

Scanning tunneling microscopy simulation study of In/Si(557)-3x1 using first principle calculation

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We observed that the subsequent annealing (at 530°C) after In deposition on clean Si(557) stepped surface gives 3x1 phase, which confirmed using low electron energy diffraction (LEED) and scanning tunneling microscopy (STM) measurements. Experimental STM images show three chains for filled state, while a single zigzag chain for empty state. We proposed structure models for this phase, and examined these models using first principle calculation. We found a structure model (2In), for which simulated STM images are very good agreement with experimental one. We could explain that the bright protrusions of experimental filled state STM image comes from step edge of honey comb structure, In atoms on the terras, and expelled Si atoms from terras.