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Simulating Ion Scattering Trajectories on a Stepped Surface

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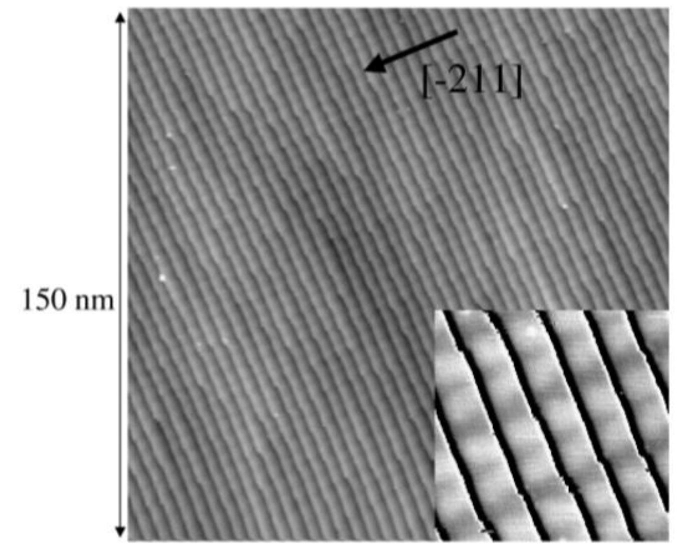
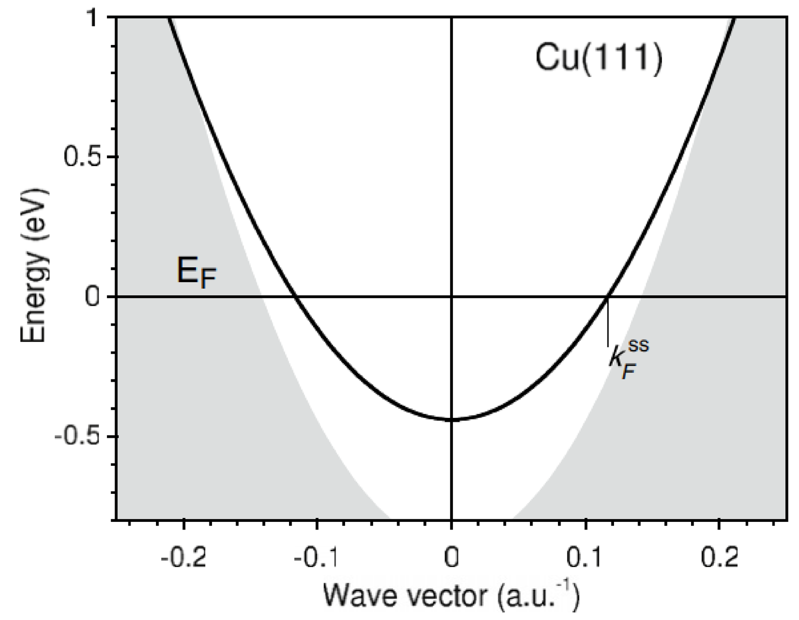
Abstract

Surfaces cut in the (111) direction exhibit isolated surface states, as the conduction band does not have any states with momentum along the z axis. These states however, are un localized, and very difficult to interact with via ion scattering. STM studies have shown that these surface states can be localized, by cutting the lattice such that it contains steps of (111) surfaces.[1] These localized states might then be able to be interacted with via ion beam studies.



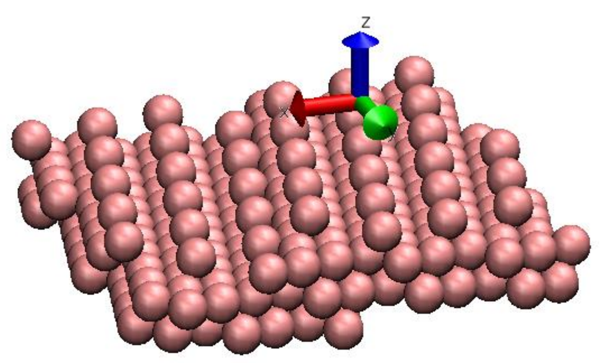
STM image of a gold (788) surface[1]



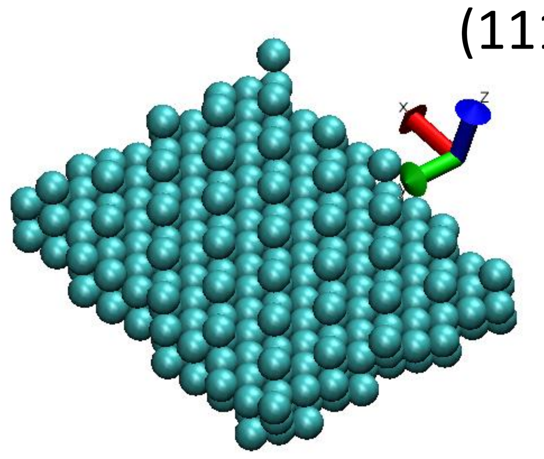
Surface State for Cu(111)[2]

- **Goal**: To identify trajectories that will probe the step-confined surface state on (111) surfaces
- Modeling of all surface trajectories using SAFARI[3], a molecular dynamics simulation
- Isolation of scattered trajectories that can be reliably detected in our facility
- Identification of step-edge and on-step collisions using impact parameters and modeled trajectories

(788)



(111)

