Electronic Supplementary Material (ESI) for Nanoscale.
This journal is © The Royal Society of Chemistry 2019
Please do not adjust margins

COMMUNICATION

Electronic Supplementary Information

Ultra-thin Ga nanosheets: analogues of high pressure Ga(III)

Yaqi Li,[‡a] Jingwei Zhang,[‡a] Fanxing Yin,[a] Yuqing Wang,[a] Haifeng Feng,[*b] Si Zhou,[c] and Yi Du[*b]

a. School of Physics, Beihang University, Beijing 100191, P. R. China.

b. BUAA-UOW Joint Research Centre, Beihang University, Beijing 100191, P. R. China.

c. Institute for Superconducting and Electronic Materials (ISEM), Australian Institute for Innovative Materials (AIIM), University of Wollongong, Wollongong, NSW 2500, Australia.

Email: ydu@uow.edu.au and haifeng@uow.edu.au

Experimental Section

STM and MBE growth were carried out in a STM/MBE combined system (Unisoku Co. 1400). The Si(111) substrate was cleaned by flashing at 1350 K for several cycles under ultra-high vacuum condition (1×10^{-10} Torr) to obtain the 7 × 7 surface reconstruction. Ga was deposited by evaporating Ga from a Ta crucible containing bulk Ga at the temperature around 450 K. The coverage of Ga was calibrated by depositing Ga on the Si(111) at a temperature of 650 K, which forms an ordered √3Ga-Si(111) surface with 1/3 surface coverage (Figure S5 in Supporting Information). After the growth, the sample was transferred to the STM chamber in UHV for further characterization at low temperature (80 K). STS measurements were performed with the lock-in technique by applying a small modulation of 30 mV to the applied voltage at 973 Hz at 80 K. The STM im-ages were analysed using WSxM software.[1]

DFT calculations were performed by the Vienna ab initio simulation package, using the planewave basis set with an energy cutoff of 500 eV,[2] the projector augmented wave potentials,[3] and the generalized gradient approximation parameterized by Perdew, Burke and Ernzerhof (PBE) for the exchange-correlation functional.4 Grimme's semiempirical DFT-D3 scheme of dispersion correction was adopted to describe the van der Waals (vdW) interactions between Ga layers.[5]To model the experimentally observed Ga supercell, we considered the (001) surface of the Ga(III) phase including five atomic layers in the vertical direction and 7 × 1 unit cells for the lateral dimensions. A vacuum space of 15 Å is added to the vertical direction to minimize the interactions between the supercell and its replica. The lateral cell parameters are fixed at the 19.00 and 2.70 Å, respectively, according to the experimental STM measurement. Note that we also considered supercells including 7 × 2 and 7 × 3 unit cells to alleviate the supercell constrain along the y direction. For each supercell, we generated various initial disordered configurations, and we obtained consistent results of structure features and STM images for the model structures. The Brillouin zone of the supercell is sampled by 2 × 14 × 1 uniform k point meshes. The model structure is fully optimized for the ionic and electronic degrees of freedom using thresh-olds for the total energy of 10^{-7} eV and the forces on each atom of 0.01 eV $Å^{-1}$, respectively. The STM image of the Ga superstructure is

Please do not adjust margins

Please do not adjust margins

simulated by using the Tersoff-Hamann approximation with a constant height of 2.0 Å above the topmost Ga atoms.[6]

