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Self-assembly of spatially separated silicon structures by Si heteroepitaxy on Ni disilicide

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A nonlithographic approach to produce self-assembled spatially separated Si structures for nanoelectronic applications was developed, employing the metal-induced silicon growth. Densely packed Si whiskers, 500–800 nm thick and up to 2500 nm long, were obtained by magnetron sputtering of Si on a 25 nm thick Ni prelayer at 575 °C. The nucleation of the NiSi 2 compound at the Ni–Si interface followed by the Si heteroepitaxy on the lattice-matched NiSi 2 is suggested to be the driving force for the whisker formation. © 2002 American Institute of Physics. [DOI: 10.1063/1.1469205]

I. INTRODUCTION

Because of the continued scaling of microelectronic devices for very large scale integration (VLSI) applications, low-dimensional silicon systems have been extensively studied in recent years. Fabrication of Si nanostructures on the size scale below 100 nm generated even greater interest after the discovery of their unique electronic and optical properties. However, it poses significant challenges for the entire semiconductor community from the technological perspective. A number of various methods to synthesize individual Si structures have been reported to date. These methods can be divided into two main categories depending on whether the formation of such structures occurs in a controlled or spontaneous manner. The vast majority of techniques, which can be classified as controlled fabrication methods, are based on the artificial cluster formation in nanolithographically defined areas. The well-established approaches are optical 1 or electron-beam 2,3 lithography followed by reactive ion 1,2 or chemical 3 etching. Many reported methods rely on the local oxidation of a Si wafer using microscope tip–substrate interactions 4–6 among which scanning tunneling microscopy 5 and atomic force microscopy 6 appeared to be the most promising techniques. All these methods involve the formation of nanostructured silicon on prefabricated Si layers. However, direct growth of Si wires through the windows in patterned SiO 2 layers, or so-called local epitaxy, has also been proposed. 7

The self-assembly methods do not employ lithographic techniques and take advantage of structural disorder at the interface between the two materials with different physical properties. Thus, the vapor–liquid–solid (VLS) model for spontaneous Si whisker growth explains the function of metallic particles as growth catalysts. 8,9 The lattice-matched metal–silicides were also shown to induce Si wire formation during the excimer laser ablation of Si powder at high temperatures. 10–12 In other studies, nanometer-scale structures formed spontaneously during Si-on-sapphire epitaxy 13 and in highly doped Si films caused by the randomly occurring fluctuations of the dopant concentration. 14

The two methodologies described above have certain advantages and drawbacks. The lithographic methods are generally considered to be superior since they can provide smaller variation in the cluster size and, therefore, a higher uniformity of the entire layer. On the other hand, the lithographically defined dots frequently reveal a characteristic instability when subjected to a subsequent chemical or thermal treatment (e.g., microscopic columns tend to coalesce, 15 etc.), while self-organized structures initially assemble at energetically favored sites. In addition, self-assembled growth techniques allow easy fabrication without further processing steps such as patterning before or after growth and etching, which is essential for reducing the technological cost.

At present, there is a critical need for nonlithographic techniques to fabricate ordered nanostructures in a well-controlled way, with improved uniformity of size and higher dot density. These techniques can be developed by understanding the physical mechanisms underlying the processes of whisker formation, which would establish unique relationships between the experimental conditions and the resulting structural film properties. In previous publications, 16,17 we described the metal-induced formation of polycrystalline silicon by depositing Si films on a thin Ni prelayer at ~500–600 °C. Silicon columnar grains grew heteroepitaxially on the lattice-matched NiSi 2 crystals nucleated at the Ni–Si interface. This article reports that the modifications to this technique can be used to produce individual Si structures. A brief discussion will be offered on how the Si-on-NiSi 2 heteroepitaxial processes and Si deposition kinetics possibly contribute to the whisker assembly process.

II. EXPERIMENT

The starting substrate in our approach was an n-type (100) oriented single crystal Si (c-Si) wafer, chosen for smoothness, coated with a 300 nm thick plasma-enhanced chemical vapor deposited SiO 2 in order to provide a diffu-
sion barrier for Ni. The experiments carried out using c-Si wafers with different crystal orientation and resistivity, glass slides, and Mo sheets have led to the conclusion that none of the substrate properties except for surface morphology influenced the Si nanowire growth, possibly due to the intermediate silica layer. A 25 nm thick Ni film was thermally evaporated at a base pressure of $2 \times 10^{-6}$ Torr. Silicon was then deposited by direct current (dc) magnetron sputtering from a 0.006 \( \Omega \) cm phosphorus-doped Si target at a substrate temperature of 575 °C and a magnetron power of 20 W, which provided a growth rate of 0.2 \( \mu \)m/h. The sputtering process took place in a 5\%\( \text{H}_2/\text{Ar} \) mixture at a pressure of 1 mTorr after an initial vacuum of better than \( 10^{-7} \) Torr was achieved. Ar served as a carrier gas, and \( \text{H}_2 \) was used to saturate dangling bonds in Si. Both the surface and cross section of the resulting Si films were examined using a Hitachi S-4000 field emission scanning electron microscope (SEM) operated at 20 keV in the secondary electron mode.

III. RESULTS AND DISCUSSION

The surface morphology of the sample grown for 6 h using the above deposition conditions is shown in Fig. 1(a). The entire surface of the sample is covered with densely packed and relatively uniformly distributed whiskers. From a higher magnification SEM image in Fig. 1(b), the whiskers have a regular wire shape with a 500–800 nm cross-sectional diameter and are 500–2500 nm in length.

