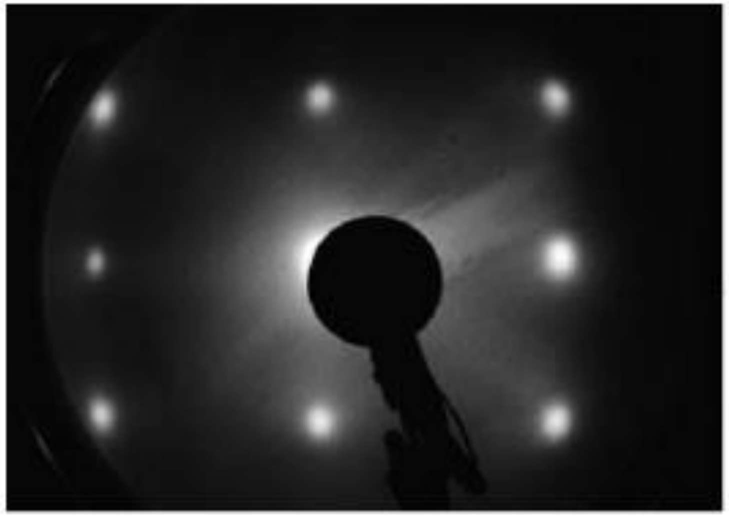
7.1 LEED pattern of a Ag single crystal surface

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

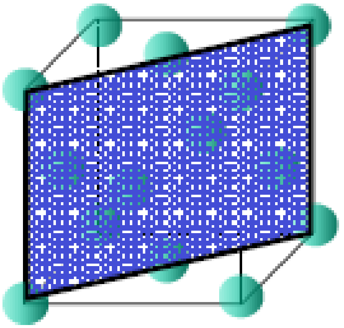
Remember that Ag has an fcc structure.

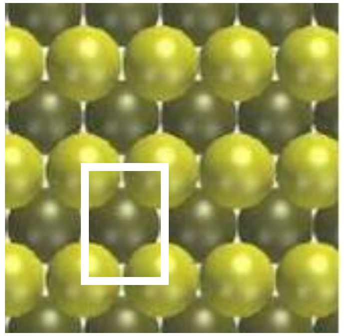


K. Aıt-Mansour *et al.*, Appl. Surf. Sci. **252**, 6368 (2006)

7.1 LEED pattern of a Ag single crystal surface - Solution

The figure on the left shows the (110) plane in a fcc crystal; the figure on the right 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).

7. 2 LEED: graphene on Cu(100)

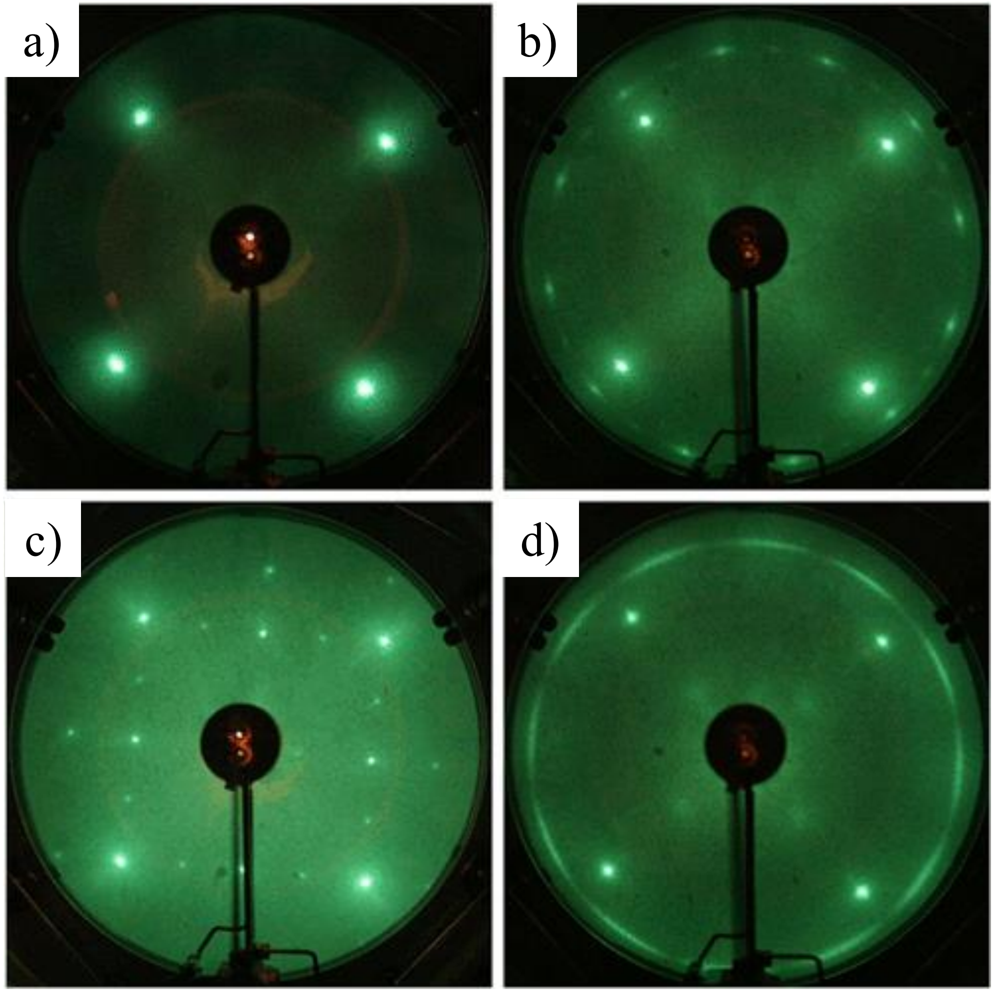
The growth of graphene by catalytic decomposition (CVD) of ethylene on both a clean Cu(100) surface and a Cu(100) surface predosed with a layer of chemisorbed oxygen has been investigated.

