Structural Evaluation of Gate-oxide / Si Interface by X-Ray CTR Scattering

Shuichi DOI, Fujitsu Laboratories Ltd,

doi.shuuichi@jp.fujitsu.com

Recent continuous scaling of the CMOS devices requires the gate oxide to be 1.0-1.5nm thick. For the development of such an ultra-thin gate oxide, to understand the gate oxide/Si interface structure, especially N incorporation effect is important to improve their electric performances. In this study, we developed the evaluation technique of the interfacial strain by using the X-ray Crystal Truncation Rod (CTR) scattering that is sensitive to the surface structure of the crystal. The strain was successfully obtained with the accuracy of 0.0005nm for the first time.

Since x-ray CTR scattering is very weak compared to the bulk diffraction peak, high flux undulator x-ray at BL16XU is desirable for the measurement. To evaluate the interfacial strain, we paid attention to that the vertical displacements of the topmost atoms introduce the asymmetry of the CTR peak profile. We measured the Si (11L) CTR from gate-oxide samples with different nitridation process. We saw the difference of the peak asymmetry for these samples that can be interpreted as the result of different interfacial strain. Applying the least squares fitting to experimental data, we determined the interfacial strain. Comparing with the N-doped interface structures from first-principles calculations, a description between the observed interfacial strain and the nitrogen distribution at the interface is obtained; the inward strain comes from the N atoms penetrated into the Si substrate, and the outward strain comes from the N atoms located in the oxide. In addition, the electric measurement revealed that the gate-oxides with the inward strain had poor electric properties, which may be due to the existence of N atoms in the Si substrate. The technique, that we developed in this study, can detect the interfacial strain with high sensitively and will be a powerful tool for the fabrication of the advanced CMOS devices with high performance and high reliability.