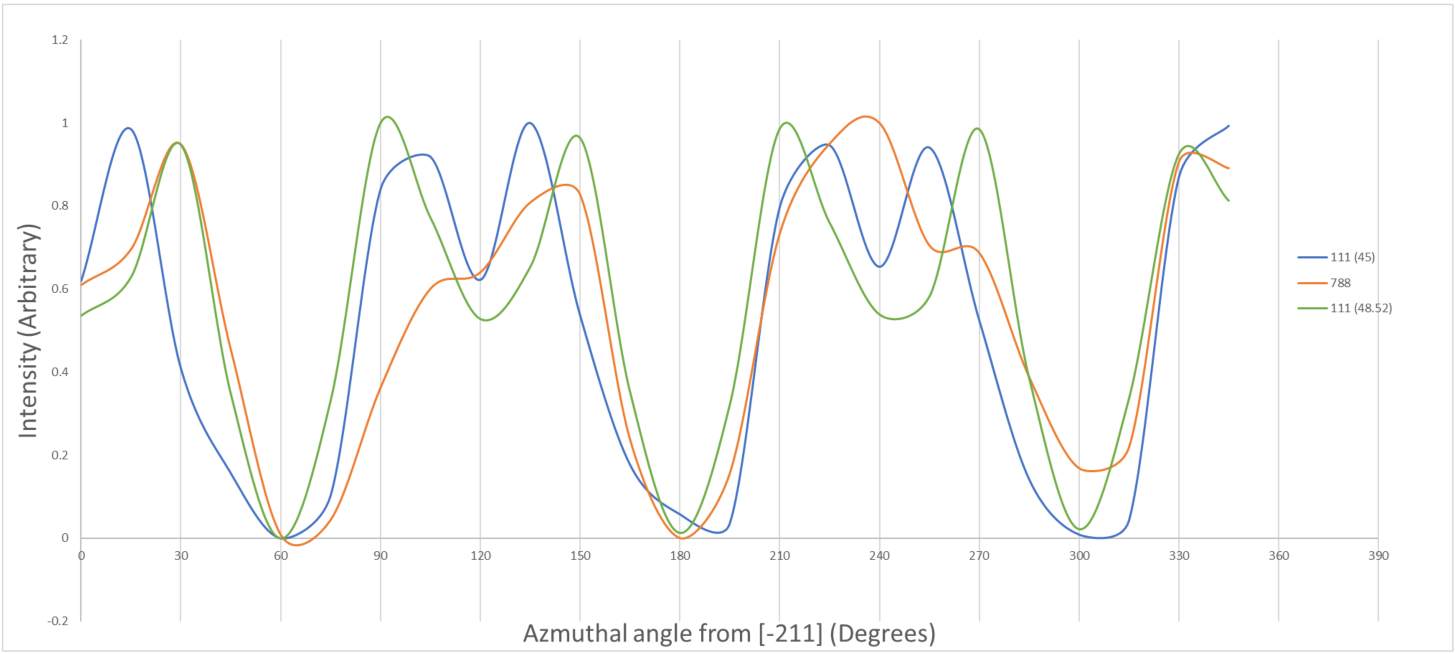


Simulation Details

SAFARI - a molecular dynamics simulation developed at Cornell University to simulate the surface and near-surface scattering of low and hyperthermal energy ions

- Simulation is optimized for rectangular symmetry, e.g. (100) surfaces
- Surface states of interest arise on (111) surfaces, which have hexagonal symmetry
- Modification of SAFARI was made to run giant "unit cells" of the entire surface+step feature
- Flexible surface slicing script developed using Python to generate SAFARI inputs

Simulation Results: Azimuthal Dependence

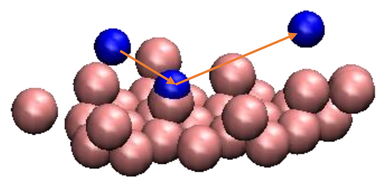


Reflectivity Integrated over all outgoing angles and energies

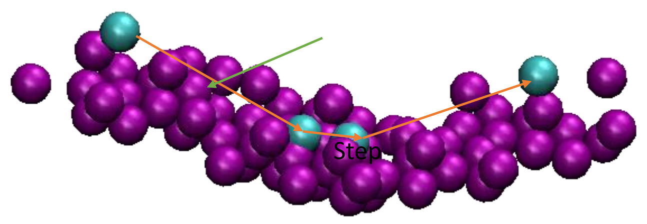
- Distinct differences between the azimuthally-resolved intensities for the stepped and unstepped surfaces
- Distinct differences between the slight offsets (3.5°) in the two unstepped 111 surfaces
- Down-step scattering between 788 and similarly aligned 111 are very similar, as expected

Simulation Results: Trajectory Comparison

- Comparing trajectories at $\phi = 240°$, the stepped surface shows increased relative intensities
- Extra scattering events are caused by down-step channelled scattering events



Quasi single scattering event at $\phi = 240°$



Channelled scattering event, due to step, at $\phi = 240°$

Conclusions

- Crystal orientation can be determined via azimuthally-resolved scattering
- Stepped surfaces can also be identified
- Location of scattering event can be determined via energy-resolved scattering at specific angles

Future Directions

- Select appropriate stepped surface(s) based on surface state energetics

Element	Face	Surface Angle
Au	2 2 3	11.4°
Au	7 8 8	3.5°
Au	21 23 23	2.4°

References

[1] A. Mugarza, A. Mascaraque, V. Pérez-Dieste, V. Repain, S. Rousset, F.G. de Abajo and J.E. Ortega, *Physical Review Letters* **87**, 107601(2001).

[2] V. Silkin, M. Alducin, J. Juaristi, E. Chulkov, P. Echenique, *Journal of Physics: Condensed Matter.* **20**, 304209 (2008).

[3] D. Goodstein, S. Langer, B. Cooper, *Journal of Vacuum Science & Technology A* **6**, 703 (1988).

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