Figure a) shows the LEED pattern on the pristine Cu(100).

1) Figure b) after graphene growth on Cu(100) . What can be deduced about the orientation of graphene wrt the copper surface?

2) Figure c) shows the LEED pattern acquired on O-Cu(100). What is the surface structure?

3) Figure d) shows the LEED pattern acquired after graphene growth on O-Cu(100). What can we say about the graphene quality? Is it better or worse than the one of sample b)?



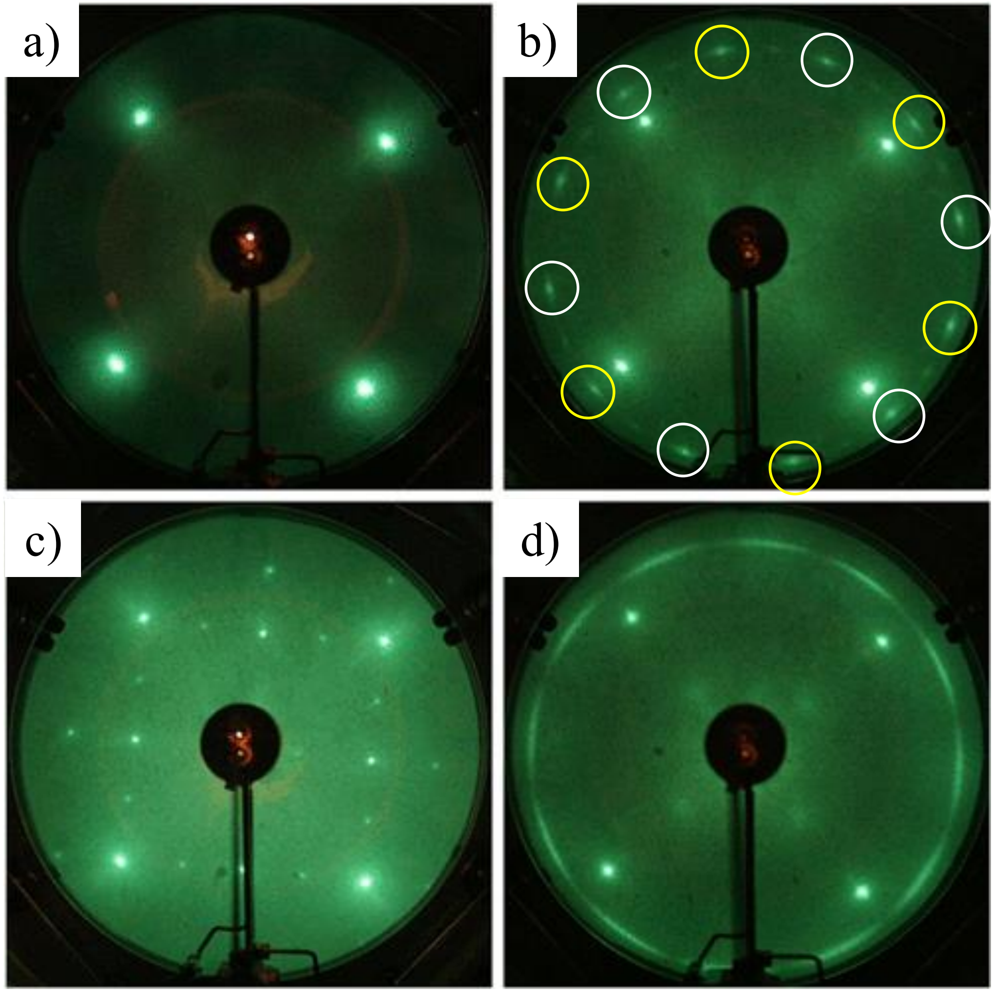
E = 70 eV

https://pubs.acs.org/doi/full/10.1021/jp410142r#

1) Graphene has a honeycomb structure and a triangular Bravais lattice. For a single domain, we expect to see six spots at corners of a hexagon. Here we observe two