X線CTR散乱による極薄ゲート酸化膜界面の構造評価

Structural Evaluation of Gate-oxide/Si Interface by X-Ray CTR Scattering

(株)富士通研究所

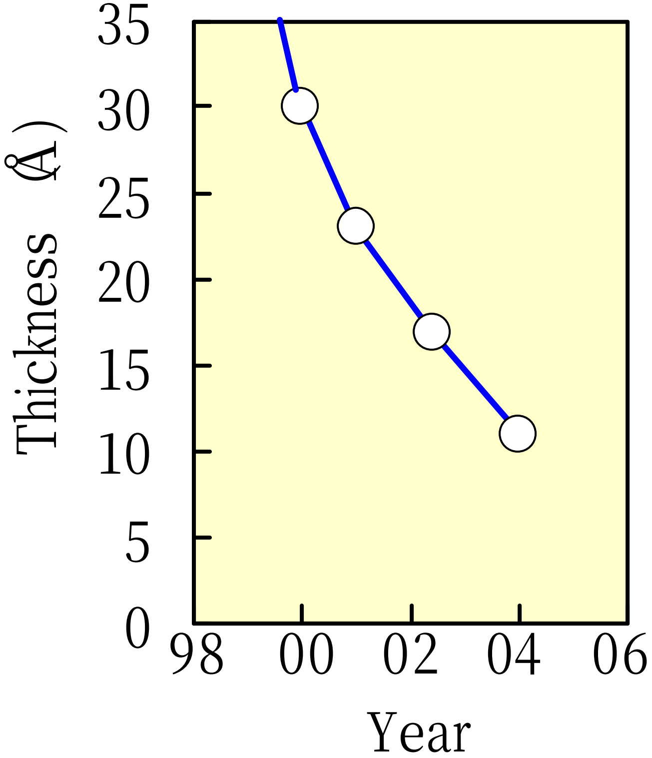
土井 修一

Shuichi Doi

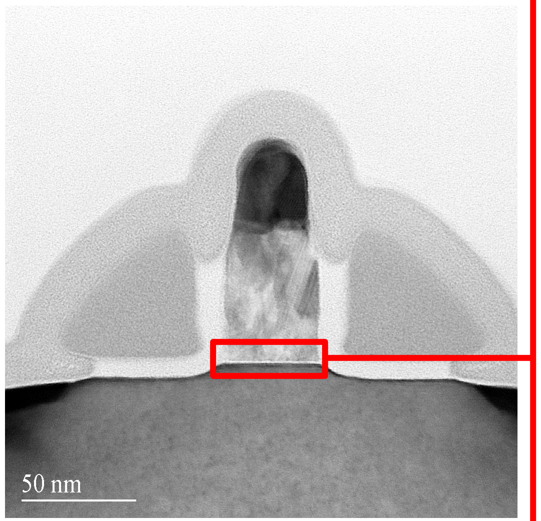
Fujitsu Laboratories Ltd.

