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Channeling studies on self-assembled Au_4Si islands on Br-passivated $Si(111)$ surfaces

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Abstract : Growth of epitaxial gold silicide islands have been observed when an Au thin film, deposited on Br-passivated vicinal (4° misoriented) $Si(111)$ substrate, was annealed around the $Au - Si$ eutectic temperature. The epitaxial silicide islands were observed over a thin uniform layer of gold silicide. Epitaxy of these islands and the thin layer underneath has been determined using Rutherford backscattering and channeling techniques. Both the gold silicide layer and the islands have been found to be epitaxial indicating a Stranski-Krastanov growth.

Keywords : gold silicide, epitaxy, Rutherford backscattering and channeling.

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1. Introduction

Studies of metal-silicon thin film reactions, kinetics of the reactions and properties of the phases formed, have been stimulated by the technological importance of these systems. Metallic silicides, which are formed by the reaction of a metal species with silicon, are finding a variety of applications in VLSI technology. Growth of an epitaxial overlayer could be a homoepitaxial growth (overlayer same as the substrate) or a heteroepitaxial growth (overlayer different from the substrate). Heteroepitaxial growth produces strained epitaxial layers due to lattice mismatch between the substrate and the overlayer. Strained epitaxial layers have interesting properties and are important in semiconductor devices [1]. For the growth of a silicide from a metal film on a silicon substrate, it is important that the diffusion across the interface is not hindered. The presence of an oxide layer at the interface is known to hinder the diffusion across the interface [2, 3]. It has been shown that the diffusion behaviour is comparable in the cases where a metal film is deposited on a chemically prepared Br-passivated $Si(111)$ substrate or an atomically clean $Si(111)(7 \times 7)$ reconstructed substrate [3, 4]. Br-adsorption in this case inhibits substrate surface oxidation.

Growth of epitaxial gold silicide islands have been observed when an Au thin film, deposited on Br-passivated vicinal (4^o misoriented) $Si(111)$ substrate, was annealed around the $Au - Si$ eutectic temperature [5]. The Br-passivated substrates were prepared by a chemical method and Au film deposition and annealing were performed under high vacuum. The composition and the general features of growth of the silicide islands are comparable to those obtained under ultra high vacuum conditions [6]. Energy dispersive x-ray (EDX) analysis results show the composition of the silicide islands to be Au_4Si. From the EDX analysis the heights of our observed islands were estimated to be $\sim 1\mu m$. We have measured the island thickness for gold silicide islands on another sample with comparable initial Au thickness by secondary ion mass spectrometry (SIMS). These silicide islands show a constant thickness of 1.23 μm and an abrupt silicide/silicon interface [7]. Also a concomitant growth of fractal patterns and nearly spherical islands of gold have been observed [8]. The islands grow in the shape of the equilateral triangle, reflecting the symmetry of the (111) substrate upto a critical size beyond which the symmetry of the structure is broken resulting in shape transition from triangle to trapezoid [5]. Such shape transition has recently been identified to be one of the ways of relieving strain from the sytem undergoing epitaxial growth [9]. The island edges are aligned along the three equivalent $\{1\bar{1}0\}$ directions of the Si(111) substrate. The elongated islands, instead of growing along three equivalent $\{1\bar{1}0\}$ directions, grow only along one preferential direction which has been attributed to the vicinality of the substrate [6].

The alignment of the silicide islands with a specific crystallographic orientation of the substrate indicates that the islands are epitaxial in nature. However this is an indirect evidence of epitaxy. Rutherford backscattering spectrometry(RBS)/channeling is a good tool to characterize the crystalline nature of a material. With this technique it is very easy to find out whether an overlayer is in epitaxy with the underlying substrate. In RBS, we detect the number of backscattered incident ions and their energy using a surface barrier detector. When any of the crystallographic axis of the substrate is aligned with the incident beam direction, there will be a drastic reduction in the number of backscattered ions. This reduction in the number of backscattered ions, is a measure of the crystalline quality of the sample under study. More reduction corresponds to better crystalline quality. This is the basic principle behind this powerful non-destructive technique. There are books [10] and review articles [11] containing the detailed description of this technqiue. Here we have employed the combined RBS/channeling technique to probe the epitaxial nature of gold silicide islands on the Si substrate. Thus in this we show thc direct evidence of epitaxy.

2. Experimental

We used a non-UHV method to obtain the gold silicide island structures on silicon substrates. The method involves gold evaporation onto a bromine-passivated $Si(111)$ polished wafer (n-type, Sb-doped, 0.005-0.02 Ωcm) substrate and subsequent annealing. The details of the substrate preparation have been discussed elsewhere [3, 4]. Br adsorption on the $Si(111)$ surfaces inhibits the surface oxidation process. A detailed x-ray photoelectron spectroscopic characterization of the Br-treated Si surfaces has been published elsewhere [12].

