Nucleation and Growth of Epitaxial Silicide in Nanowire of Silicon

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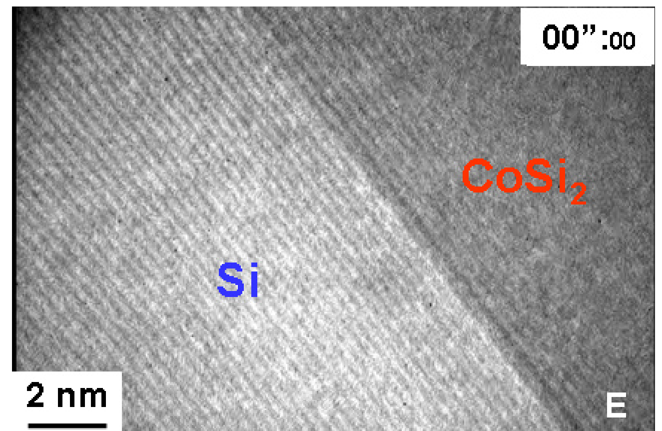
***Abstract*- When two nanowires cross each other, they form a point contact. Point contact reaction between a nano metal wire and a nano Si wire has been studied by using ultra-high vacuum and high resolution transmission electron microscopy. Axel epitaxial growth of nano silicides of NiSi and $CoSi_2$ in nanowires of Si has been observed. The nucleation stage and stepwise growth stage of the reactive epitaxial growth of nano silicide on nano Si have been measured. A repeating event of homogeneous nucleation has been found, which enables us to estimate the number of molecules in a critical nucleus to be about 10 using the Zeldovich factor. A comparison to heterogeneous nucleation will be made. The nucleation-controlled or supply-controlled growth mode of point contact reactions is different from the well-known diffusion-controlled and interfacial-reaction-controlled modes of growth in thin film and bulk samples.**

I. Introduction

Our ability to synthesize and fabricate nanostructures over the past decade has fueled the tremendous growth in the area of nanoscience and nanotechnology. [1, 2] A wide range of well developed "bottom-up/self-assembly" techniques is now available to the researchers to create nanoscale materials, often with unique and technologically appealing properties. One of the common requirements of practical applications of nanodevices is the ability to pattern nanoscale electrical contacts and interconnects. Low resistance ohmic contacts and low RC interconnect delay, for example, are essential for optimum performance of the traditional Si-based CMOS circuits. Similar requirements hold true for Schottky or rectifying contacts in Si nanowire based devices. To assess the new properties of nanocontacts, a detailed experimental determination of structural and electronic properties of contact interfaces is needed. First, we should be able to control the growth of epitaxial silicide in nanowires of silicon. Silicide is a metal-silicon intermetallic compound; C-54 $TiSi_2$, NiSi, and CoSi2 have been used widely as contacts and gates in CMOS devices. Understanding of the kinetics of nucleation and growth of these silcides in nanowires of silicon is essential. [3, 4]

Point contact reaction between a nanowire of Si and a nanowire of metal to form silicide is of interest because it eliminates the use of a large area of metal contact pads. In point contact reactions, the metal contact has the nano dimension as the nanowire of semiconductor. [5]

Because the nanowires of Ti oxidize very quickly, we studied the formation of Ni and Co silicides in nanowires of Si.



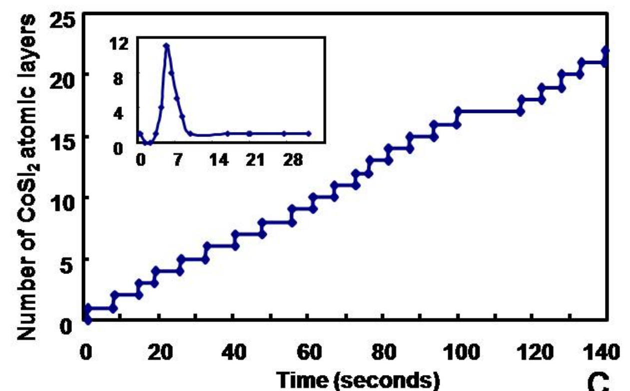


Fig. 1. High resolution TEM images of epitaxial $CoSi_2$/Si interfaces. The stair-type growth curves $CoSi_2$. The insets are the distribution curves of incubation periods of nucleation.

Axel epitaxial growth of nano silicides of NiSi and $CoSi_2$ in nanowires of Si has been observed by using ultra-high vacuum and high resolution transmission electron microscopy. This talk will report experimental and theoretical analysis of kinetics of homogeneous nucleation and heterogeneous nucleation and step-wise epitaxial growth of silicides in nanowires of Si. [6]

II. Results and Discussion

Both the metal nanowires of Ni and Co and the Si nanowires have diameters ranged from 20 to 70 nm and lengths of a few microns. *In situ* annealing for point contact reactions and high-resolution lattice imaging were performed in a JEOL 2000V ultrahigh vacuum TEM. The annealing temperature of Co and

Si samples was at 800 ^{o}C and that of Ni and Si samples was from 450 to 750 ^{o}C. The vacuum in the sample stage was about 3 x 10^{-10} Torr. Figure 1 shows high resolution TEM images of epitaxial $CoSi_2/Si$ and step-wise curves of repeating nucleation and growth from video recording.

On the basis of assumption of thermally activated process of fluctuation of sub-critical nucleus, the steady state homogeneous nucleation rate has been given as,

$$I^{s}_{n^*} = \beta_n^* C_{crit} Z = \beta_n^* C_o e^{-\frac{\Delta G_n^*}{KT}} \left[-\frac{1}{2\pi KT} \left(\frac{\partial^2 \Delta G_n}{\partial n^2} \right)_{n^*} \right]^{1/2} \quad (1)$$

where β_n* is the micro-reversible frequency of atomic jump toward an critical nucleus and convert it into a stable nucleus, and $C_{crit} = C_0 \exp(-\Delta G^*_n/kT)$ is the equilibrium concentration of critical size nucleus, and Z is the Zeldovich factor. We have estimated that the number of molecules in a critical nucleus to be about 10.

III. Conclusions

We observed in high resolution video recording the stepwise growth of each atomic layer of silicide in nanowire of Si. It leads to axial stair-type of growth mode. The growth of every new atomic layer of silicide requires an independent event of nucleation accompanied by a long incubation time. The nucleation stage and the growth stage of each layer of NiSi and $CoSi_2$ can be separated. The distribution of incubation time of nucleation has been measured, and it enables us to determine the steady state nucleation rate per unit area per unit time. The number of molecules required to form a stable NiSi or $CoSi_2$ nucleus for homogeneous nucleation has been calculated to be about ten on the basis of Zeldovich factor and the measured activation energy of nucleation. The calculated and the measured homogeneous nucleation rates are in good agreement. The super-saturation needed for the homogeneous nucleation is about 1000.

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