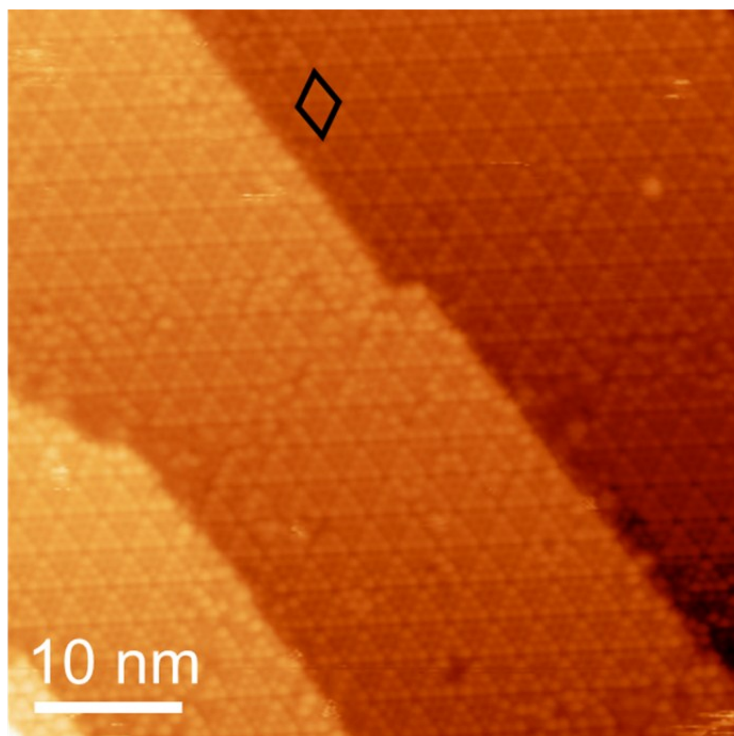

Figure S1. STM image of the Si(111) with 7 × 7 surface reconstruction (-1.4 V, 50 pA). The black rhombus represents the unit cell of 7 × 7 reconstruction.

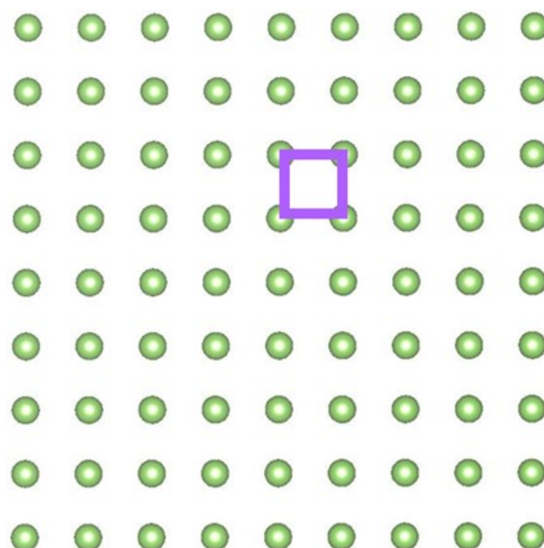

Figure S2. The top view of the monolayer (001) plane of Ga(III).

This journal is © The Royal Society of Chemistry 20xx

Please do not adjust margins

Please do not adjust margins

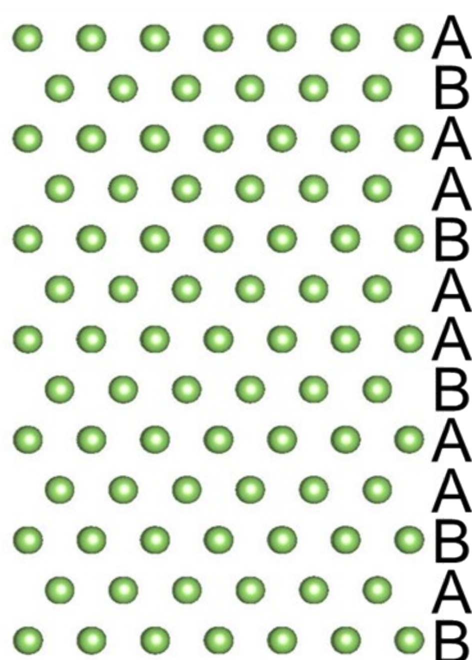

Figure S3. Side view of Ga(III) (001), showing AB stacking with B locating at the centrosymmetric position of plane A.