Trend of the gate-oxide thickness

Trend

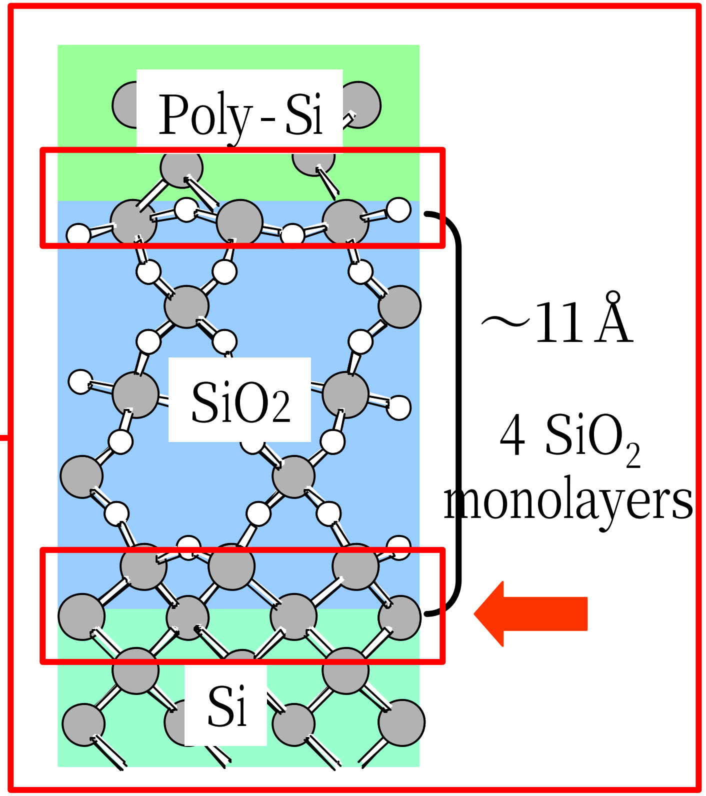


MOSFET



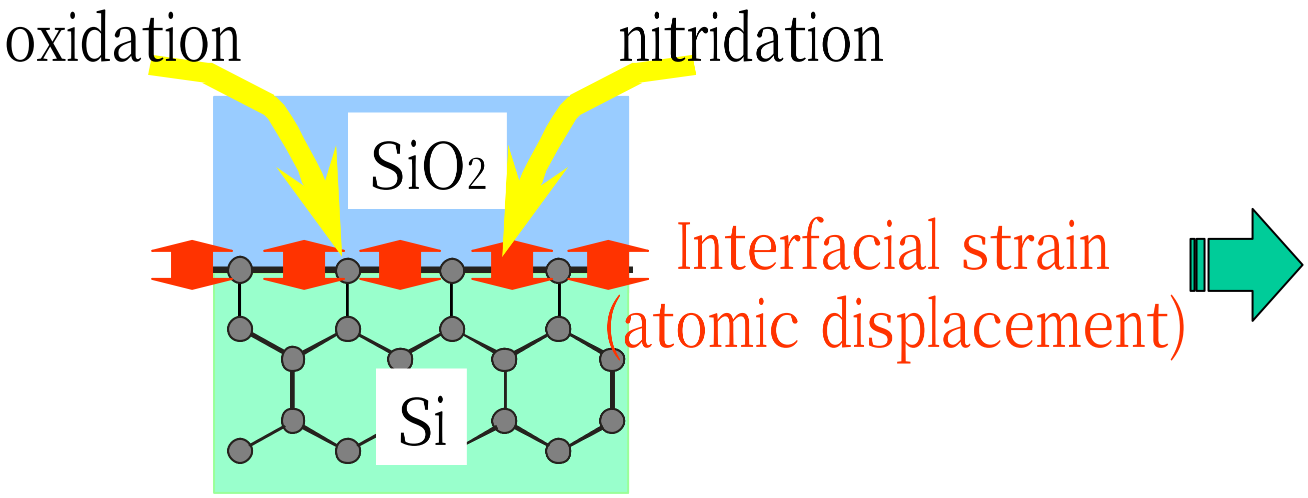
TEM image

Ultra-thin Gate-oxide film

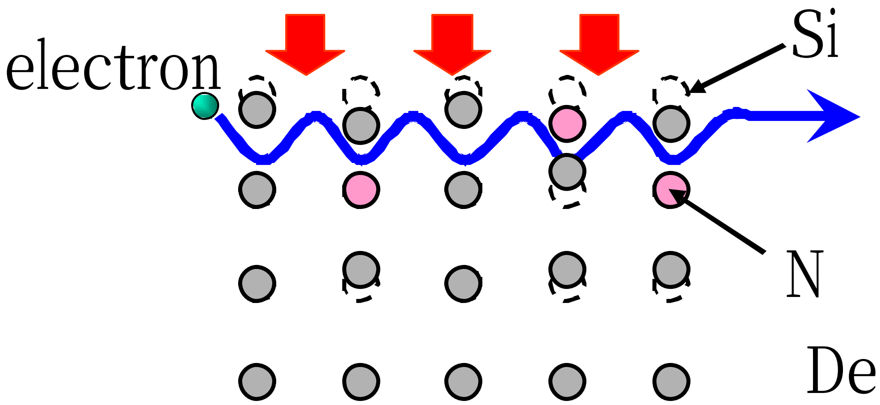


The interface structure affects the electric properties of the gate-oxide more than before

Effect of the interfacial strain



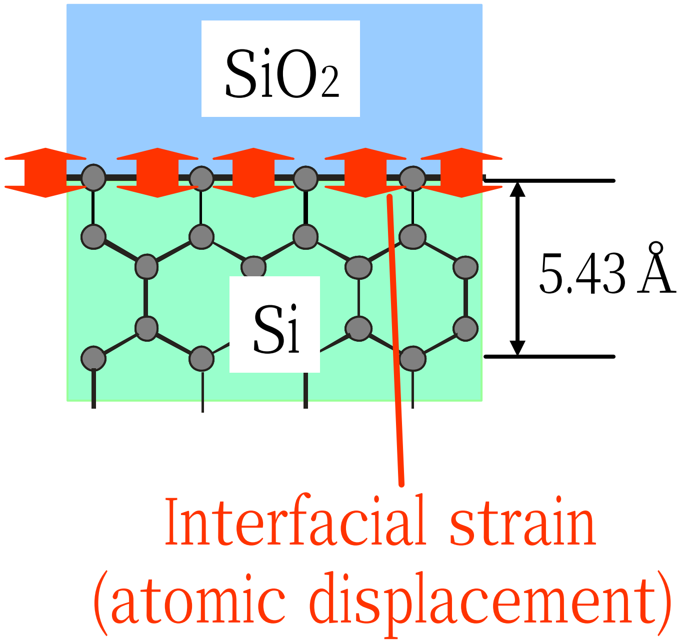
- carrier mobility
- leakage current
- interface states



