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Epitaxial insertion of Au_5Si nanodiscs during the growth of silicon nanowires

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1. Introduction

Recent studies of one-dimensional (1D) silicon nanostructures have focused mainly on cylindrical nanowires with very high aspect ratios for use in field effect transistors and sensors [1]. In this process, metal (usually gold) is used to catalyze the decomposition of a Si source gas [2]. Au and Si then form a eutectic liquid phase alloy. Finally, Si nanowires (SiNWs) crystallize and grow from the supersaturated Au-Si alloy. These alloy tips were known to locate only at the growth front of SiNWs, avoiding the incorporation of Au inside the nanowire bulk. Here we alter the typical feature of nanowire growth by using the hydrogen enriched ambient. Crystalline (110)-oriented Au_5Si nanodiscs were found to be epitaxially inserted in between the (111)-oriented segments of a crystalline SiNW. These silicided nanodiscs would be useful as a nanosized electrical junction for the future applications in the nanowired interconnection.

2. Experimental

P-type, 4-in. Si(111) wafers were cleaned by diluted HF (deionized water:HF = 10:1) and piranha (H_2O_2:H_2SO_4 = 1:4) solutions. Au thin films (1-nm-thick) were thermally evaporated on substrates. For silicidation, all samples were thermally annealed at 700°C for 10 min under H_2. After ramp-up to 900°C in Ar ambient, SiNWs were then synthesized for 10 min in hydrogen ambient mixed with Ar. $SiCl_4$ was used for silicon source gas.

3. Result and discussion

Figure 1 shows the different morphologies of SiNWs with varying hydrogen content. Diameter and length of SiNWs were found to increase with increasing hydrogen content in ambient. This feature can be explained by thermodynamic coefficient, η which can quantify the dissociation reaction of $SiCl_4$ in H_2 ambient [3].

$$\eta = \frac{(Si/Cl)_i - (Si/Cl)_f}{(Si/Cl)_i}$$

According to Fig. 2 showing the residual silicon content based on the above equation in Si-H-Cl gas phase system, initial $(Si/Cl)_i$ ratio was 0.25, but the H_2 overflow lowered a Cl/H ratio, inducing a $(Si/Cl)_f$ of <0.25. Each experimental regions corresponding to Figures 1(a), (b), and (c), respectively, were depicted in Figure 2. In case of Fig. 1(a) (η<0.25), higher dissociation of $SiCl_4$ can produce more silicon atoms nearby the alloy tips, which then increases silicon content inside the catalyst tips with increasing tip size. This feature results in larger diameter with longer nanowires shown in Fig. 1(a).

However, if the degree of Si supersaturation inside the catalyst tips becomes too high, silicon atoms likely diffuse out to the catalyst surface because the free energy of silicon-bonded surface is lower than that of gold-bonded one [4]. This behavior leads to a locally gold-rich phase close to catalyst core regions (see Fig. 3), so a liquid state of alloy at 900°C likely phase separate into gold-rich solid silicide and silicon-rich liquid phase as shown in Au-Si phase diagram of Fig. 4.

Figure 5 shows that SiNW can be further grown after precipitation of gold-rich silicide. Despite the phase separation, interestingly, epitaxial relation in between the nanowire-silicide-nanowire segments maintains very well. Diffraction pattern shown in Fig. 5 reveals the presence of crystalline (111)-oriented SiNW segments jointed with a (110)-oriented Au_5Si nanodisc. Note that the diameter of nanodisc is slightly smaller than the one of nanowires because the precipitation of Au_5Si is confined to gold-rich core regions inside alloy droplets. Figure 6 describes why silicided nanodiscs align along the (110) directions in between (111)-oriented SiNW segments. In case of superposition of Au_5Si BCC (110) onto a Si FCC (111) plane, two kinds, i.e., *Nishiyama-Wassermann* and *Kurdjumov-Sachs*, of epitaxial lattice matching are possible in spite of crystallographic difference [5]. If this epitaxial rearrangement is not enough upon silicide precipitation due to unsuitable kinetics, SiNW likely bends just after the formation of nanodiscs, as shown in Fig. 1(a).

