SYSTEMATIC SEARH FOR THE Si(553)-Au RECONSTRUCTION.

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Gold deposited on silicon surfaces at the monolayer regime results in a variety of reconstructions. The most peculiar ones are the (quasi-) one dimensional phases, featuring monatomic wires of gold. They promise exotic physical phenomena, such as the Luttinger liquid [1]. These wires can be grown on the flat Si(111) surface which yields three possible directions for the wires to grow [2]. Stepped silicon surfaces avoid this problem; the wires grow parallel to the step edges. These systems have been manufactured now for years [3].

We present an *ab-initio* study of the Si(553)/Au surface reconstruction using the SIESTA method [4]. Very recently the Si(553)/Au surface has been studied with growing intensity [3],[5],[6],[7],[8],[9],[10]. The reason for this is the peculiar band structure seen in the photoemission that features one half-filled and another quarter-filled band [5]. As the temperature is increased, these bands show Peierls-like distortions with different periodicities in the atomic structure [7].

Big amount of experimental information is available, including STM, photoemission and x-ray diffraction studies [5],[6],[7],[8] but an atomic structure [3],[8],[9],[10] that would give consistent results with the experiments has not been found up-to-date. We present a systematic method for searching any quasi one-dimensional surface reconstruction based on a tetrahedric coordination of both Au and Si atoms in the surface (we are able to search through all the surface reconstructions that include the most typical Si(111) building blocks: honeycomb-chains, surface-dislocations, stacking-faults, etc.). We have arrived at a model that produces the experimental band structure extremely well. The half-filled band has a strong gold-character as it should in order to feature the (spin-orbit) splitting [11] seen in the experiment [5],[7], while the quarter-filled band originates from the silicon atoms at the step-edge. The structure does not feature the honeycomb-chain structure, as proposed earlier [9] and is very different from the well-known Si(557)-Au reconstruction [11]. We present also simulated STM-images of the new structure.

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