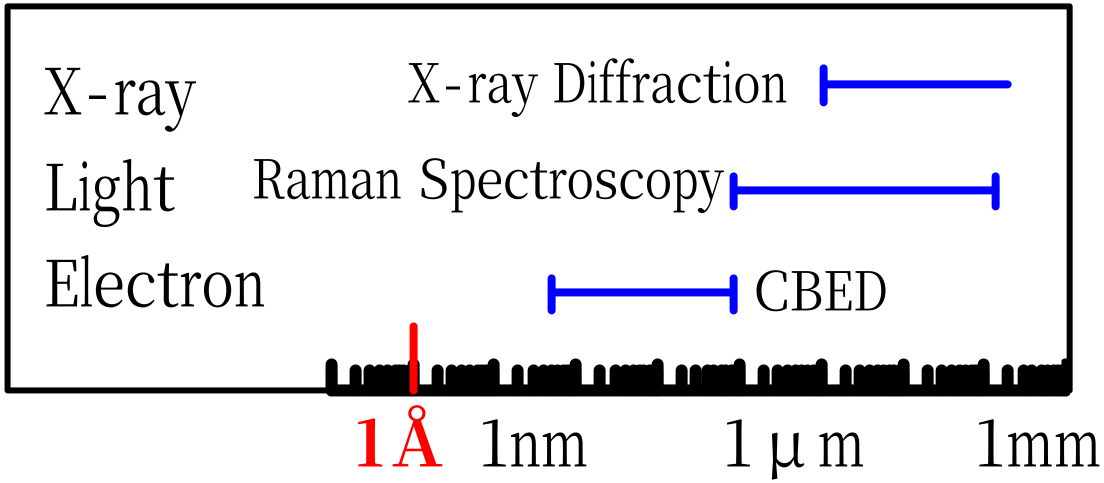
Degradation of mobility

The interfacial strain influences on the electric properties of the gate-oxide

Evaluation techniques of the interfacial strain

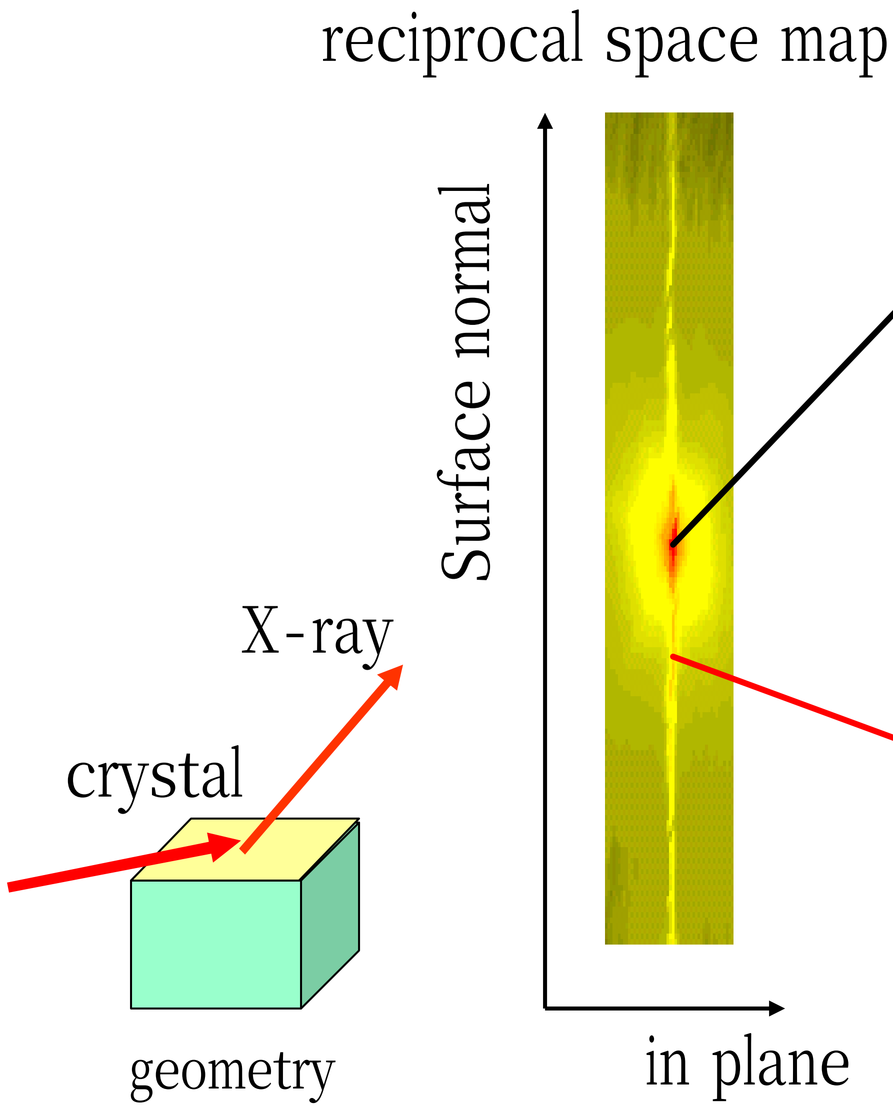


Evaluation techniques for the strain



