Atomic and electronic structure of Co induced identical clusters grown on Si(111)-(7×7) template

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ABSTRACT

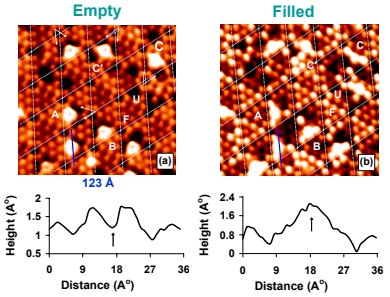
Cobalt-induced identical clusters have been grown on Si(111)-(7×7). *In situ* scanning tunneling microscopy (STM) studies show that the clusters are accompanied by voids created by two missing adatoms. We explain the atomic structure of these clusters by first-principles total energy calculations. The electronic structure of the clusters are investigated by bias dependent STM, scanning tunneling spectroscopy and real-space multiple-scattering calculations. Spectroscopic studies on the clusters indicate a band gap of ~0.8 eV, suggesting localized *nonmetallic* behavior.

INTRODUCTION

The template nature of Si(111)-(7×7) has been frequently used to grow nano-dots of different elements with identical size and shape comprising fixed number of atoms i.e. identical clusters and, attracted much interest in recent days [1-2]. Such low dimensional structures with interesting quantum properties are important not only for fundamental scientific interest but also for wide variety of potential nanotechnology applications. We have studied the early stage interaction of reactive metal Co with Si(111)-(7×7) [3,4]. At lower coverages Co-induced identical clusters are formed on Si(111)-(7×7) at specific adsorption sites in the faulted half of the unit cell [3]. *In situ* STM studies identify the interaction sites of the clusters. Each cluster is closer to one side of the FHUC, breaking the local three-fold symmetry, in stark contrast to all previous group-III cluster systems where the symmetry is preserved on Si(111)-(7×7) [2]. Based on first-principles total energy calculations and experimental observations, we propose a model to explain the atomic structure and formation mechanism of these clusters. The electronic structure of these clusters has been unveiled by a combined study of bias dependent STM, scanning tunneling spectroscopy and real space multiple scattering calculation [5].

RESULTS AND DISCUSSION

A. Co induced identical cluster formation on Si(111)-(7×7)

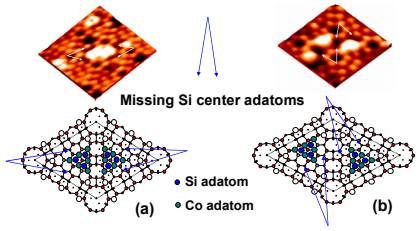


STM images, ~0.06 ML Co at temperature 230±20 °C. F and U for faulted and unfaulted triangular half.

Cluster Features:

- Shifted to one side of the HUC (not at the middle)
- 2 Si center adatom vacancies with every cluster
- 3 equivalent orientation within FHUC: A, B & C
- C' is at mirror position of C and within UFHUC
- Small depression at the middle at empty state

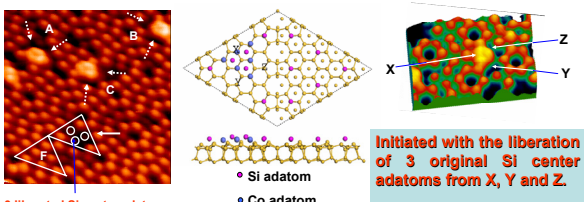
B. Two magic clusters at both halves of a single unit cell



More evidence of cluster interaction site on 7×7 template

(a) Two oppositely-directed clusters are connected back to back
(b) Voids of the two oppositely directed clusters share a common axis

C. Formation mechanism and atomic Structure



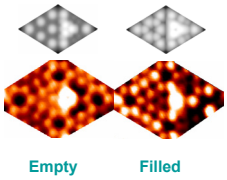
- 3 Si atoms at topmost layer
- 6 Co atoms at next layer

Initiated with the liberation of 3 original Si center adatoms from X, Y and Z.

