

Preparation of ultra-clean hydrogen and deuterium terminated Si(111)-(1x1) surfaces and re-observation of the surface phonon dispersion curves

H. Kato, T. Taoka, P. Murugan¹, Y. Kawazoe¹, T. Yamada², A. Kasuya³ and S. Suto

Department of Physics, Tohoku University, Sendai 980-8578, Japan

¹Institute of Materials Research, Tohoku University, Sendai 980-8577, Japan

²RIKEN, Saitama 351-0198, Japan

³Int. Advanced Research and Education Org., Tohoku University, Sendai 980-8577, Japan

The surface phonon is defined as a coherent vibrational excitation of surface atoms propagating along the surface. It is characterized by a phonon dispersion curves, which were extensively studied in 1990's using helium atom scattering and high-resolution electron-energy-loss spectroscopy (HREELS)[1]. The understanding is mainly based on the theoretical framework of a classical bond model or cluster calculations. The recent sample preparation and first principles calculations open the new way to deep insight for surface phonon problems.

The surface phonon dispersion on the hydrogen-terminated Si(111)-(1x1) surface [H:Si(111)] is the typical system and already reported experimentally [2] and theoretically [3], although the understanding is incomplete. The sample contaminated by the oxygen atoms on the surface and the calculations were also classical. In this study, firstly, we have prepared an ultra-clean H:Si(111) surface [4] and measured the surface phonon dispersion curves using HREELS. Secondly, we have performed first-principles density functional calculations with the projector augmented wave functionals, as implemented in VASP, using generalized gradient approximations. We used a slab of six silicon layers and both top and bottom surfaces were terminated with hydrogen atoms. Finally, we have compared with the surface phonon dispersion of deuterium-terminated Si(111)-(1x1) surface [5] and led to our conclusions.

The Si-H stretching and the bending modes are observed at 258.5 and 78.2 meV, respectively. These energies are the same as the previously reported values [2], but the energy-loss peaks at the lower

energy regions are dramatically shifted. Through this combination study, we have formulated the procedure of preparing ultra-clean H:Si(111)/D:Si(111), which was confirmed by HREELS vibrational analysis. The Si surface will be utilized for further nano-physics research as well as for the materials for nano-fabrication.

References

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