Ordered submonolayer arrangements of adsorbate atoms on semiconductor surfaces constitute a rich playground for investigating electronic correlation effects. These effects are tightly connected with the local atomic arrangement. For many material systems, the detailed arrangement is quite complicated and still under debate. E.g. for the (5x2) reconstructed Au-Si(111) system, various structural models are presently under discussion [1,2]. Vibration mode analysis constitutes a powerful tool for resolving these ambiguities. It is not only a valuable extension to electron diffraction (LEED) with regards to atomic arrangement, but also gives access to local bond strengths. Thanks to high-sensitivity spectrometers and detection systems, even very weak surface- and adsorbate-induced vibration modes have become accessible to optical analysis by Raman spectroscopy.

We applied polarized Raman spectroscopy to Au-covered Si(111) surfaces, either with (5x2) or with (√3x√3) reconstruction, and to clean Si(111) (7x7) surfaces for reference. On clean annealing-induced (7x7) surfaces, six surface vibration modes appear, in the energy range between 7.7 meV and 52.1 meV, and with different polarization dependence. As a further proof for their surface phonon character, these modes are fully quenched upon gold coverage. They are replaced by new modes, whose detailed behavior is governed by the Au reconstruction. For the (5x2) - Au reconstruction, five Au-induced surface vibration modes occur at rather low frequencies, ranging between 3.2 meV and 18.7 meV. The surface phonon spectrum of the (√3x√3) Au reconstruction shares two of these modes, but also shows two new reconstruction-specific peaks in the same range.

For the clean Si(111) (7x7) surface, these results should enable refined calculations of the dynamic properties of the established DAS structural model [3]. For the Au-covered surfaces, the reconstruction-specific vibration modes may contribute to the clarification of the atomic geometry, extending the base for more sophisticated calculations of atomic and orbital properties of ordered adatom arrangements for correlated-electron systems.

Keywords: Raman Spectroscopy; surface phonons; Au/Si(111) surface

References