

## Strain due to Ni diffusion beneath Hydrogen-terminated Si(111) surface

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### Introduction

Understanding and controlling of silicide reaction are important for improving electronic device technology. Silicide reaction occurs at low temperature between silicon and almost every metal present. These reaction cause problem, such as electric leakage, as the feature size is decreased in large-scale integration (LSI) devices. Hydrogen (H) termination of Si surface is one common technique for controlling the silicide reaction, because hydrogen acts either as a passivating layer or as a surfactant. There have been many studies about metal film growth on hydrogen-terminated Si surfaces. Hirose et al. [1] investigated Ni film growth on a hydrogen-terminated Si(111) surface (Si(111)-H) at room temperature. They found two growth regimes in Ni film growth. Up to deposited Ni film thickness,  $t_{\text{Ni}} = 0.8$  nm, Ni atoms migrate into the Si crystal and form an “Ni diffusion layer”. For deposition of the thicker films, Ni films grow on the hydrogen-terminated surface. They suggested that the hydrogen suppresses the silicide reaction at room temperature.

In this paper, we studied affection of this “Ni diffusion layer” to the substrate by using extremely asymmetric X-ray diffraction. Comparing measured and calculated rocking curve, we found that the “Ni diffusion layer” compresses the {111} spacing near Si surface. Moreover such compressive strain fields begin to relax after deposited Ni films become thicker than 0.6 nm[2].

We found that the wavelength dependence of the integrated intensity of the rocking curve is sensitive to the strain fields. From dynamical diffraction calculations, the wavelength dependence is not only sensitive to the strain fields, but is also insensitive to absorption effects of the overlayer [2].

### Results and Discussion

The sample were either H-terminated Si(111) or Ni deposited H-terminated Si(111) surfaces. For the Ni deposited Ni films,  $t_{\text{Ni}} = 0.2, 0.4, 0.6,$  and  $0.8$  nm. H-terminated surfaces were prepared by dipping of Si wafers in a conventional pH-controlled HF solution.

To evaluate strain fields near sample surfaces, rocking curves of extremely asymmetric Si 113 reflections were measured. The {113} planes of crystals with a diamond structure make 29.5 degrees to the {111} planes. Therefore the rocking curves for the Si 113 reflection strongly reflects distortion of the Si crystal along [111] direction.

Figure 1 shows X-ray wavelength dependencies of the integrated intensities of the measured rocking curves. The

integrated intensities can be fitted by using linear functions, as shown in Fig. 1.

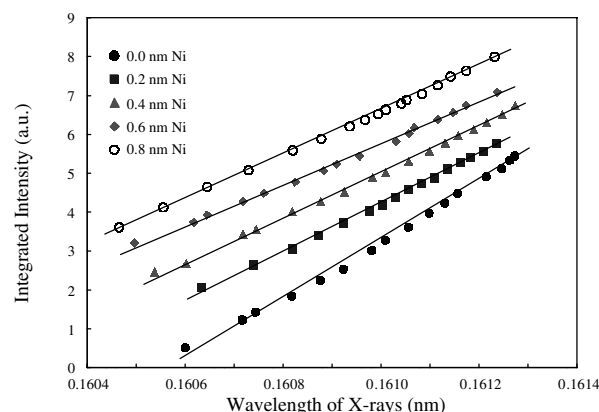


Fig.1 Dependence of integrated intensities for the measured rocking curve.

We quantified the wavelength dependence of the integrated intensities by using the slope,  $m$ , of the fitted, linear functions to the X-ray wavelength versus intensity plots. The relation of  $m$  to  $t_{\text{Ni}}$  is shown in Fig. 2.

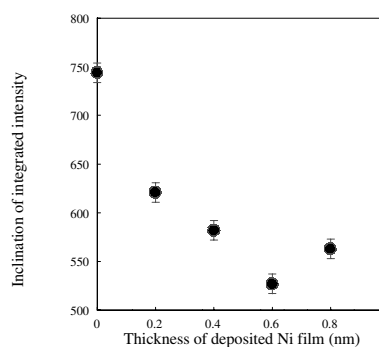


Fig. 2 Relationship between the slope of the measured integrated intensity vs. X-ray wavelength, and the thickness of deposited Ni.

Figure 2 indicates that with increasing  $t_{\text{Ni}}$ , for  $t_{\text{Ni}} < 0.6$  nm  $m$  decreases, but that for  $t_{\text{Ni}} > 0.6$  nm  $m$  increases. We found the slope  $m$  is explained by the strain fields near surface[2].

### References

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