S-P10

Origin of the type-C defect on the Si(001) surface

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We studied the water molecule adsorption on the Si(001)-2x1 surface by using Scanning Tunneling Microscopy and the ab initio pseudopotential calculations. The water molecules exist even in the UHV(Ultra High Vacuum) chamber. Hence the residual water molecules adsorb dissociatively on the Si(001)-2x1 surface to form Si-H and Si-OH bondings into ID(Inter dimer) and OD(On dimer) configurations. Both the residual and direct dosed water molecules creates type-C(ID) and the U-shape(OD) defects with the ratio of ~5:1 at RT. We also made to measure the thermal dissociation C/U ratio under the different temperature(~600℃) conditions.

In conclusion, the type-C defect and U shape defects are identified water molecule dissociation. In addition, most of the 1DV like features in the filled state images, not a intrinsic vacancy but a U-shape(OD) features.