[III-13]

CAICISS study for the buckled Si(001) surface structure

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Although the (2×1) dimer structure for the clean Si(001) surface was proposed by Schiler and Fransworth using LEED about thirty years ago, there still remains controversy about the details for the surface. Theoretically, while some of total energy calculation have predicted the buckled dimer to be stable in comparison with the nonbuckled dimer, some other calculations such as a pseudopotential method, a core-level-shift calculation and ab initio molecular dynamics study have reported the stability of symmetric dimer. Another recent theoretical results have been predicted that c(4×2) structure of p(2×2) structure are energetically more favorable than the asymmetric (2×1) dimer. On the other hand, most of the experimental studies have supported the asymmetric dimer structure with buckling. Moreover, the p(2×2) and c(4×2) structures have been reported by recent experimental results such as STM, X-ray standing wave measurements, X-ray photoelectron spectroscopy and UHV-TEM. In the case of the models proposed by theoretical calculation, the phases and 3-dimensional geometric structure have been described in detail. However, most of experimental results have been mentioned about only phase, there are few experimental one which is described about geometric structure.

CAICISS(Coaxial Impact Collision Ion Scattering Spectroscopy) experiment is a very powerful technique for solving surface geometric structure at the atomic level. So the geometric structure of Si(001) surface is investigated using CAICISS system. We confirmed that the Si(001) surface is certainly buckled, and the asymmetric (2×1) and c(4×2) structure coexists. In this representation, thus, the reconstruction structure of Si(001) surface will be discuss using data obtained from CAICISS experiment, and, based on our experimental results, we will also report the geometric structure such as bond length and bonding angle of surface atoms.