sets of 6 spots (yellow and white) rotated by 30°, meaning that graphene patches/domains grow with two different orientations wrt the Cu(100) surface. Fainter spots are also visible with other rotational angles.

2) The O-Cu(100) has a 2x1 structure (domains rotated by 90° are present)

3) The diffraction pattern due to graphene is almost a ring, meaning that many different orientations exist. Still, some parts of the ring are brighter, indicating that some orientation are more favorable. Overall, in this case we have graphene overlayers with considerable rotational disorder.



E = 70 eV

https://pubs.acs.org/doi/full/10.1021/jp410142r#

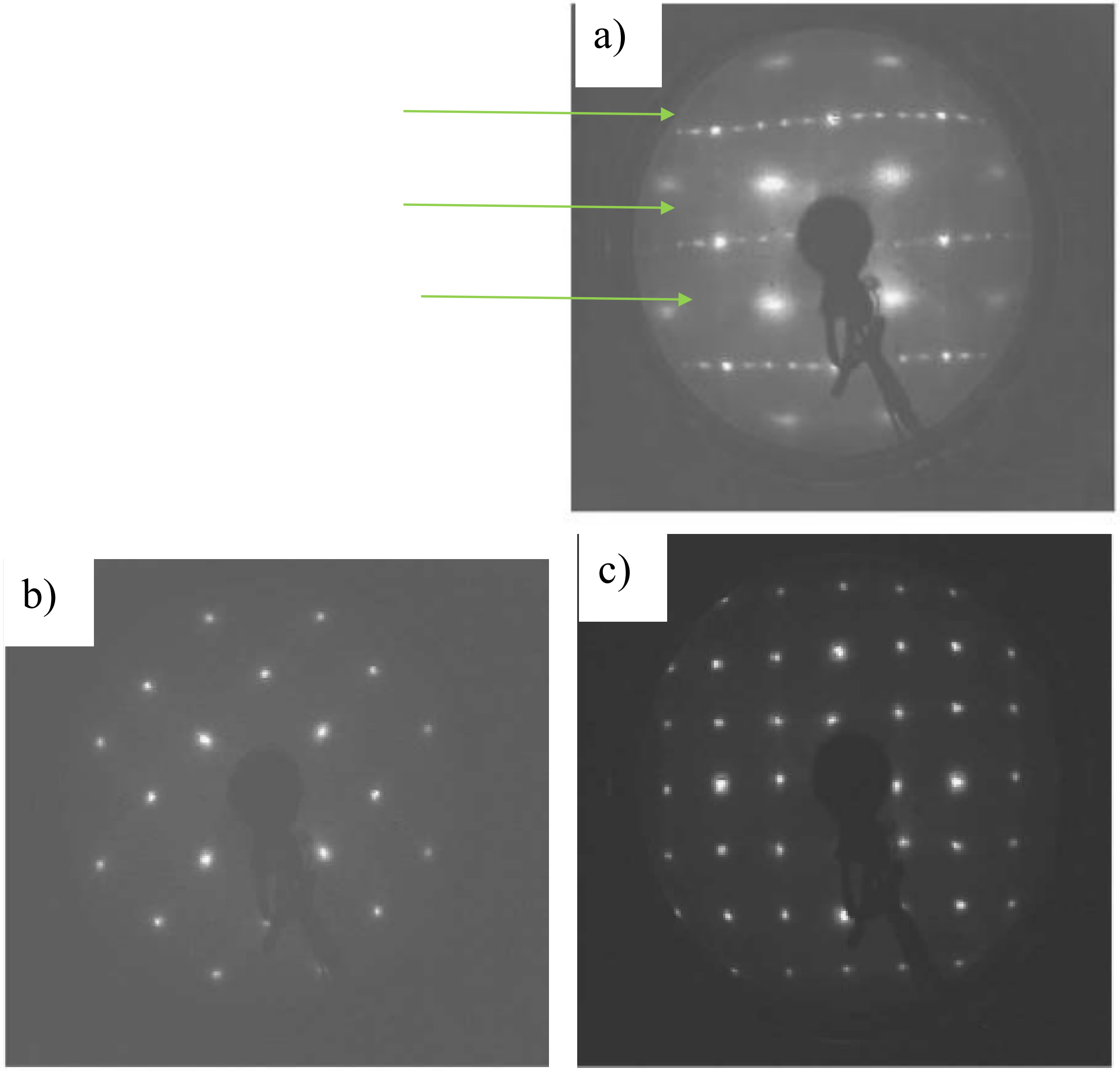
7.3 H_2S adsorption on Ir(100)

