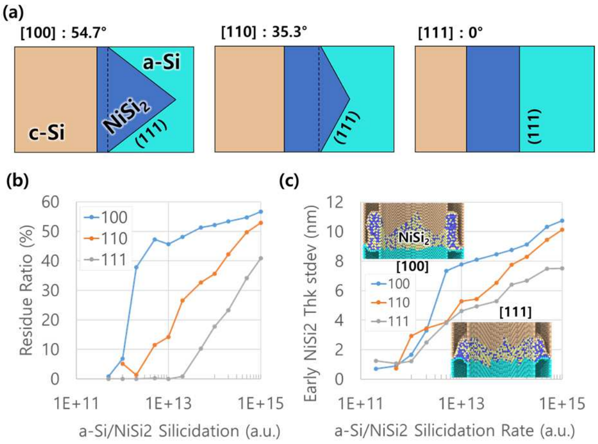


Fig 6. (a) The angle between stable {111} facet and the MILC direction with respect to the grain orientation. On the <100> grain orientation, the angle between the facet is the largest, and hence has the largest variation of the thickness. Since this thickness difference is purely geometric, the trend might be universal regardless of the reaction condition. (a) Size of the residue on each silicon orientation with respect to the silicidation rate reveals that for all possible parameter cases, <100> direction shows the largest number of residual Ni atoms, indicating the unstable MILC process. (b) On the eargy stage of MILC, the silicide thickness variation differs with respect to the crystallographic orientation. The <100> orientation has the highest variation of the thickness.

Unlike simple epitaxial growth, MILC process has two distinct reactions on separate interfaces, which is connected by diffusion through the silicide. On the amorphous silicon interface, during the silicidation reaction, a nickel atom is consumed on the interface, by forming the $NiSi_2$ layer on the originally amorphous silicon region. This reaction could only happen when a free nickel atom is supplied. The source of this free nickel is at the amorphous silicon interface. On this side, the silicon crystallizes, releasing a free nickel atom inside the silicide. This nickel atom could reach on the amorphous silicon interface by diffusing through the silicide.

This diffusion mechanism provides the dynamic instability inside the system. When the thickness of the $NiSi_2$ becomes thicker, it will take longer time for a nickel atom diffuses to the amorphous silicon interfaces. This slowing by the diffusion could slows down the MILC rate. It has been reported that the thinner silicide leads the faster growth, due to shorter diffusion length [5]. This slowing of MILC in the thick silicide provides an origin of the intrinsic dynamic instability of the MILC process. Fig 4(b), shows the schematic demonstration of the dynamic instability. Because the reaction is dealing with the diffusion, it is physical to expect stochastic variation in the random walk diffusion process. This randomness can be captured in the KMC simulation. Once the thickness variation occurs, the overall crystallization rate at the thicker region becomes slower, even though the interface reactions are unchanged. This slowing is due to lack of source at the interface. Then this growth rate difference would increase the thickness variation, because the thinner region proceeds further, while leaving the thicker region behind as a residue. On Fig. 5, we captured the residual silicide forming moment. The thicker point becomes very slow, and the original interface stuck at the original position, while other parts precedes to the amorphous region. This reduces total volume of the silicide, and may lead failure due to complete consumption of the silicide. The only way to avoid forming of residue is to reduce the thickness deviation, which could dynamically emerge throughout the MILC process. One simple solution is to increase the diffusivity of free nickel atoms inside the $NiSi_2$. By this way, even under small thickness variation, the diffusion would smear out the variation, and might make the whole system in more uniform way.

Furthermore, we investigated the stability of the MILC reaction with respect to the grain orientation and found out the geometric origin of the stability. From Fig. 3, we can expect that on a stable MILC regime, crystalline silicone can stable form regardless of the initial grain direction of the silicide. This uniformity is originated from the stable {111} facet formation during the crystallization process. This facet formation is pure geometric, and only happens on specific angle with respect to the crystal structure. On different grain orientation, this stable facet might have different orientation. Fig 6. (a) shows the angle between the energetically stable facet and the crystallization direction on each key orientations. We found that on the <100> grain, the {111} facet has the largest angle, and hence might have the largest thickness variation of the $NiSi_2$ layer. As Fig. 4 shows, this variation is a seed of residual silicide formation during the process.

