Solving a long-standing problem regarding atomic structure of Si(100)2×3-Ag

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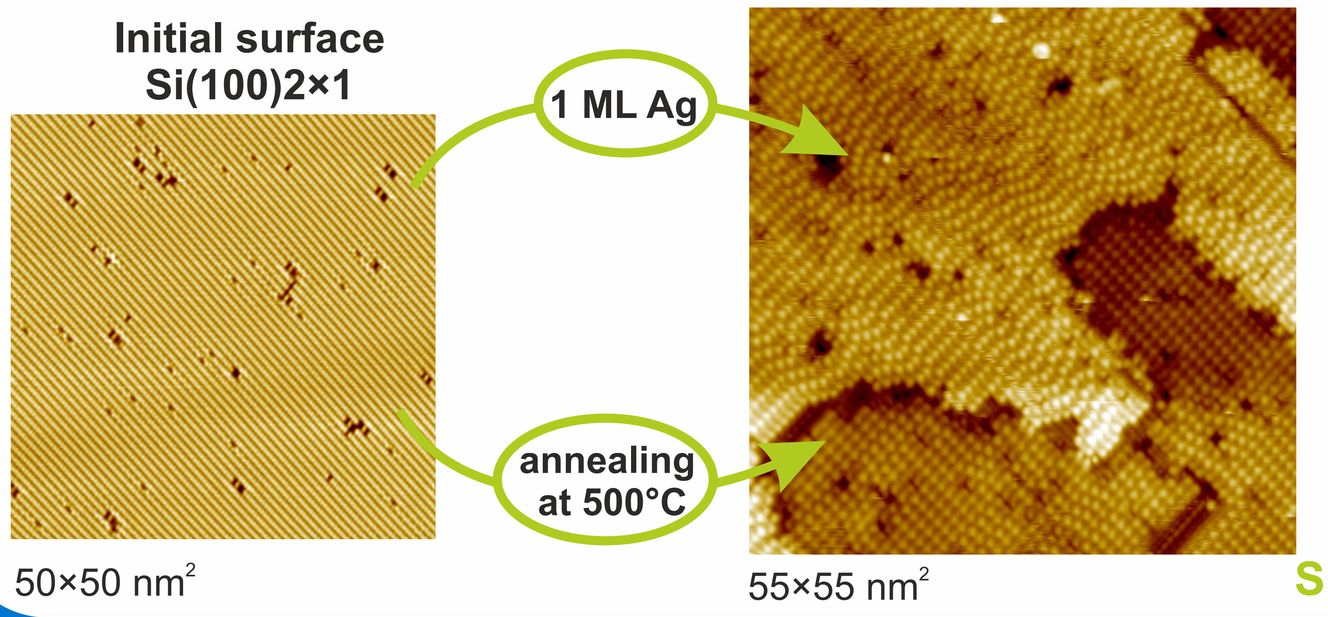
Introduction

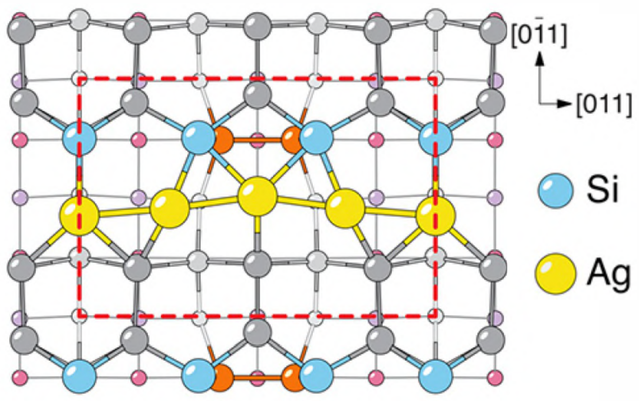
Low-dimensional systems composed of atomically thin metal films on semiconductor surfaces have attracted great attention due to their intriguing electronic properties and potential prospects for applications in atomic-scale devices.

Breakthrough in assessing the prospects of a given reconstruction has typically been trigged out by the conclusive determination of its atomic arrangement. Sometimes it takes decades to reach this goal. The Ag/Si(100) system can serve as an example. Though onset of the extensive study of the system dates back to the mid-1990s, atomic arrangement of its surface reconstructions still remains unknown.

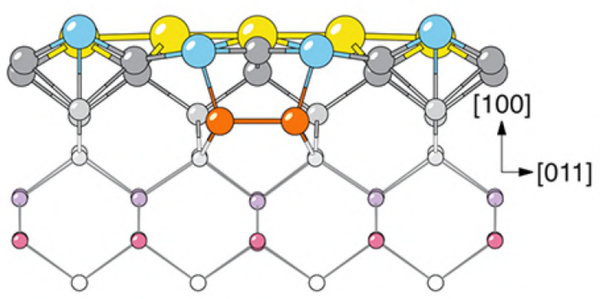
Formation of the Si(100)2×3-Ag reconstruction