Atomic level evaluation of the interface strain is requested

Surface X-ray Diffraction (CTR scattering)



CTR (Crystal Truncation Rod)

Bulk X-ray Diffraction
Bragg peak
↓
3D crystal structure

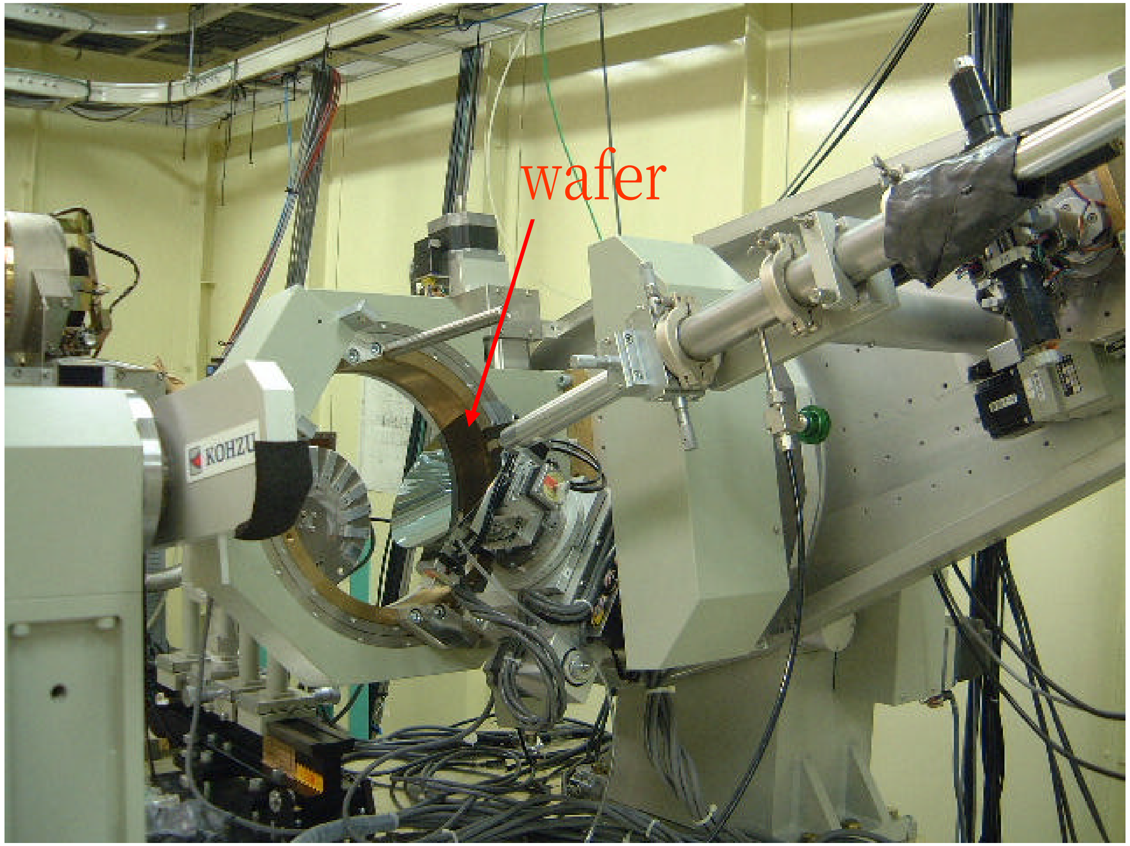
Surface X-ray Diffraction
↓
2D surface structure

