

## Chapter 3. Step Structures on Semiconductor Surfaces

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### 3.1 Phase Behavior of the Si(112) Surface

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The structural properties of various silicon surfaces have been studied very widely during the last decade both because of their interesting physical behaviors and for practical applications. Key questions include: Is a specific surface stable against faceting? If so, what is the microscopic atomic structure, i.e., the structure of surface reconstruction? Does the reconstruction undergo phase transformation? If not, what is the macroscopic (or mesoscopic) morphology as a result of faceting transformations? And, what are the properties of the steps for vicinal surfaces?

Most studies have been concerned with silicon surfaces near the cubic [001] or [111] orientations. Although much less studied than (001) and (111), surfaces of high-index have been attracting considerable interest for several reasons: First, they often show rich physical phenomena, for example, a  $(3 \times 1)$ -to-disorder phase transformation for the Si(113) surface<sup>1</sup> or step tricriticality for stepped Si(113) surfaces.<sup>2</sup> Second, the unique structure of a

high-index surface may be suitable for use as a substrate for a special purpose. For example, Si(112) and Si(113) have been proposed as effective substrates for heteroepitaxial growth of compound semiconductors on silicon.<sup>3</sup>

Even though the Si(112) surface has such possibilities, neither the atomic structure nor the orientational stability of Si(112) surface is fully known. Here, we report the results of an x-ray scattering study of the orientational phase behavior of the Si(112) surface for temperatures between 300 and 1400 K. In these experiments, five different kinds of profiles of x-ray scattering may be discerned, corresponding to five different morphologies depending on temperature.

First, at the highest temperatures (above 1155 K), the x-ray scattering profile shows just one sharp resolution-limited peak at  $K = 0$ , which corresponds to the specular reflection of x-rays, the so-called specular peak. Therefore, we conclude that above 1155 K, Si(112) is a stable surface. Second, for temperatures between 1139 and 1155 K, in addition to the specular peak, there are two more sharp peaks symmetrically displaced from the specular peak. This may be explained by scattering from a grooved structure with well defined period. Further measurements reveal that mean periodicity of the grooved superstructure is  $670 \pm 15 \text{ \AA}$  and that one of the groove sides is tilted at an angle of  $2.2 \pm 0.1^\circ$  from [112] towards  $-K$ . Remarkably, we also find that this tilted surface is reconstructed with a periodicity of  $67 \pm 6 \text{ \AA}$ . The tilt angle of the other coexisting groove side is  $1.2 \pm 0.2^\circ$  from the [112] direction towards  $+K$ . Similar scatter-

1 D.L. Abernathy, R.J. Birgeneau, K.I. Blum, and S.G.J. Mochrie, *Phys. Rev. Lett.* 71: 750 (1993); D.L. Abernathy, S. Song, K.I. Blum, R.J. Birgeneau, and S.G.J. Mochrie, *Phys. Rev. B* 49: 2691 (1994).

2 S. Song and S.G.J. Mochrie, *Phys. Rev. Lett.* 73: 995 (1994); S. Song and S.G.J. Mochrie, *Phys. Rev. B* 51: 10068 (1995); S. Song, M. Yoon, and S.G.J. Mochrie, *Surf. Sci.* 334: 153 (1995).

3 S.L. Wright, M. Inada, and H. Kroemer, *J. Vac. Sci. Tech.* 21: 534 (1982); G.H. Olsen, T.J. Zamerowski, and F.Z. Hawrylo, *J. Crystal Growth* 59: 654 (1982).

ing profiles were found for all temperatures between 1139 and 1155 K, which we identify as the second temperature region for the orientational phase behavior of the Si(112) surface.