4. Conclusion

Utilizing hydrogen-enriched ambient, we could find that crystalline (110)-oriented Au_5Si nanodiscs were epitaxially inserted in between the (111)-oriented segments of a SiNW. Our finding suggests a potential as silicided nanojunctions at the cross-points of nanowired interconnection.

Acknowledgements

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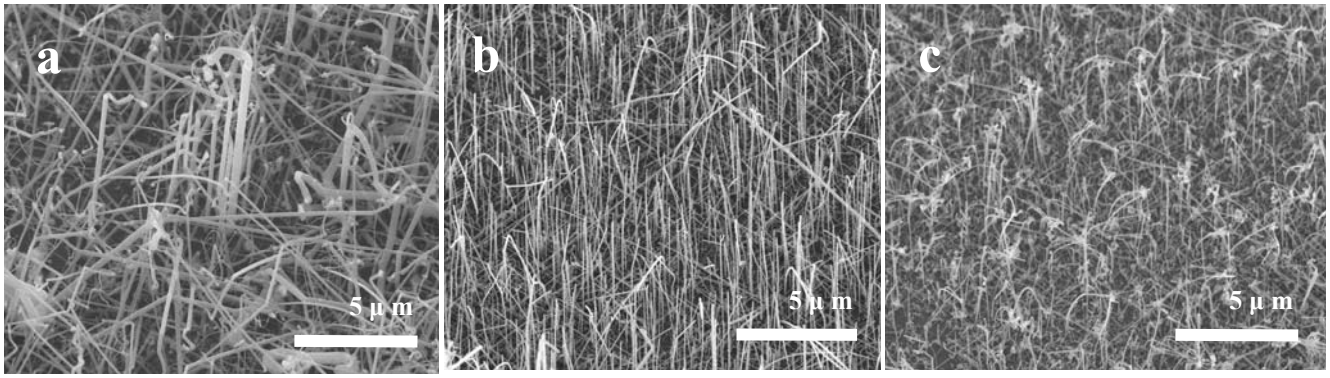

Fig. 1 SEM images of Si nanowires synthesized in various ambient: (a) 200 sccm H_2 with 100 sccm Ar, (b) 100 sccm H_2 with 200 sccm Ar, (c) 50 sccm H_2 with 250 sccm Ar.

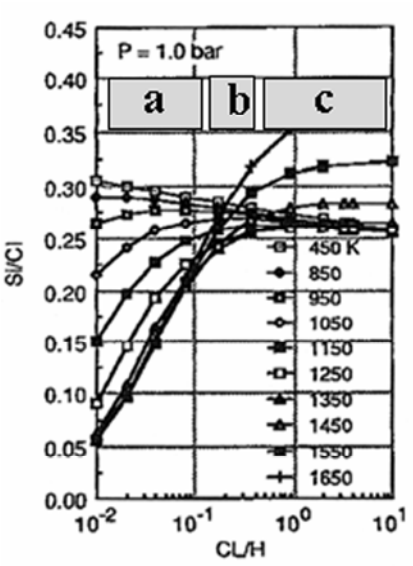

Fig .2 Final silicon contents in the residual gas ambient as a function of the concentration of the starting species (Cl/H) in the Si-H-Cl system at equilibrium (Ref. 3). The inset, a, b, c, correspond to figure 1 (a), (b) and (c), respectively.