Weak scattering intensity

High flux x-ray from synchrotron radiation is necessary

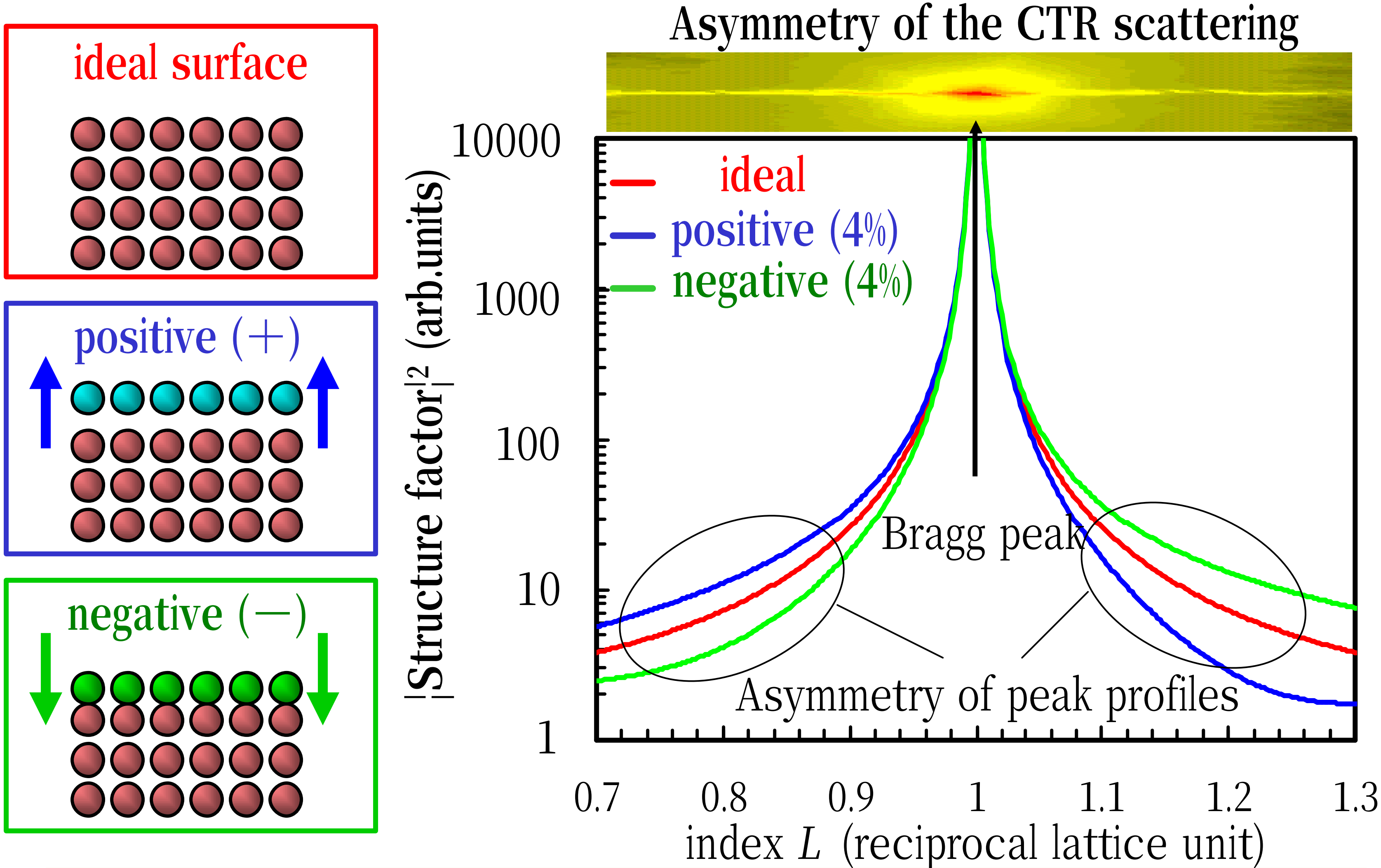
Equipment

- Wave length : 1.16 Å (10.69 keV)
- Si(111) analyzer crystal was used



High-resolution 4-circle diffractometer at BL-16XU

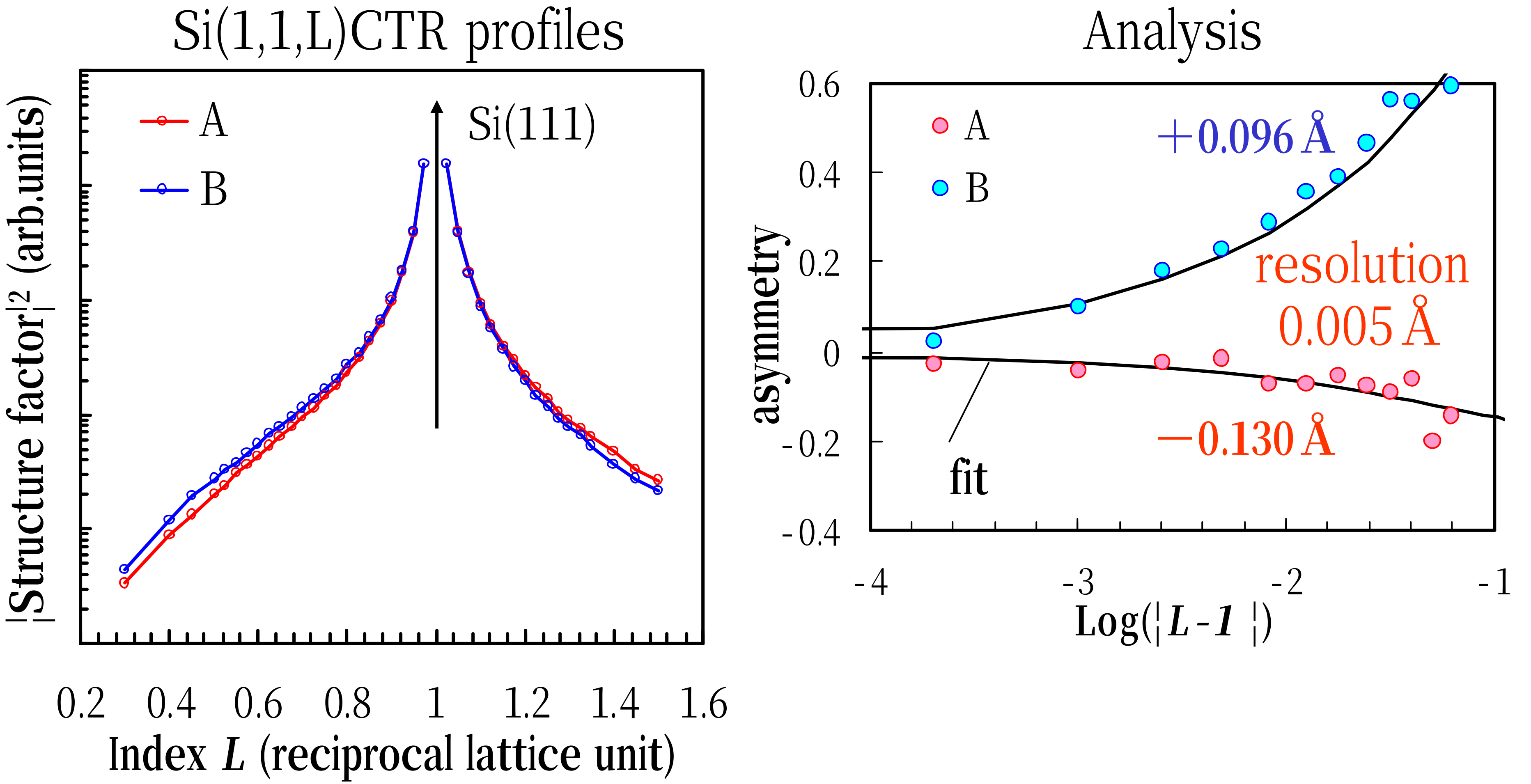
Model Calculation



Monolayer strain introduces the asymmetry of CTR profile

Evaluation of the ultrathin gate-oxide samples

The oxynitrided samples with different nitridation process



Monolayer strain at gate-oxide/Si interface was successfully measured for the first time