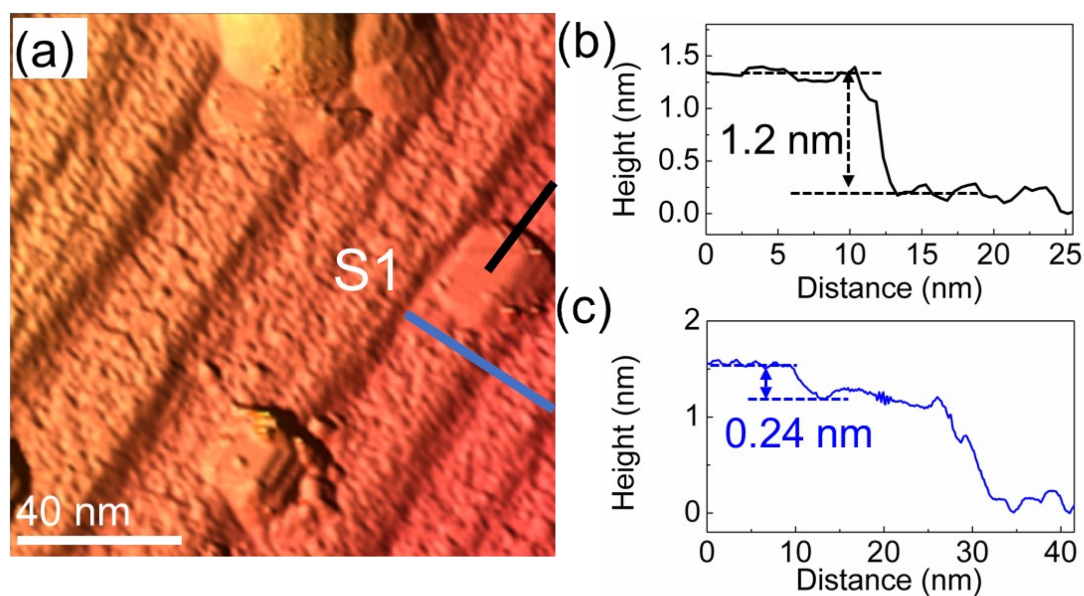

Figure S4. (a) STM image of Ga nanoislands on Ga/Si(111) wetting layer. (b) The height profile of an island S1 of 5 layers. (c) The height profile of an island S1 of 2 layers.

Please do not adjust margins

Please do not adjust margins

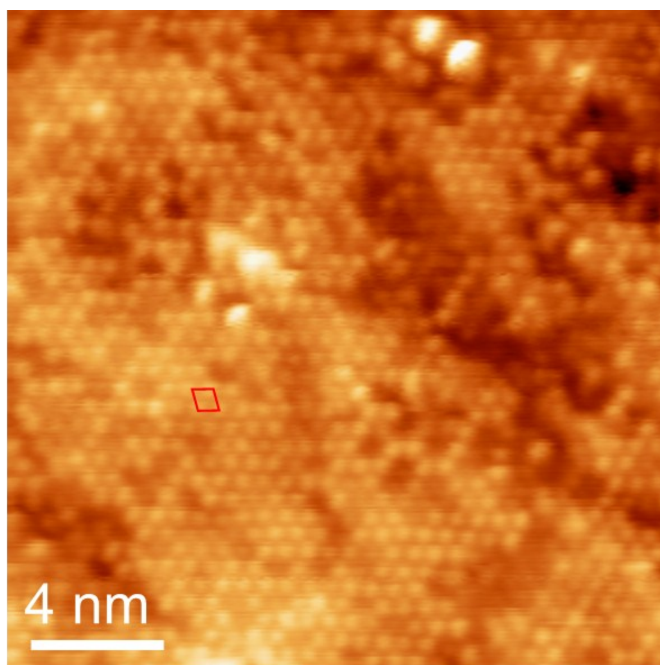

Figure S5. STM image of the √3Ga-Si(111) with 1/3 monolayer Ga on the surface (1.2 V, 50 pA), with the red rhombus representing the √3 × √3 unit cell.

References

1 I. Horcas, R. Fernández, J. M. Gómez-Rodríguez, J. Colchero, J. Gómez-Herrero and A. M. Baro, *Rev. Sci. Instrum.*, 2007, **78**, 013705.

2 G. Kresse and J. Furthmüller, *Phys. Rev. B,* 1996, **54**, 11169.

3 G. Kresse and D. Joubert, *Phys. Rev. B,* 1999, **59**, 1758.

4 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865.

5 S. Grimme, J. Antony, S. Ehrlich and H. A. Krieg, *J. Chem. Phys.,* 2010, **132**, 154104.

6 J. Tersoff and D. Hamann, *Phys. Rev. Lett.,* 1983, **50**, 1998.

This journal is © The Royal Society of Chemistry 20xx

Please do not adjust margins