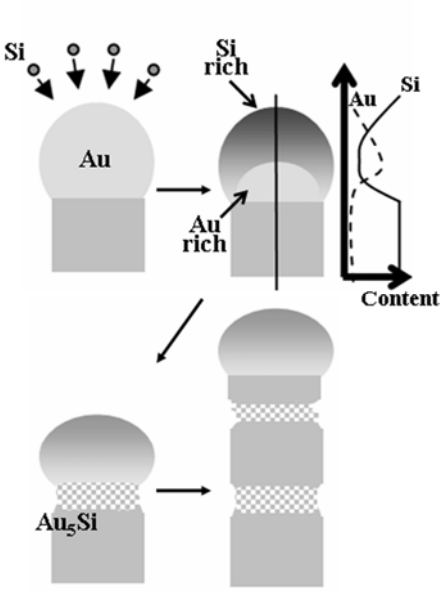

Fig. 3 Conceptuals chematic showing the possible insertion mechanism of the Au_5Si nanodiscs. Note that the core region of droplets gets Au-rich while making the surface Si-rich so as to decrease the total free energy of a droplet system.

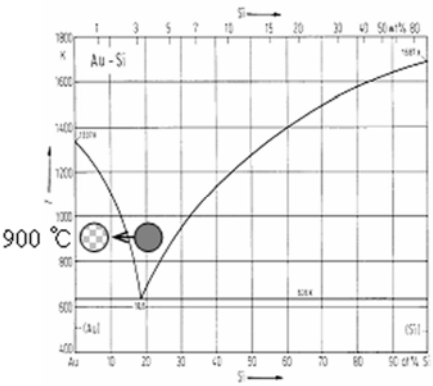

Fig. 4 Phase diagram of Au-Si binary system. At 900C, a gold-rich tendency of eutectic liquid droplets leads to precipitation of Au-rich silicide (Au_5Si) below a liquidus line.

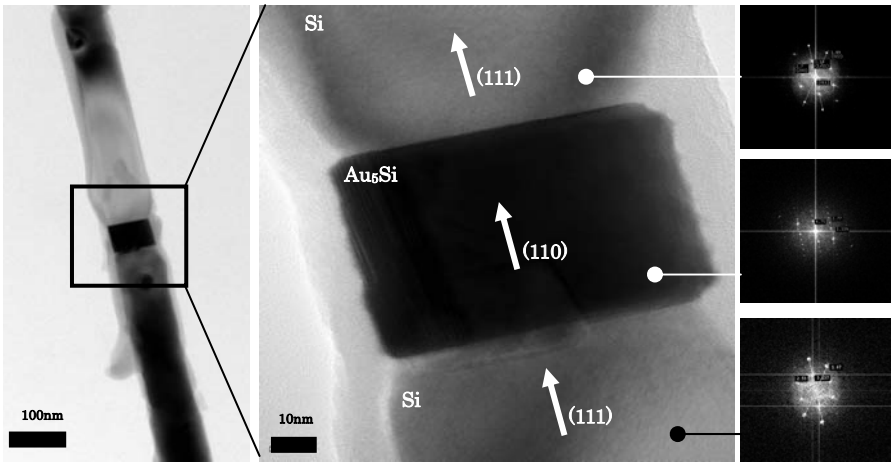

Fig. 5 High resolution TEM images showing the epitaxial relation of inserted Au_5Si nanodisc having a zone axis of [011]. Corresponding SADPs are shown in the right column.

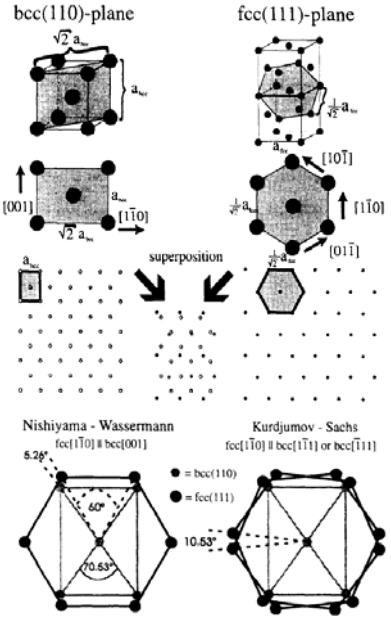

Fig. 6 Epitaxial superposition of Au_5Si-bcc (110) onto a Si-fcc (111) plane at the interface. Two kinds of epitaxial relationship are shown. (Ref. 5)