The Ir(100) surface naturally reconstructs in a Ir(100)-(*a* x *b*)-H structure. This reconstruction gives rise to the horizontal lines of spots visible in a), indicated by the green arrows.

1) Give the values for *a* and *b*

2) Fig. (a) actually shows the LEED patterns after exposing the Ir surface to 5 Langmuir of H_2S at 300 K and (b) after flashing the crystal to 700 K.
Explain the evolution of the LEED pattern.
Identify the periodicity and draw the atomic arrangement corresponding to the LEED pattern in Fig.(b). Is the answer unique?

3) Further exposing the Ir surface to 0.5 L of H_2S at 200 K produces the LEED pattern in Fig.(c). Draw the corresponding atomic arrangement.

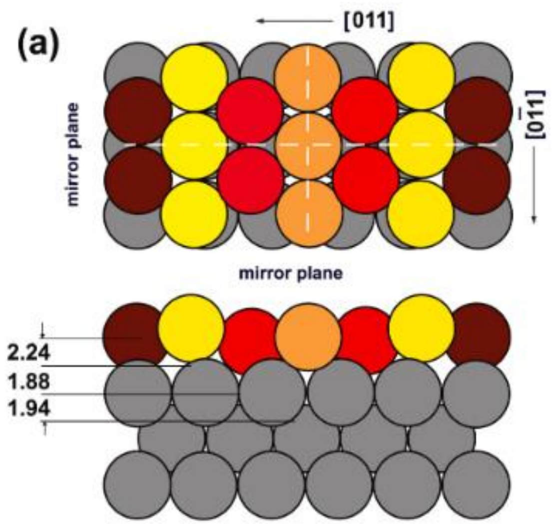


E = 136 eV

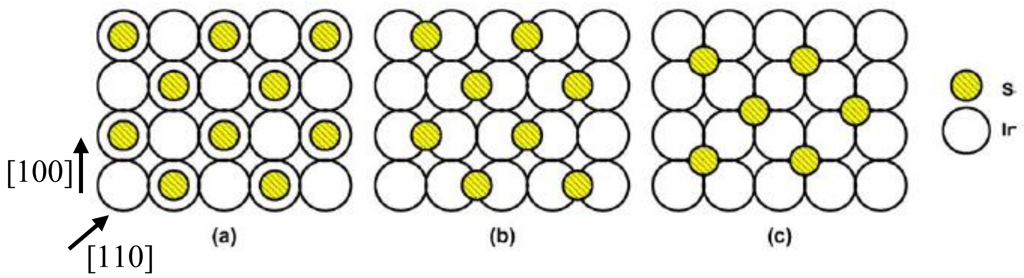
T. J. Lerotholi *et al.*, Surf. Sci. **600**, 880 (2006)

7.3 H_2S adsorption on Ir(100) - Solution

1) The surface reconstructs in the Ir(100)-(5 x 1)-H (there are 4 spots between the bright spots of the substrate). In general, domains rotated by 90° could also be present, but it's not the case here. The "H" means that the topmost layer has a hexagonal structure (see figure on the right).

