Dynamics of Sn adatoms at the single steps on the Si(111)-$\sqrt{3}\times\sqrt{3}$-Sn surface

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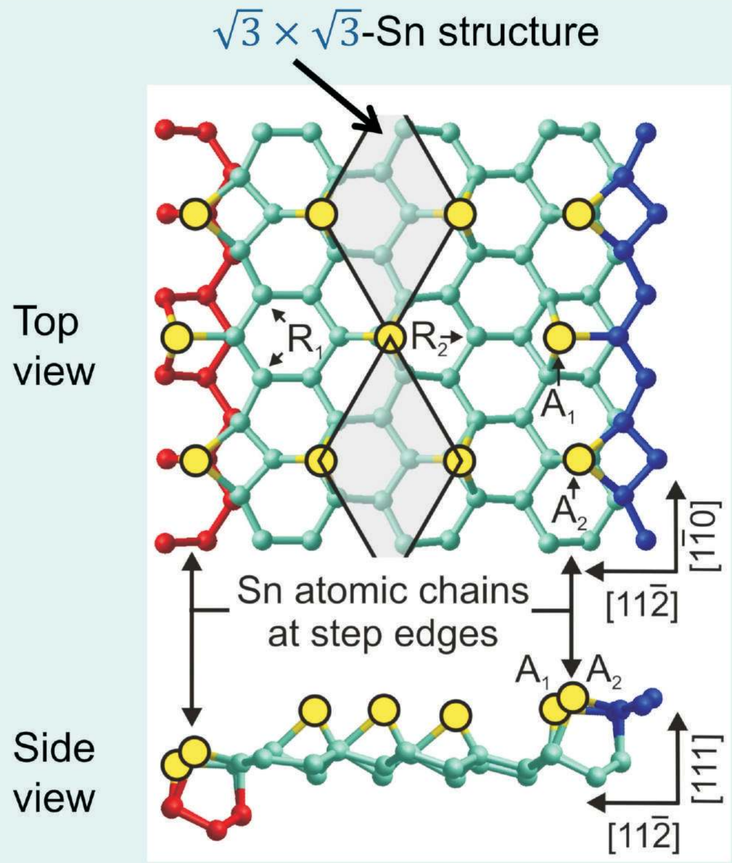
Methods: low-temperature scanning tunneling microscopy (LT-STM, Omicron), density functional theory calculations (SIESTA) using generalized gradient approximation (GGA).

References:

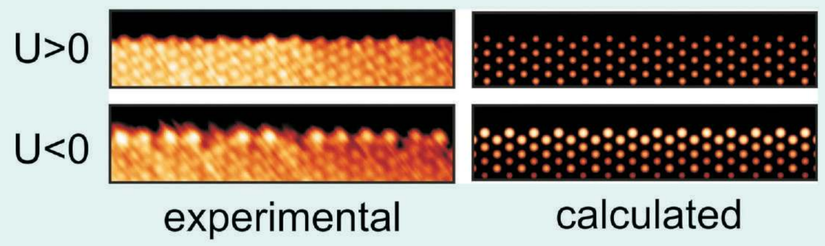
1. R. A. Zhachuk at al., Phys. Rev. B 104 (2021) 125437
2. F. Ronci et al., Phys. Rev. Lett. 95 (2005) 156101.
3. F. Ronci et al., Phys. Rev. Lett. 99 (2007) 166103.
4. F. Ronci et al., J. Phys.: Condens. Matter 22 (2010) 264003.

Atomic structure of a single step

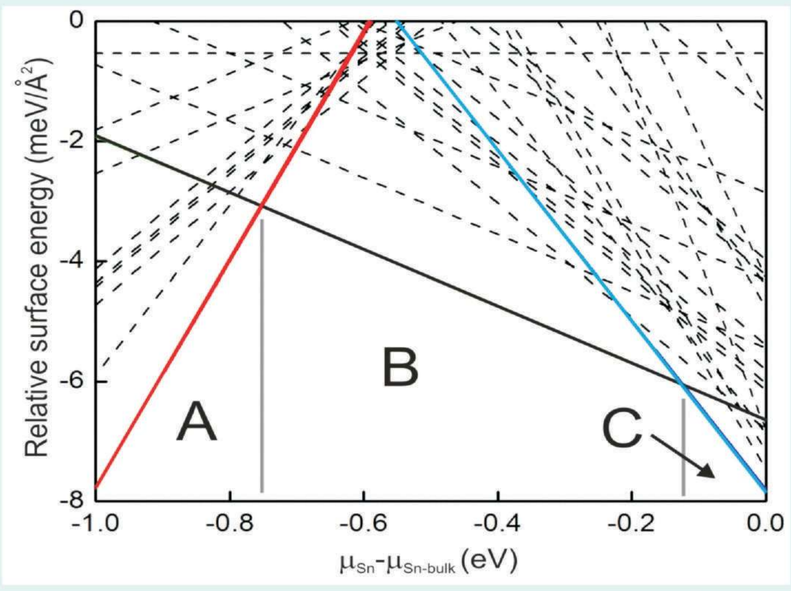


Model "B". Yellow balls – Sn atoms, R_1, R_2 – rest atoms, A_1, A_2 – Sn adatoms forming Sn chains along step edges, red, cyan and blue balls are Si atoms of the lower, middle and upper (111) terraces, respectively.

1) Proof: STM images.



2) Proof: Lowest calculated surface energy among 50 tested models.