In the present work a 120 nm thin Au film was evaporated from a W basket onto a Br-passivated $Si(111)$ substrate at room temperature in high vacuum $(3 \times 10^{-4}$ $Pa)$. Then the sample was annealed at 360^oC, that is around the $Au - Si$ eutectic temperature (363^oC), for 20 minutes in high vacuum. Upon annealing the Si substrate contained a very thin layer of Au_4Si ($\sim 40\AA$) and on top of this uniform layer, in addition to the triangular and trapezoidal gold silicide island structures, stray gold was present. The stray unreacted gold was removed by dipping the sample in aqua regia for 2 minutes. This process left the gold silicide islands unaffected. The aqua regia etched sample was taken for the RBS/channeling studies. RBS/channeling measurements were made using a 2 MeV He^+ beam from the 3 MV tandem Pelletron accelerator in our laboratory. The experimental set up has been described elsewhere [4, 11].

3. Results and discussions

RBS measurements were made on as-deposited samples, i.e., on the Au film deposited on a Br-adsorbed $Si(111)$ surface as well as on annealed samples. The spectrum for the as-deposited sample (not shown here, but shown in Ref. [6]) indicates that the Au-film is laterally uniform. The thickness of the film has been determined from the RBS spectrum. The crystallinity of Au_4Si islands has been determined with Rutherford backscattering spectrometry (RBS) and channeling measurements along [111] direction (which is closer to the surface normal of the substrate) as well as along the [110] axial direction using 2 MeV He^+ beam. The size of the ion beam was 1.5 mm while the island size was of the order of microns to tens of microns.

Fig. 1. shows the backscattering spectra for the He^+ beam incident from a random direction and also for the beam aligned along the [111] crystallographic axis of the substrate. A tiny peak appearing around higher channel number or energy (around ch. no. 1160), is due to Au from a thin uniform layer of

Au_4Si. (Here this peak signal is blown up by a factor of 10 for clarity). It is clear from this tiny peak that the thickness of the uniform Au_4Si layer is very small, around ~ 40 Å (obtained from RBS simulation). Tailing towards the low energy side is due to the presence of about a micron thick gold silicide islands. Appearance of tails in an RBS spectrum could be due to real diffusion or due to non-uniformity of the surface of the sample. The spectrum for the aligned case (along [111] direction), shows a reduction in the backscattered signal in the tailing region though not prominent. This confirms that the Au_4Si islands are epitaxial. There is little reduction in the backscattering yield from the thin uniform layer.

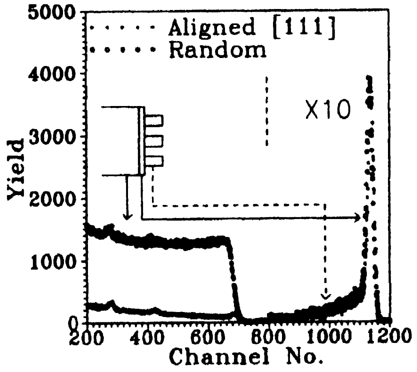

Fig. 1. RBS spectrum for the random and aligned condition for the goldsilicide/Si sample aligned along [111] direction of the Si substrate.

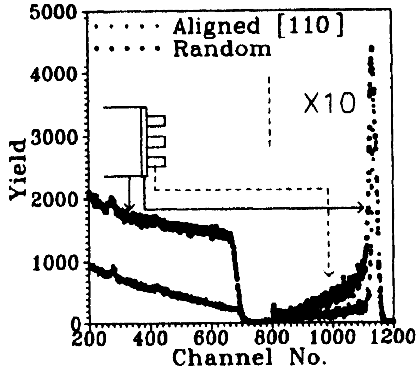

Fig. 2 RBS spectrum for the random and aligned condition for the goldsilicide/Si sample aligned along [110] direction of the Si substrate.

Fig. 2 shows the backscattering spectra for the He^+ beam incident from a random direction and also for the beam aligned along the [110] crystallographic axis of the substrate. In this case one can notice a clear reduction in the backscattering yield, from the thin uniform layer as well as from the tailing region (from the islands). It is obvious from these two figures that there is reduction in the backscattering yield of gold in the aligned condition from the thin uniform layer as well as from the islands along both [111] and [110] directions. This confirms the crystallinity and alignment of the gold silicide islands. Greater reduction in the backscattering yield is seen in aligned spectrum along the [110] axis compared to the [111]. This implies that Au_4Si islands have better lattice matching with the $Si(111)$ substrate along [110] direction. This is in good agreement with the results of Green and Bauer [13]. They have shown for an ultrathin silicide layer, using low energy electron diffraction that either the [01] or the [10] direction of the gold silicide layer is parallel to the $[1\bar{1}0]$ direction of the Si(111) substrate. In the present work we have demonstrated that on the $Si(111)$ surface, there is a thin uniform layer of epitaxial silicide on top which there are epitaxial silicide islands. This layer-plus-island growth conforms to the Stranski-Krastanov growth mode.

4. Conclusions

RBS/channeling techniques have been used to characterize the epitaxial nature of the gold silicide islands on Br-passivated vicinal $Si(111)$ substrate. The silicide islands, grown over a thin uniform layer of gold silicide, and the thin uniform layer were found to be in epitaxy with the underlying Si substrate. Although indirect evidence of epitaxy was obtained in previous works [5, 6], application of the combined RBS/channeling technique has provided direct evidence of epitaxy.

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