Third, for temperatures between 1130 and 1139 K slightly different scattering profiles are found. The overall behavior is qualitatively the same as for 1146 K. The mean period of the superstructure determined from the displacement of the peaks was  $670 \pm 15 \text{ \AA}$ , within errors, the same as the mean period obtained at slightly higher temperatures. However, now, the inclination angle of one of the coexisting surfaces is  $1.1 \pm 0.1^\circ$  (shown as squares and dashed lines) towards  $-K$  and the reconstruction of this surface has a periodicity of  $91 \pm 3 \text{ \AA}$ . The inclination angle of the other side of the groove was found to be the same as for the previous temperature region,  $1.2 \pm 0.2^\circ$ .

Below 1130 K, the measured scattering profiles change considerably, corresponding to a surface morphology with groove sides composed of surfaces approximately  $1.0^\circ$  misoriented towards  $+K$  and surfaces approximately  $2.1^\circ$  misoriented towards  $-K$ . The average period of the grooves is  $260 \text{ \AA}$  at this temperature. Between 1055 and 1130 K, the same scattering profiles were found, therefore, we identify this as the fourth temperature region for the orientational phase behavior of the Si(112) surface.

On further cooling to temperatures below 1055 K, yet another different scattering profile, corresponding to yet another surface morphology, is found. Based on extensive measurements in this temperature range, we conclude that here the surface is composed of grooves with a mean size of  $210 \pm 15 \text{ \AA}$ , and each groove is composed of a  $4.1 \pm 0.2^\circ$  misoriented surface towards the  $-K$  direction with respect to [112] and a  $10 \pm 0.5^\circ$  misoriented surface towards the  $+K$  direction with respect to [112]. Unfortunately, it is not possible to obtain the angles of coexisting phases more accurately because of their small facet sizes. For example, the calculated average sizes of these surfaces are approximately  $150 \text{ \AA}$  and  $60 \text{ \AA}$  for the  $4.1^\circ$  and  $10.0^\circ$  misoriented surfaces, respectively. For all temperatures below 1055 K, we observed the same scattering profiles. Therefore, we identify this as the fifth temperature region for the orientational phase behavior of the Si(112) surface. Noting that the angle between [112] and [337] is  $4.0^\circ$  and the angle between [112] and [5512] is  $4.8^\circ$ , we speculate that the  $4.1^\circ$  misoriented surface, that we observed, is composed of [337] and/or [5512], which have previously been observed to be stable surfaces. Note

also that the angle between [112] and [557] is  $10.0^\circ$ . In this case, we may suggest that our  $10.0^\circ$  misoriented surface is [557].