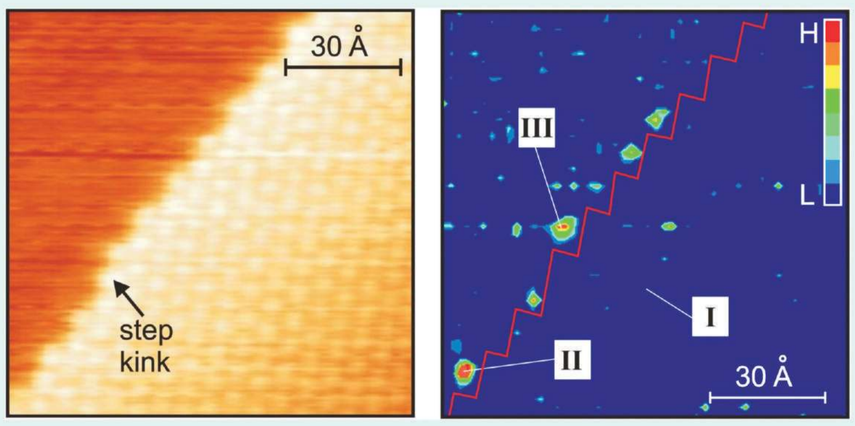


Sn-depleted ⟷ Sn-rich

Dynamics of Sn adatoms at T=80 K

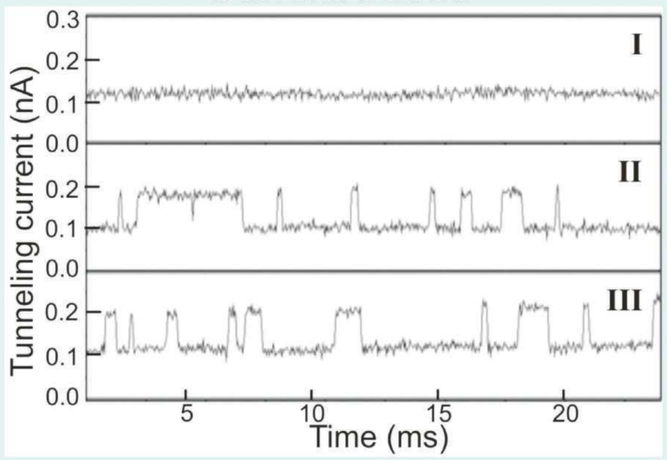
Constant current STM image

Ξ-map: standard deviation of the current traces



feedback loop is ON feedback loop is OFF

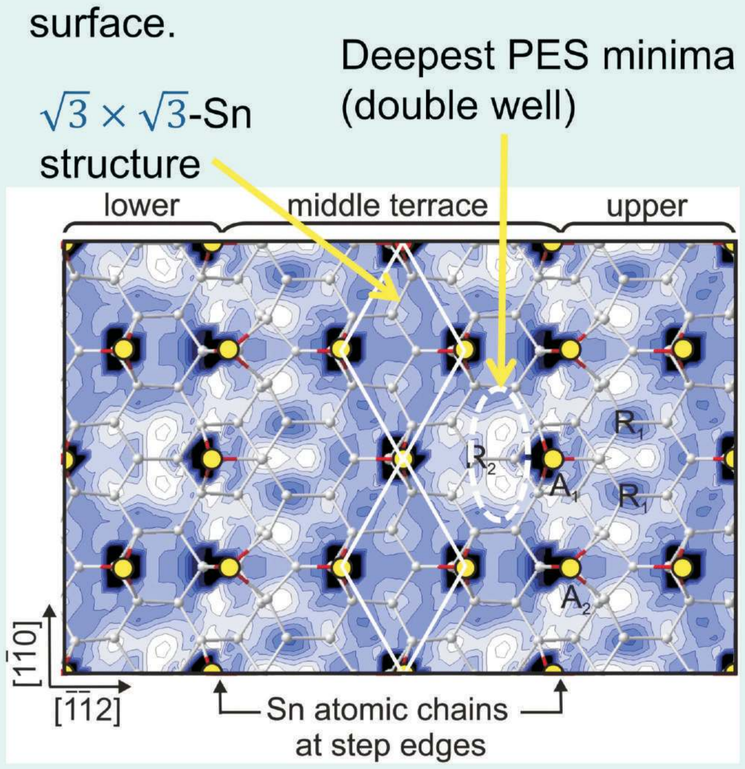
Current traces



feedback loop is OFF

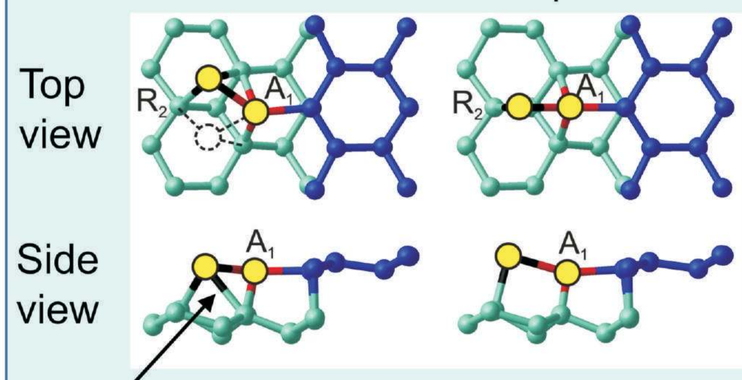
The dynamics of Sn adatoms was detected near the steps (bright spots on the Ξ-map).

Calculated Potential Energy Surface (PES) for Sn atoms on the Si(111)-$\sqrt{3}\times\sqrt{3}$-Sn surface with steps: describes the energetics of adsorbed Sn atom on the reconstructed surface.



Bright (dark) regions indicate energy minima (maxima). The contour spacing is 0.2 eV. White circles are Si atoms; yellow circles are Sn atoms.

How does the double well look like?



Conclusions:

1) Step atomic structure is determined.
2) Dynamics of Sn adatoms near step edges is explained by formation of double wells.