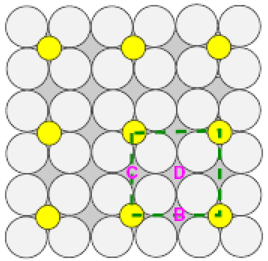


2) Sulphur partially lifts the (5 x 1) reconstruction at 300 K, while annealing to 700 K results in the complete lifting of the reconstruction. The LEED pattern in Fig.(b) corresponds to a centered (2x2) arrangement (c(2x2)) of the S adsorbed atoms. Three different atomic configurations are possible on the simple basis of the LEED pattern (see figure below)

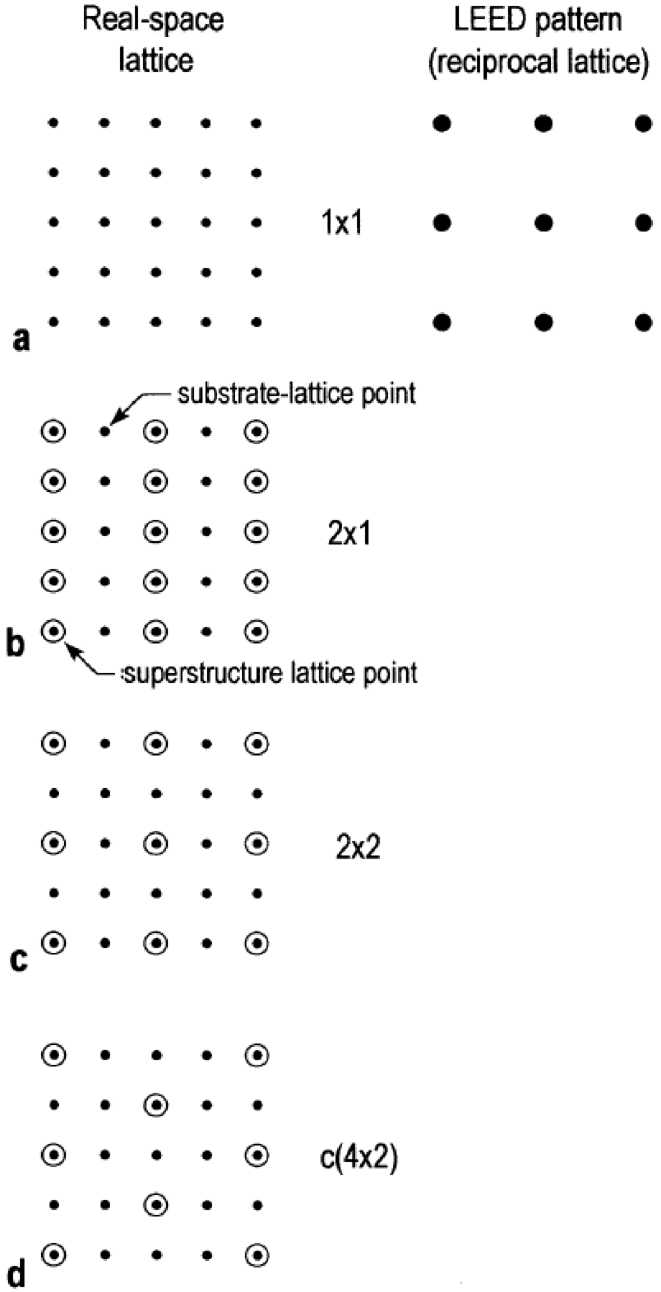


Top view of 0.5 ML c(2 x 2)-S possible structures: (a) atop, (b) bridge and (c) hollow adsorption sites.