Site X filled by a Co

Permanent vacancy left at Y and Z

D. Calculation of STM images



Method:

Calculations are based on DFT and ultrasoft pseudopotential plane-wave method.

Vacuum layer ~10 Å, atomic slabs with 8 layers Si.

Total 6 Co, 396 Si and 49 H atoms considered per unit cell.

Cutoff energy of 17.5 Ry

Bias voltages of ± 1.9 V

Comparison of calculated and experimental STM images

References:

[1] M. Y. Lai and Y. L. Wang, *Phys. Rev. Lett.* 81, 164 (1998).
[2] Li *et al.*, *Phys. Rev. Lett.* 88, 066101 (2002).
[3] M. A. K. Zilani, Y. Y. Sun, H. Xu, Lei Liu, Y. P. Feng, X.-S. Wang, and A. T. S. Wee, *Phys. Rev. B* 72, 193402 (2005).
[4] M. A. K. Zilani, Lei Liu, H. Xu, Y. P. Feng, X.-S. Wang and A. T. S. Wee, *J. Phys: Cond. Matt.*, 18, 6987 (2006).
[5] M. A. K. Zilani, H. Xu, T. Liu, Y. Y. Sun, Y. P. Feng, X.-S. Wang, and A. T. S. Wee, *Phys. Rev. B* 73, 195415 (2006).

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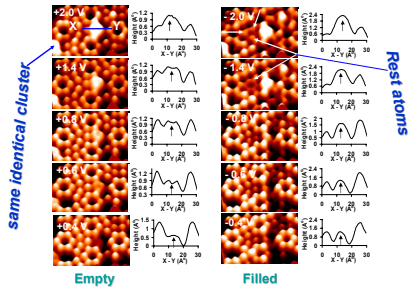
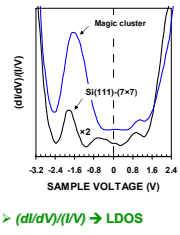
E. Electronic structure

(i) Bias Dependent STM



All images are for same magic cluster and taken with same tip

(ii) STS Measurements on a magic cluster



For clean Si surface area:

-0.35 V: Partially filled adatom bands

-0.7 V: Completely filled rest atoms

-1.8 V: Corner hole and Si-Si backbonds surrounding the adatoms

+0.95 V: Si adatom backbonds in the surface double-layer

On a magic cluster:

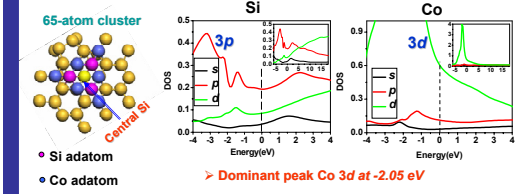
Two surface states at -1.7 V and 1.2 V, and a flat gap region from -0.3 V to +0.5 V

➢ *(dI/dV)/(I/V)* → LDOS

➢ **Si surface:** Considered as metallic due to dangling bond states

➢ **Magic cluster:** Localized nonmetallic with a band gap ~0.8 eV

(iii) RSMS calculations of element and momentum projected DOS



➢ Dominant peak Co 3*d* at -2.05 eV

➢ Flat region around Fermi level for Si 3*p*

➢ **STM:** Localization of charge at magic cluster sites

➢ **STS:** Band gap of 0.8 eV

➢ **STS and RSMS:** STS peak at -1.75 V is due to 3*d* orbital of Cobalt

Conclusion

The atomic and electronic structure study of low-dimensional systems such as 3*d* ferromagnetic metal induced clusters is important for understanding their electrical, optical and magnetic properties. The STS results suggest that the identical clusters are responsible for a local removal of the metallicity of Si(111)-(7×7) and a band gap of 0.8 eV opens near the Fermi energy. This bandgap opening suggests the gain of electronic energy as a driving force for the formation of the clusters.