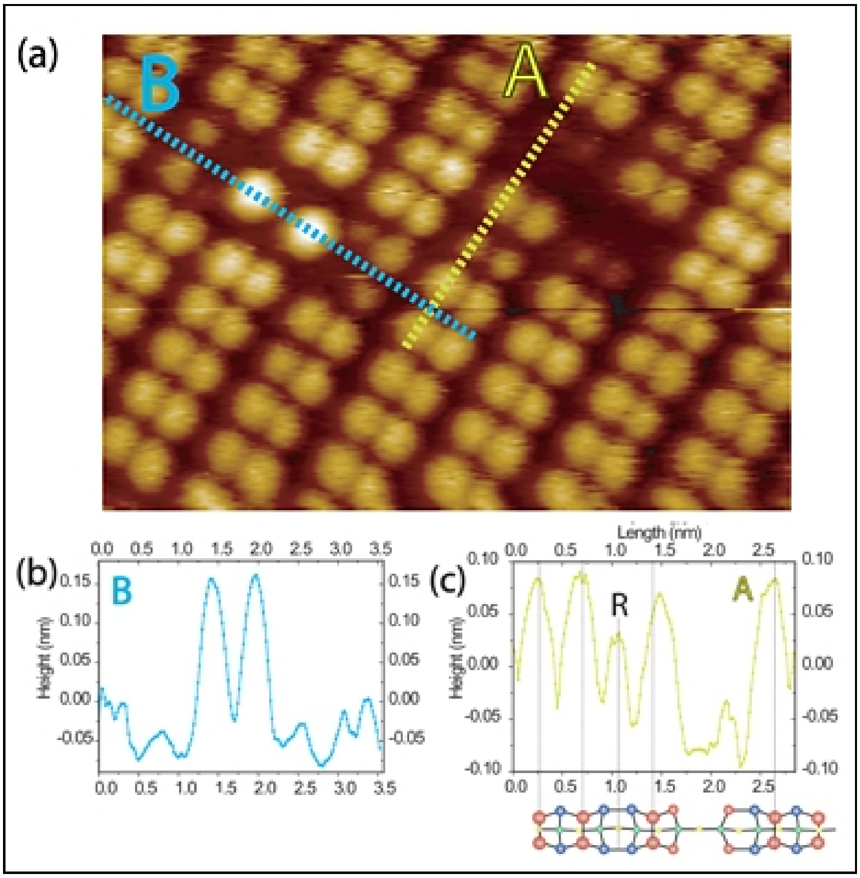
qPlus atomic force microscopy of the Si(100) surface:
Buckled, split-off, and added dimers
(Result of the month 10/2009)

We have used an Omicron LT qPlus system, operating at 77 K, to image dimer configurations at the Si(100) surface, using both large (10 nm peak to peak) and small (0.5 nm peak to peak) oscillation amplitudes. In addition to the p(2x1), p(2x2), and c(4x2) reconstructions of the pristine surface, a variety of defect types including ad-dimers, vacancies, and split-off dimers have been imaged. Our data appear at odds with the currently accepted structural model for split-off dimers. At low oscillation amplitudes the degree of apparent dimer buckling can be tuned by varying the frequency shift set point.



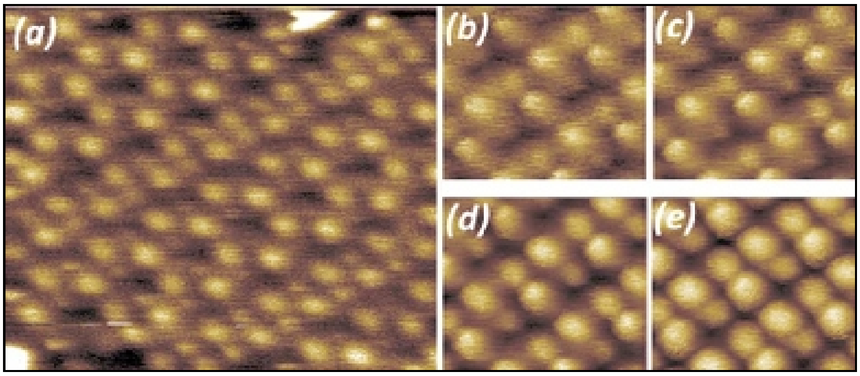
NC-AFM image taken using a qPlus sensor (5.42x3.75 nm2) of the Si(100) surface taken at 77 K with an oscillation amplitude of 10 nm peak to peak, df =−4.9 Hz, and Vsample=±0.1 V. In addition to the p(2x1) surface reconstruction, two surface defects are observed.

a) boron-induced ad-dimer (labeled B) and a 1+2-DV vacancy cluster;

b) Line profile through the ad-dimer defect;

c) Line-profile through1+2-DV defect cluster and comparison with currently accepted structural mode. R represents the position of the "recessed" dimer observed in our images

We first imaged the Si(100) surface at 77K using a high oscillation amplitude (10 nm pk-pk) in order to compare our data with previously published conventional silicon cantilver-based NC-AFM measurements of the Si(100) surface. Our images of the clean surface Si(100) dimers are in very good agreement with the results of, for example, Sawada et al. [Japn. J. Appl. Phys. 47 6085 (2008)]. Similarly, qPlus AFM images of the boron-induced defect agree well with the structural model very recently put forward by Liu, Zhang, and Zhu [Phys. Rev. B 77 035322 (2008)]. However, qPlus images of split-off dimer defects appear to be at odds with the currently accepted structural models for these defect complexes



a) qPlus AFM image of the Si_100_ surface taken at 77 K with a peak to peak oscillation amplitude of 0.7 nm, a sample bias of +0.3 V, and df =−10.9 Hz;
b)   e) Effect of changing the setpoint df on the resolution of the lower atom of each buckled dimer; df =−26.1 Hz, -27 Hz, -28 Hz, and -30 Hz for images b) e), respectively. [For b)   e) the oscillation amplitude and sample bias are 0.5 nm peak to peak and +0.8 V, respectively.

There has been a great deal of debate (spanning a number of decades) regarding the precise structure of the Si(100) surface and, in particular, the nature of the ground state of this surface: does it comprise buckled or symmetric dimers? A key difficulty lies with the sensitivity of the surface to scanning probes: as the energy barrier between buckled states is ~ 100 meV, it is easy to affect the surface structure while scanning. We therefore investigated the Si(100) surface at 77 K using small oscillation amplitudes (0.5 nm pk-pk) with a range of different set-point frequency shifts (see Fig. 2). Buckled dimers (in both c(4x2) and p(2x2) arrangements) are observed (Fig. 2(a)). The degree of apparent dimer buckling observed depends sensitively on the setpoint frequency shift (Fig. 2(b)   (e)).

Authors:
A. Sweetman, S. Gangopadhyay, R. Danza, N. Berdunov, and P. Moriarty

Institute:
The School of Physics and Astronomy,
The University of Nottingham, Nottingham NG7 2RD,United Kingdom
www.nottingham.ac.uk/physics/research/nano

Publication(s)
*APPLIED PHYSICS LETTERS **95**, 1 (2009)*

This result has been obtained with : **OMICRON LT STM**