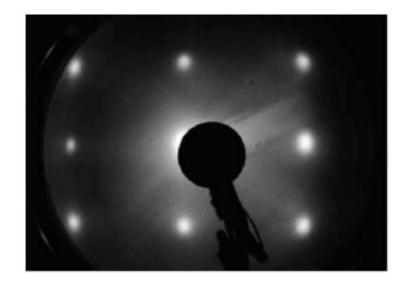
# LEED pattern of Ag single crystal surface

The clean surface of a Ag single crystal was investigated by LEED (see figure). What is the orientation of the investigated surface?

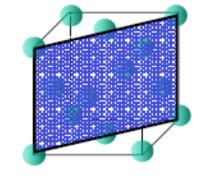
(Ag has an fcc structure.)

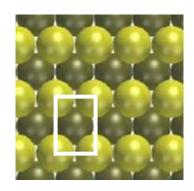


# Solution: LEED pattern of a Ag single crystal surface

The left figure shows the (110) plane in a fcc crystal; the right figure the corresponding top view with the unit cell, which is a rectangle.

The (100) surface has square symmetry. The (111) surface has triangular (hexagonal) symmetry.

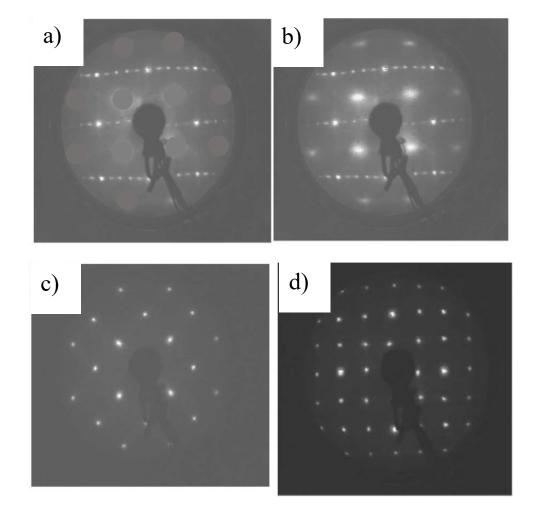




The LEED shows a rectangular pattern; then, the Ag single crystal surface investigated by LEED is the Ag(110).

# H<sub>2</sub>S adsorption on Ir(100)

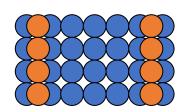
- 1) The Ir(100) surface naturally reconstructs in the Ir(100)-( $a \times b$ )-H, as shown by the LEED pattern in fig.(a). Draw the corresponding structure in the real space and give the values for a and b. (Iridium has an fcc structure.)
- 2) Fig (b) shows the LEED patterns after exposing the Ir surface to 5 Langmuir of H<sub>2</sub>S at 300 K and (c) after flashing the crystal to 700 K. Give an explanation for the evolution of the LEED patterns. Draw the atomic arrangement corresponding to the LEED pattern in fig. (c). Is the answer unique?
- 3) Exposing the Ir surface to 0.5 L of H<sub>2</sub>S at 200 K produces the LEED pattern in fig.(d). Draw the corresponding atomic arrangement.



E = 136 eV

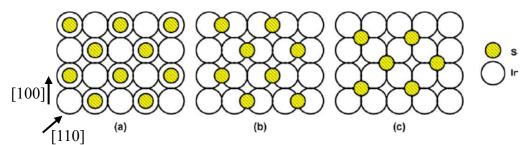
# Solution: H<sub>2</sub>S adsorption on Ir(100).

1) The surface reconstructs in the Ir(100)-(5 x 1) (there are 4 spots between the bright spots of the substrate). In general, domains rotated by 90° could also be present



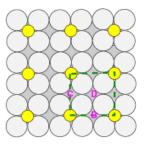
2) The Sulphur partially lifts the (5 x 1) reconstruction at 300 K, while annealing to 700 K results in the complete lifting of the reconstruction.

The LEED pattern in fig. (c) corresponds to a centered (2x2) arrangement (c(2x2)) of the S adsorbed atoms. Three different atomic configurations are possible on the simple basis of the LEED pattern (see figure below)



Top view of  $0.5 \text{ ML c}(2 \times 2)$ -S possible structures: (a) atop, (b) bridge and (c) hollow adsorption sites.

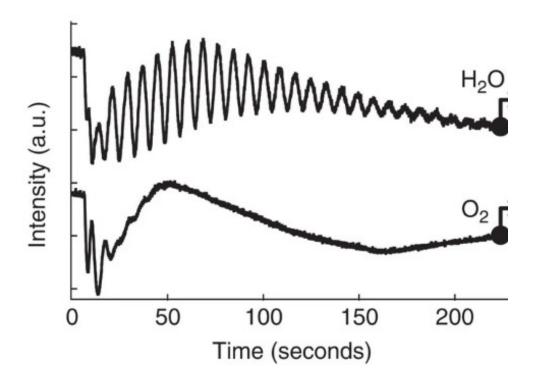
3) The LEED pattern in fig (d) correspond to a (2x2) structure as shown in the figure below. Also in this case we have 3 possible structures as in point 2)



#### Growth of CaO on GaN

Growth of CaO on a given substrate requires MBE deposition of Ca in an O rich atmosphere. The figure on the left compares the growth of CaO film on GaN with the O supplied as an ambient of either molecular oxygen or water vapor. We measure with RHEED the dependence of the specular beam intensity vs deposition time. The result is shown in the figure.

