Identification of Tetramers in the Silver Film Grown on Si(001) Surface at Room Temperature

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The growth of metal films on silicon is of interest in the fabrication of miniaturized semiconductor devices, including integrated circuits, microelectronics and opto-electronics.[1] Amongst the numerous systems in this field, the growth of Ag-films on Si(001) has been heavily examined,[2-18] since it serves as a prototype model for an abrupt metal/semiconductor interface.

At room temperature (RT), the growth of silver on Si(001) follows the Stranski-Krastanov mode.[6,8,11] Adsorbed Ag-atoms aggregate to form a film up to one full monolayer, beyond which Ag-islands are formed. What remains unclear, however, is the atomic structure of the initial silver monolayer because earlier measurements at RT were often obscured by the high-mobility of silver on Si(001).[4,8,17] At RT, this film appears to have either a 2×1 or 2×2 structure with a high degree of disorder. Various models[7,8,12,15] have been proposed where both the 2×1 and 2×2 structures are all based on a Ag dimer structure.

Here, we present the atomic structure of the sliver film grown on Si(001) at RT that challenges the notion of Ag-dimers as the building block. Experiments, using Scanning Tunneling Microscopy (STM) between 15 K and 140 K, succeeded in supressing the mobility of silver on Si(001), and allow the identification of Ag-tetramers in the silver film for the first time, as shown in Figure 1. Ag-tetramers are found to be adsorbed exclusively at the trough between two Si-rows, interacting with four adjacent Si-dimers via covalent bonding. Consequently, the π-bonds of the Si-dimers underneath the silver film are eliminated. This interpretation is supported by Density Functional Theory (DFT) calculations of the Ag-tetramer adsorption geometry, providing further insight into the surface bonding of silver adsorbed on Si(001).

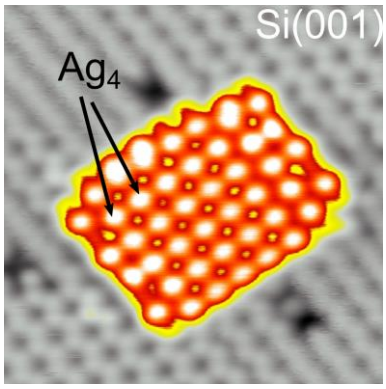

Figure 1 | STM image of 0.15 ML Ag on Si(001) at 65 K.

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