[22-S18]

Atomic structure of the Si(113) surface studied by coaxial impact collision ion scattering spectroscopy

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The atomic structure of Si(113) has been studied using time of flight-coaxial impact collision ion scattering spectroscopy (TOF-CAICISS) and reflection high energy electron diffraction (RHEED). RHEED observations showed that the phase transition from 3x2 to 3x1 occurs during annealing at high temperatures above ~450C and it is reversible. In the CAICISS measurements, the intensity of He ions scattered from Si atoms was investigated as a function of polar- and azimuth-angles. It was found that in all measurements the CAICISS yields of 3x2 are most probably consistent with those of 3x1, which indicates that the atomic geometry of 3x2 would be consistent with 3x1. In both phases, the CAICISS yields of two selected polar-angle measurements, which were carried out along the directions deviated +45 and -45 from the [332] direction, are almost the same. This means that the atomic geometry of the Si(113) reconstructions, which have the unit of five atoms including a dimer, is symmetric on the [332] direction.

These remarkable features are likely to be explained by the Ranke's adatom and dimer (AD) model(1). Furthermore, it has been known that as observed by Knall et al.(2) the STM images corresponding to filled and empty states of Si(113)3x2 are in accordance with the Ranke's AD(3x2).

In order to certify these findings we have carried out an ion-scattering simulation using some structural models including the Ranke,s AD model, and compared with the experimental results. From these comparisons we discuss the atomic structure of the Si(113) reconstructions.

[References]
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2. J. Knall, J. B. Pethica, J. D. Todd, and J. H. Wilson, Phys. Rev. Lett. 66, 1733 (1991).