Interfacial strain v.s. Electric properties

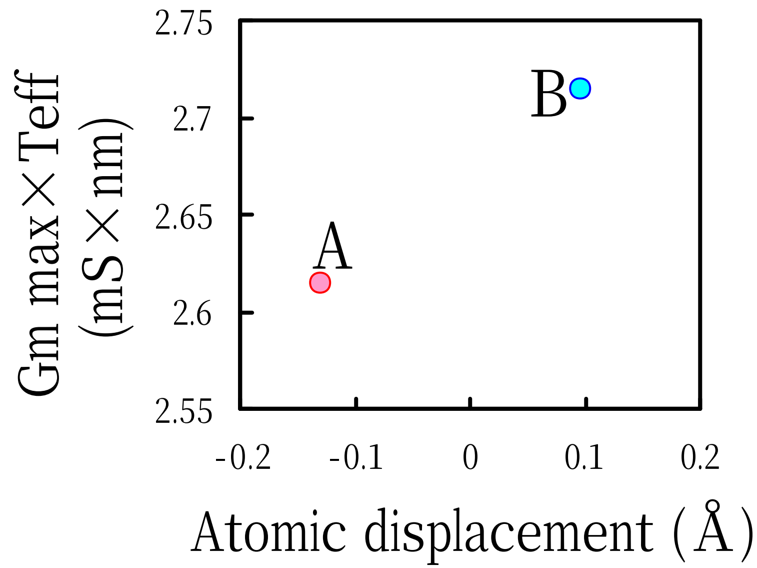
Mobility

positive strain → **Good**
negative strain → **Poor**

Gate Leakage Current

positive strain → **Good**
negative strain → **Poor**

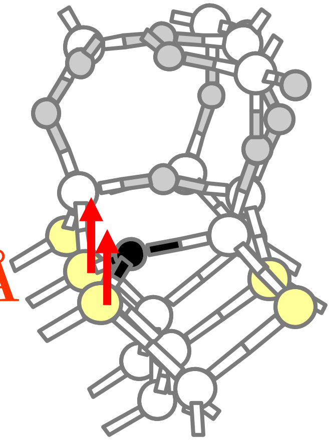
Mobility property



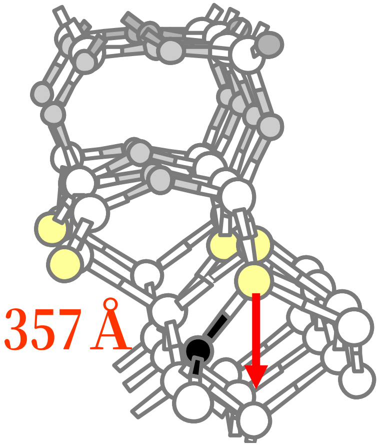
Positive strain provides superior electric properties compared to the negative strain

First-principles calculations

N-doped interface structures



In the oxide



Into the substrate

- ● N
- ○ Si
- ○ Si at interface
- ○ O

Positive strain ← N atoms located in the oxide region
Negative strain ← N atoms penetrated into the substrate

T. Yamasaki and C. Kaneta
"Mechanisms of Nitrogen Segregation and Hole Trap Generation at the Interface of SiO_2/Si(100)"
Extended Abstracts of the 2002 International Conference on Solid State Devices and Materials, Nagoya, 2002, pp.750-751

Summary

- A new evaluation technique of monolayer strain at the Si interface has been developed with the accuracy of 0.005 Å by analyzing the asymmetry of the CTR scattering.

- For the case of oxynitrided films,
  positive strain → superior electric properties
  negative strain → inferior electric properties

- The interfacial strain is sensitive to the nitrogen distribution.
  positive strain ← N atoms located in the oxide
  negative strain ← N atoms penetrated into the Substrate