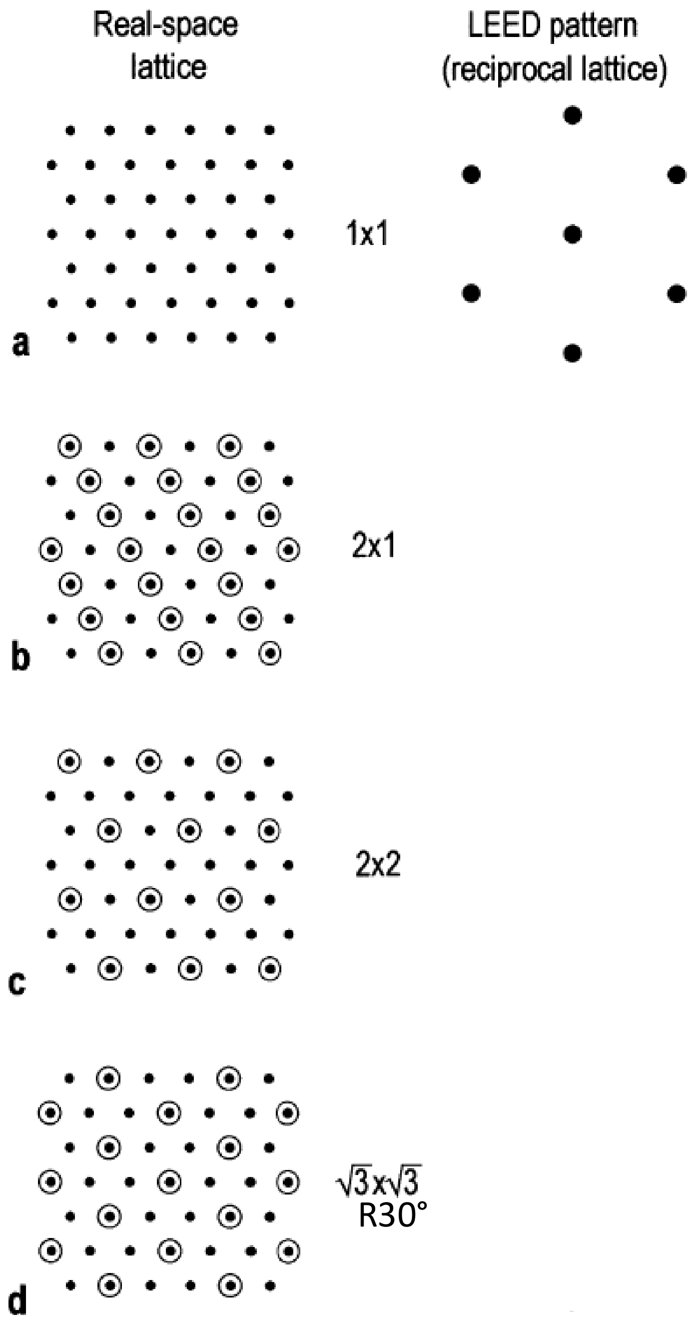
3) The LEED pattern in Fig.(c) correspond to a (2x2) structure as shown in the figure below. In this case we have 3 possible structures as in point 2).



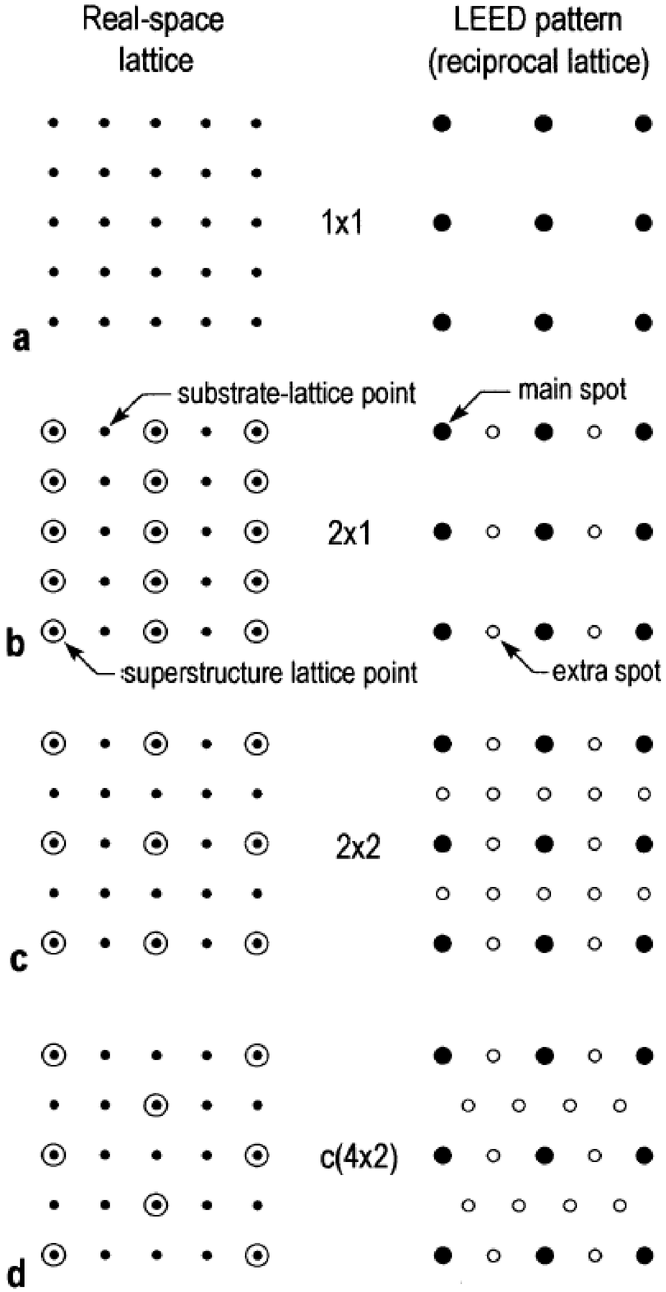
7. 4 Superstructures and expected LEED patterns