The cross-sectional SEM images shown in Fig. 2 were taken in order to provide mechanistic insights into the whisker-growth process. Previously,17 we proposed the scenario for the Si epitaxy on NiSi\(_2\) in the case of Si deposition onto a Ni prelayer, which is as follows. At the beginning of deposition, sputtered Si atoms react with Ni to form Ni silicide. When Ni is completely consumed, Si saturates in the NiSi\(_2\) compound, the most energetically favorable silicide phase,\(^{18}\) with a cubic lattice structure and a lattice constant of 5.416 Å (0.4% lattice mismatch with Si). As a result, the Si atoms that continue to arrive at the growth front attach to the already established NiSi\(_2\) crystalline network more strongly than to each other, completing uniform monolayers. We have also shown previously that the Si overgrowth is essentially free from Ni Ref. 16 due to the complete Ni consumption by the stable NiSi\(_2\) compound, which leaves no atomic Ni available for diffusion. The Si monolayers reproduce the surface morphology of the Ni disilicide crystals due to the heteroepitaxial phenomenon, and the initial Si film growth follows an atomic layer-by-layer sequence.

Although the precise mechanism of the whisker formation is yet to be clarified, it is most likely related to the...
heteroepitaxial processes in the Si-on-NiSi$_2$ system. The
grains comprising the Si epilayer have a cubic lattice with a
lattice constant equal to that of NiSi$_2$, i.e., the Si film grows
mechanically strained. It follows from the classical theory of
heteroepitaxy that the strain energy increases linearly with
the film thickness until the latter reaches some critical value
which is a function of the lattice mismatch between a film
and a substrate.$^{19}$ Above this critical thickness, the strain
energy exceeds the sum of the substrate surface energy and
the interface energy and is released via rapid and spontaneous
structural changes. One of the most common ways for
the relaxation of a strained system is the introduction of mis-
fit dislocations which lie at the interface between the sub-
strate and epilayer, as was observed in the Stranski–
Krastanov growth mode, previously adopted for the lattice-
matched systems.$^{20}$ It has also been established that misfit
dislocations at the epilayer–substrate interface represent an
ideal source for stacking faults that propagate from the inter-
face into the bulk of the growing layer.$^{21}$ This, in turn, im-
plies that the inverted pyramids seen in Fig. 2 are in fact the
nuclei containing stacking faults, which coalesce with nor-
mal nuclei and grow into the bulk of the film. The schematic
of this process can be illustrated as in Fig. 3. When such
clusters exceed the surrounding grains in size, they begin to
grow faster, extending into the growth ambient transversely
to the base of the substrate, and form spatially separated
individual wire-shaped structures.

On the other hand, no cluster development was observed
at high levels of the magnetron power. Increasing the mag-
netron power threefold, i.e., to $\sim$60 W (0.5 $\mu$m/h growth
rate), led to the formation of a dense polycrystalline Si film
with a columnar structure.$^{16,17}$ Although a high concentration
of stacking faults was introduced at the grain boundaries (be-
tween the columns), no individual structures were formed on
the film surface. According to the VLS model,$^8$ the morphol-
ogy of a growing film is strongly dependent on the adatom
surface mobility. Whisker growth is initiated when the ada-
tom diffusion length is sufficiently small to provoke the ada-
tom trapping at the sites located near the nuclei. The diffusion
length of adatoms is determined mainly by their kinetic
energy, ambient pressure, and deposition rate. The adatom
kinetic energy, in turn, consists of two portions: the initial
kinetic energy, which depends on the atom acceleration to the
substrate in the electric or electromagnetic field, and the kinetic energy acquired due to the elevated substrate tem-
perature. Reducing the dc power of the magnetron sputtering
gun results in a corresponding almost linear decrease in the
initial kinetic energy of the silicon atoms which, in turn,
limits the migration of the Si atoms on the growing film
surface.$^{22}$ Although a lower magnetron power also results in a
lower deposition rate, this effect apparently is less pro-
nounced. As follows from the discussion above, most of the
incident sputtering flux is deposited on high points on the
film, with little material reaching the valleys (shadowing ef-
fect). The larger grains grow at the expense of the smaller
ones, becoming thicker closer to the surface as seen in Fig. 2.

Despite the fact that the density of the synthesized Si
whiskers is relatively high, they are not suitable for device
fabrication in their present form. Such issues as the whisker
size and the pattern uniformity still need to be addressed.
Because the quantum effect was demonstrated for the struc-
tures with features smaller than 100 nm,$^{22}$ further decrease in
the whisker cross-sectional diameter is needed. The most
convenient and readily available technique to reduce the lat-
eral dimensions of the Si whiskers is thinning of prefabri-
cated structures by oxidation. Since the oxidation rate of sil-
icon and, respectively, the oxide thickness are easily
controlled, this method may offer a simple way to produce
arrays of nanostructures with the desired size.

IV. CONCLUSIONS

In summary, a method to fabricate spatially separated
individual Si structures by Si deposition on a thin Ni prelayer
was developed. The Si whiskers produced are 500–2500 nm
long and 500–800 nm thick with the potential of further
decrease their dimensions by oxidation. The strain relaxation
in the Si-on-NiSi$_2$ heteroepitaxial system was proposed to be
the driving force for the whisker formation. In addition, the
kinetics of Si deposition was suggested to contribute to the
final structure.

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