Materials Science and Technology
Scanning Tunneling Microscopy

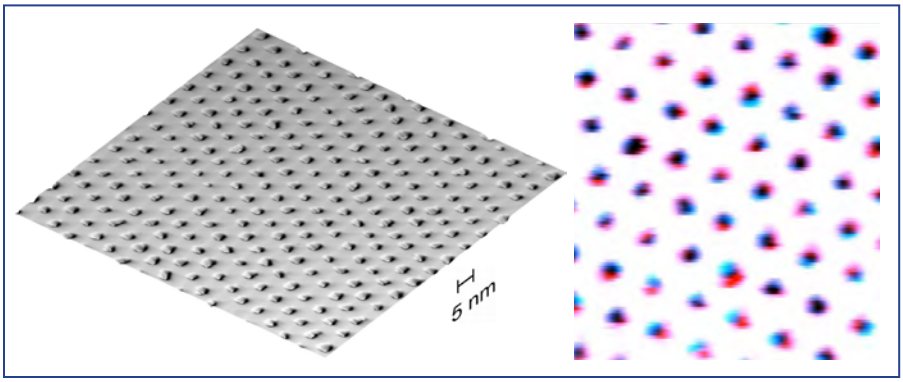

Figure 1: Left - STM image of a very regular array of vacancy islands (holes) embedded in a 1-atom-thick silver film grown on a ruthenium crystal. Right - The overlay of two STM images (red and cyan) acquired 12s apart at T=80°C shows the thermal vibrations in this self-organized triangular lattice.

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Using STM to determine the origins of self-organized patterns on surfaces

A novel combination of quantitative real-time microscopy measurements and atomistic modeling helps Sandia researchers solve the problem of manipulating structures at the nanoscale.

Thin films and solid surfaces are often observed to spontaneously "self-organize" into ordered patterns at nanometer length scales. At this length scale, structures are too large to be manufactured by chemical synthesis and too small to be accessible to existing microtechnologies based on photolithography. Having the ability to work in the nanometer range offers the prospect of continuing the drive to miniaturization in electronics and designing novel devices with specific properties that rely on such small dimensions.

Understanding the physics of nanoscale self-organization is challenging because it is difficult to manipulate structures at this length scale in a controlled way. This difficulty is compounded by the complexity of the involved nanometer-scale forces.

To surmount these difficulties, we quantitatively analyze the naturally occurring thermal vibrations in these structures using variable-temperature atomic-resolution Scanning Tunneling Microscopy (STM).

We chose a system simple enough to allow a precise determination of its atomic structure – a triangular array of vacancy islands (holes) in a monolayer (1 atom) thick silver film (Fig.1) that develops spontaneously when a monolayer of silver grown on a ruthenium crystal is exposed to a tiny amount of sulfur. We found that although the holes wander about their respective average positions, their arrays are extremely stable. Our novel combination of quantitative real-time STM measurements and atomistic modeling allowed us to determine the origin of this stabilizing force.

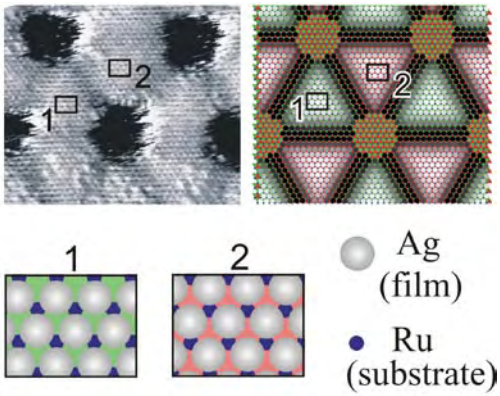

Figure 2: Left: Atomically resolved STM image of the hole-array structure. Right: Corresponding unit cell used in a Frenkel-Kontorova model. The inserts 1 and 2 show the different stacking in the two types (green and red) of triangular building blocks.

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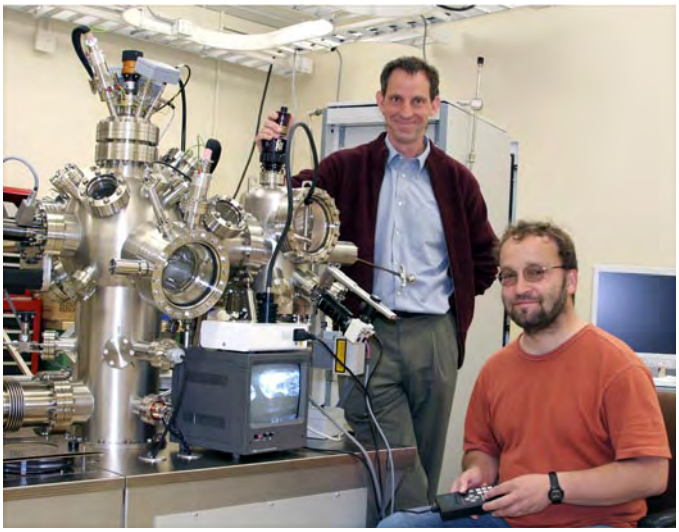
We observed thermal hole vibrations inconsistent with the conventional explanation for the surface ordering, which involves elastic distortions of the substrate. In our search for an alternative ordering mechanism, we used an atomically resolved STM image. We established that the hole-hole interaction originates in the preference of dislocations, which often form to accommodate a mismatch between the lattice constants of film and substrate, to run along specific crystallographic directions.

Since dislocations are extremely common in crystalline solids, we expect to discover other systems where self-organization is accomplished through similar dislocation-mediated mechanisms. The value of such ordered nanostructures could be greatly enhanced if one could tailor their properties. In the case of the presented vacancy island lattice, we could achieve some tailoring if the mechanism for self-organization remains intact even if the film material (pure silver) is replaced by an alloy, possibly silver/copper. We should then be able to control the hole-hole spacing simply by adjusting the composition of the film.

Publications:

K. Thürmer, C.B. Carter, N.C. Bartelt, R.Q. Hwang, "Self-assembly via adsorbate-driven dislocation reactions," *Physical Review Letters* **92**, 106101-4 (2004).

K. Thürmer, R.Q. Hwang, N.C. Bartelt, "Surface self-organization caused by dislocation networks," *Science* **311**, 1272-1274 (2006).



While employing state-of-the-art microscopy, the true hallmark of our approach is very tight integration of experiment and theory.