

Hydrogen-Enhanced Schwoebel Barriers and Anisotropic Strontium Diffusion on Vicinal Si(001)

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Functional oxides such as BaTiO₃ can add electro-optic functionality to silicon devices [1]. Epitaxial integration commonly uses a SrTiO₃ buffer [2–4], initiated by depositing half a monolayer of Sr at 625 °C to protect silicon from oxidation. Growth on vicinal Si(001) substrates [5,6] introduces terraces and steps that complicate Sr migration. We examine how hydrogen affects Sr migration on double-step Si(001) surfaces with a (2×1) reconstruction.

In this talk, we present first-principles calculations for bare and H-passivated surfaces with a 6.8° miscut and 22.59 Å terrace width (Fig. 1). On the bare surface, Sr moves from a terrace trough into a secondary minimum between step-edge dimers before descending. Hydrogen raises the initial barrier toward the step from 0.983 to 1.055 eV and adds two intermediate minima. Our multistate model predicts approximately tenfold slower step crossing. Conversely, hydrogen lowers the barrier along the trough above the step from 0.917 to 0.812 eV, yielding an approximately tenfold faster transition rate.

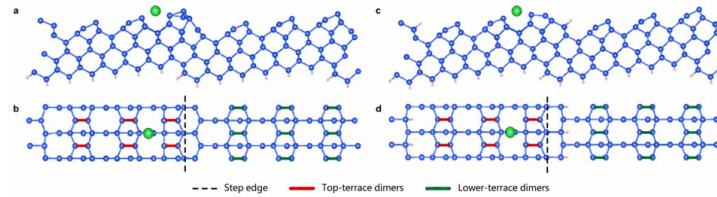


Figure 1: (a, c) (110) projections of Sr in an upper-terrace trough for bare and H-passivated models, respectively. (b, d) (001) projections: upper- and lower-terrace dimers are red and green, respectively; dashed lines mark the step edge.

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