We found out that on a unstable MILC regime, the <111> grain shows the most stable growth kinetics. In order to investigate both stable and unstable regime of MILC, we have changed the silicidation reaction rate on the amorphous silicon interface. On Fig. 6 (b), by changing this rate, we counted the number of residual atoms. This number of residue atoms represents the stablility of the reaction. Through the reaction range, the <100> direction shows the most residual atoms, indicationg the most unstable growth. As shown in Fig 6(A), this deviation migh be originated from the crystal angle with respect to the growth direction. To confirm this, we checked the correlation between stabilith and thickness deviation of the early stage with no residues (Fig. 4(c)). As we expectec, the <100> case shows most rough silicide for all parameter range, and hence becomes the most unstable direction.

Finally, we have simulated the MILC process in a real device scale. A 5 µm long silicon channel is chosen as a reference structure. Fig. 7 shows the snapshots of the MILC process for both stable (a) and unstable (b) cases. On a stable case, a perfect crystallization without defect proceeds to the bottom of the silicon. In contrast, the unstable one leaves the residual nickel atoms, surrounded by the crystalline silicon. By carefully changing the reaction parameters, our model can explore both stable and unstable cases within a single model. In addition to that, it shows a possibility to simulate the MILC process in a real device dimensions, by using efficient atomistic KMC simulation.

IV. CONCLUSIONS

In this work, we have developed device scale KMC simulation method of MILC process, which efficiently deals change of morphology in atomistic scales. By this method, we could simulate real device scale process in fully atomistic manner. We found out that even for defect-free cases, dynamic instability could make structural fault, which leads failure of the whole process. Our new methodology could be applied not only to Ni related silicidation, but also any other silicidation processes in crystalline silicon.

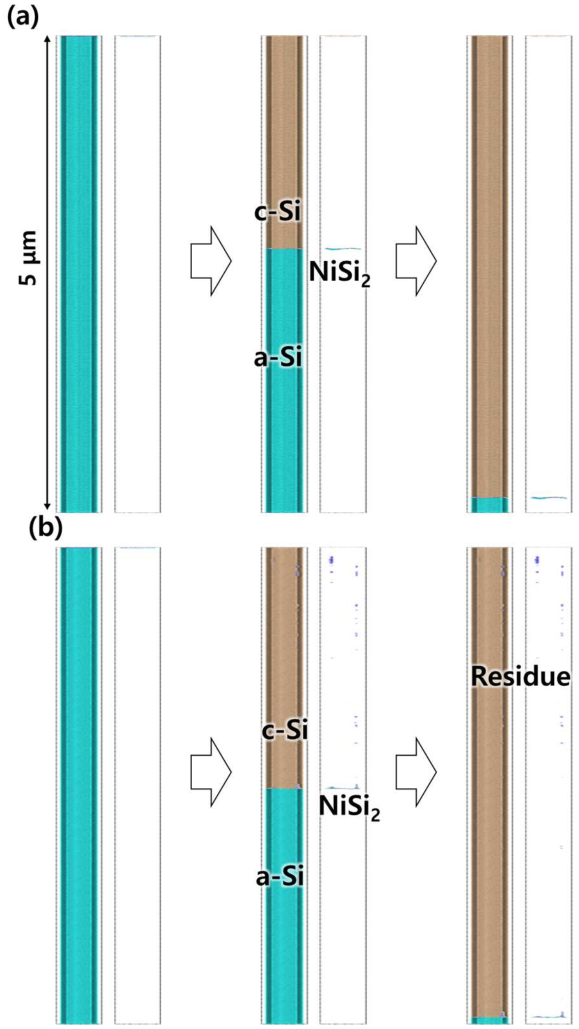


Fig 7. Growth snapshots of a 5 µm silicon channel structure. (a) shows stable growth and (b) shows forming of a residue during the crystallization. A single model can demonstrate both stable and unstable behavior by only changing reaction rates.

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