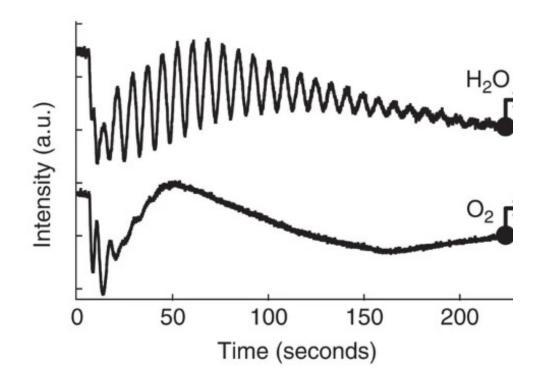
- 1) Describe the growth modes observed in the two cases
- 2) Assuming we want a flat surface, what is the maximum number of layers we can grow before the CaO becomes very rough?



Taken from: doi.org/10.1038/ncomms1470

### Solution: Growth of CaO on GaN

- 1) Depositing Ca in presence of H<sub>2</sub>O results in a FM (layer-by-layer) growth mode. Deposition in O<sub>2</sub> results in a SK growth mode with a layer-by-layer growth for the first 2 layers and then islands formation for larger amounts of CaO
- 2) The FM growth mode obtained in presence of H<sub>2</sub>O allows to grow a flat film of about 15-20 atomic layers. Adding more CaO results in a very rough surface

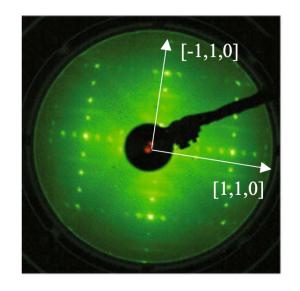


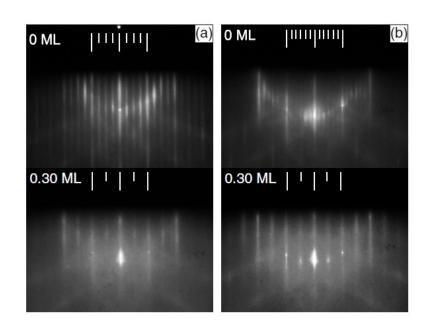
### The GaAs(001) surface

GaAs is a well know semiconductor. Its surface is unstable and shows several reconstructions depending on the surface stoichiometry which, in turn, depends on the preparation method. The Ga rich surface is characterized by the reconstruction shown in the LEED picture.

1) Describe the periodicity of the reconstruction with respect to the bulk structure

- 2) The same surface is imaged with RHEED with the electron beam aligned along two different directions (a and b, top panels). What are these directions?
- 3) After these measurements, 0.3 ML of Mn are deposited on the surface and then the RHEED patterns are measured again (a and b, bottom panels). Does the surface reconstruction remain the same or does it change?



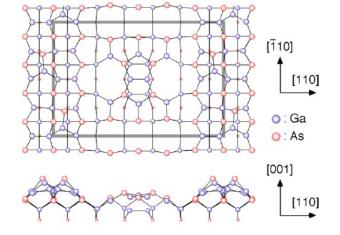


adapted from: doi:10.1088/0953-8984/26/39/395006 and doi:10.1186/1556-276X-8-169

# Solution: the GaAs(001) surface

1) The periodicity of the reconstruction is a 6 x 4 compared to the bulk lattice constants.

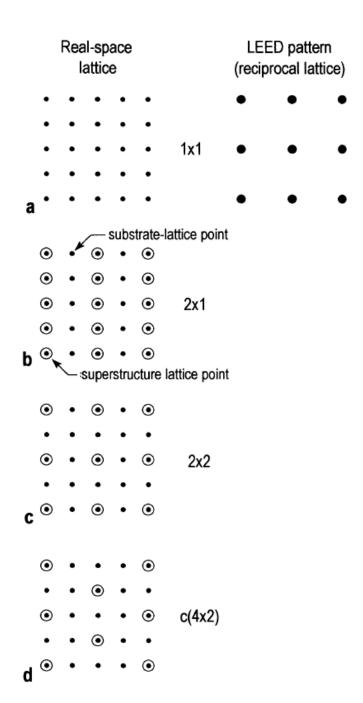
Top and side view are shown on the left



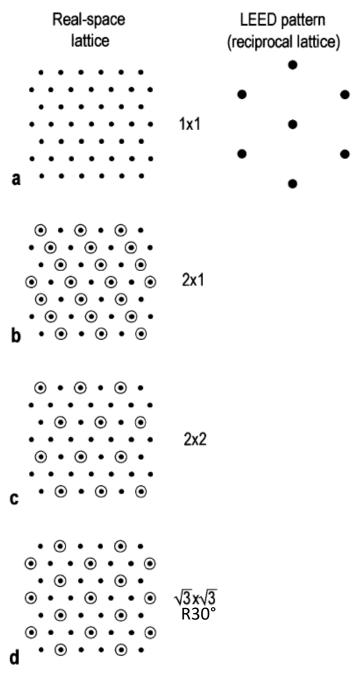
- 2) Image a) is taken with the electron beam along the [1 1 0] while image b) is taken along the [-1 1 0] direction.
- 3) After Mn deposition the surface reconstructs into a (2 x 2) structure

Taken from: doi:10.1088/0953-8984/26/39/395006 and

# **Superstructures and expected LEED patterns**



For each real-space surface lattice, draw the expected LEED pattern, starting from the pattern for 1x1 lattice already shown.



### Solution: Superstructures and expected LEED patterns