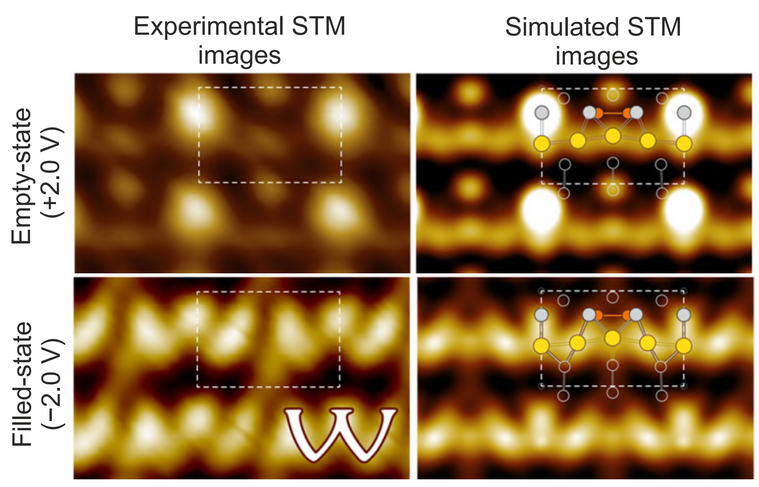
Structural model of the Si(100)2×3-Ag reconstruction



- The structural model was determined by using the AIRSS technique.
- The AIRSS technique was applied to the three possible cases, in which the number of Ag atoms was either 3, 4, or 5 per 2×3 unit cell, while the number of Si atoms was always 3.
- As a result, it was found that the structure with 4 Ag atoms is the most appropriate. The structure consists of slightly meandering chains of Ag atoms and almost straight chains of Si atoms.



The underlying top layer of the Si(100) substrate is dimerized. In the second Si(100) layer, there are also Si dimers (shown by a pair of orange balls in figure). Occurrence of such dimers appears to be very important for stabilization of the Si(100)2×3-Ag reconstruction. It lowers the formation energy by 630 meV, as compared to that of a similar structure having the same atomic arrangement of the top Ag and Si chains but without the inner Si dimers.

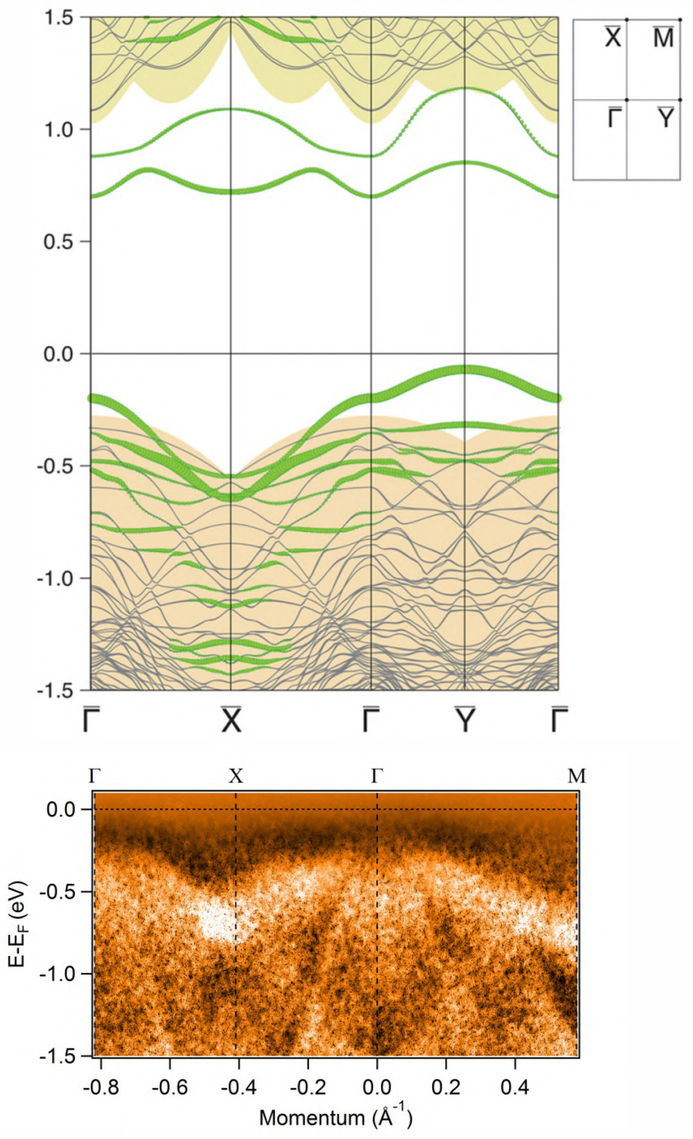


The further support for the model with the inner dimer was gained from the comparison of the experimental high-resolution STM images with the simulated ones.

The simulated filled-state (−2.0 V) images reproduce well the characteristic W-shaped features seen in the experimental STM image.

As for the experimental empty-state (+2.0 V) images, the most principal features there are the pair of almost round protrusions, large bright and small faint, within the 2×3 unit cell. There is also a faint wavy-line feature "underlining" the bright features.

Electronic band structure of the Si(100)2×3-Ag reconstruction



The electronic band structure calculated for the Si(100)2×3-Ag reconstruction model with the inner Si dimer and experimental data obtained by using ARPES technique. One can clearly see that it is semiconducting with an indirect band gap of ~ 0.8 eV. .

Conclusion

A structural model of the reconstruction Si(100)2×3-Ag was proposed. The model incorporates 3 Si atoms and 4 Ag atoms per 2×3 unit cell, forming linear atomic chains running along the $3a_{Si}$-periodic direction of the reconstruction. The essential feature of the Si(100)2×3-Ag structure is the occurrence of the inner Si dimer in the second atomic layer from the top of Si(100) substrate. The model properly fits the principal experimental findings, including our own and those reported before.