### 3.2 Development of Beamlines for Condensed-Matter Physics and Materials Science at the Advanced Photon Source

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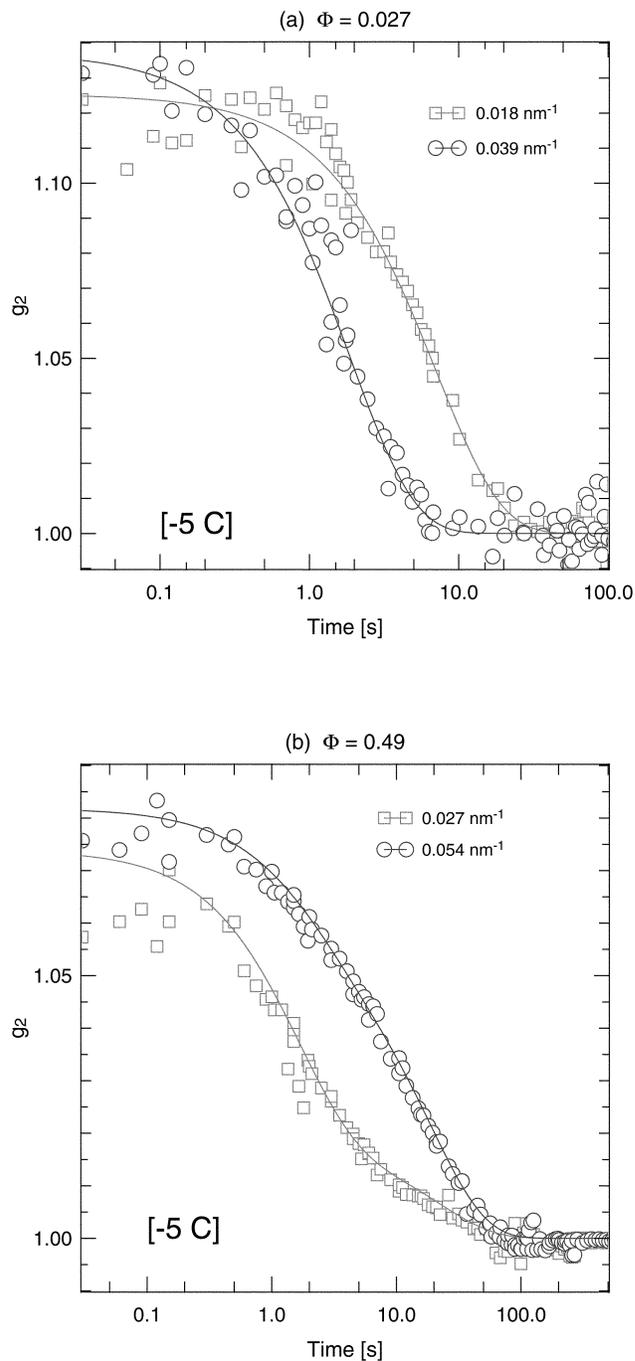
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The Advanced Photon Source (APS) is the United States' major new synchrotron x-ray source. Use of the APS presents new opportunities for x-ray scattering experiments. In the last year, we have made a major effort to bring the MIT-McGill-IBM beamline (8-ID) there into operation. Our first important technical goal at 8-ID was the realization of the "pink beam" concept, to deliver high-intensity, highly-collimated, wide-bandpass x-ray beams into the experimental enclosures using a mirror as the first optical component of the beamline. At the same time, this strategy reduces the heat-load on downstream optics and facilitates radiation shielding. This has now been successfully accomplished: pink-beam is delivered into the 8-ID-D/E experimental enclosures and is available for experiments. Specific examples of test experiments carried using pink beam will be described below.

Our second technical goal was the implementation of a transmission monochromator side-station using a thin diamond monochromator crystal to allow two experiments to run simultaneously on the insertion device (ID) line. This has also been accomplished: A thin, diamond-(111) crystal transmission monochromator, with 40% transmission at x-ray energies of 7.66 keV, was installed in the 8-ID-D hutch and commissioned. In addition, it is also possible to use a Ge(111) crystal in the side station monochromator for experiments that require higher intensity than available with the diamond monochromator. In this case, two experiments may operate in alternate shifts. Refinement and development of side-station diffractometers and other equipment for specific experimental set-ups is ongoing and will continue.

We have carried out several test experiments to exercise and demonstrate the capabilities of our beamline. One exciting opportunity is to carry out x-ray photon correlation spectroscopy (XPCS) measurements to investigate *dynamics*. The ability to carry out XPCS measurements depends on making a coherent x-ray beam and resolving the resultant x-ray speckles in the scattering pattern. To demonstrate XPCS at 8-ID, we initiated studies of the concentration dependence of the structure and dynamics of colloidal polystyrene (PS) latex spheres suspended in glycerol.

With XPCS, the relaxation of density fluctuations may be quantified by means of the autocorrelation of the scattered x-ray intensity versus time [ $g_2(t)$ ]. Such data, measured at 8-ID, are shown in Figure 4. Notably, these data are the first XPCS measurements of equilibrium dynamics to be carried out at the Advanced Photon Source. The evident decrease of  $g_2(t)$  versus time in the plots reveals the spheres' diffusive dynamics on time scales from 50 milliseconds to 50 seconds.



**Figure 4.** Intensity autocorrelations, plotted on a linear scale, versus time, plotted on a logarithmic scale, over nearly four decades in time, for PS latex spheres suspended in glycerol at  $-5^\circ\text{C}$ . (a) volume fraction of 0.027. (b) volume fraction of 0.49.