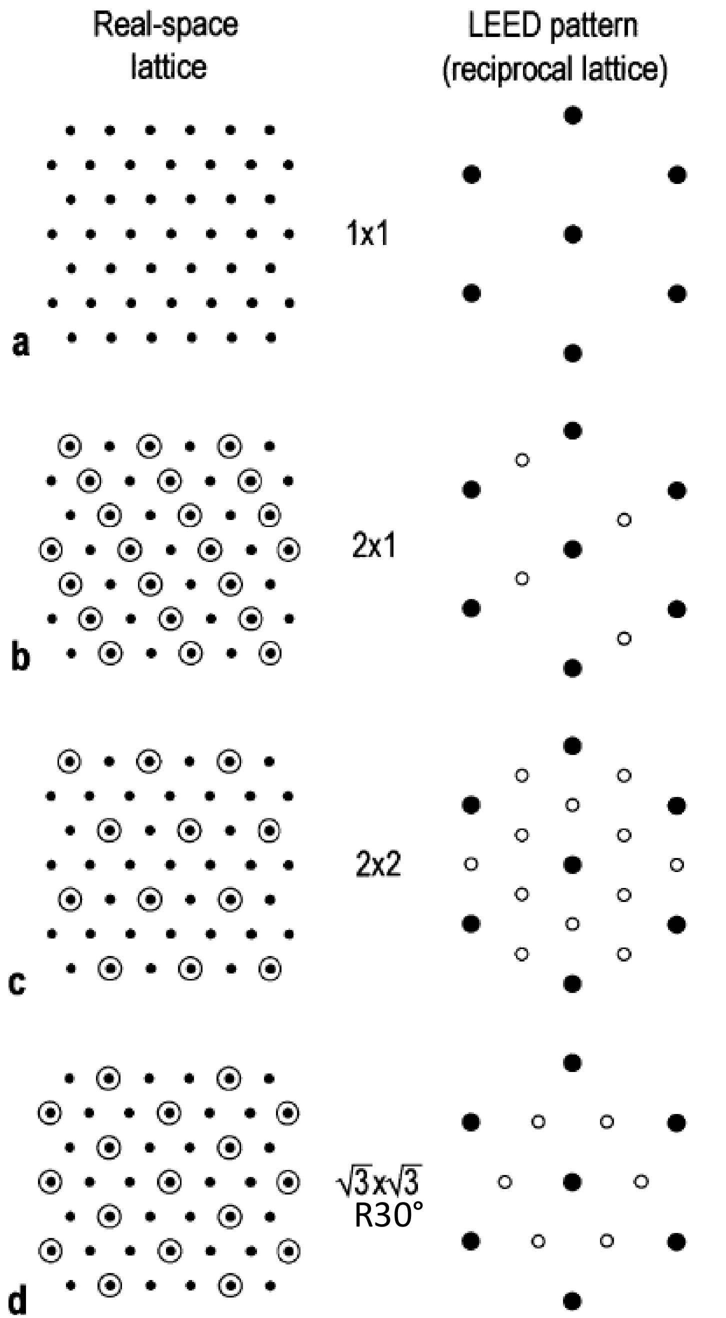


For each real-space surface lattice, draw the expected LEED pattern, starting from the pattern for 1x1 lattice already shown.



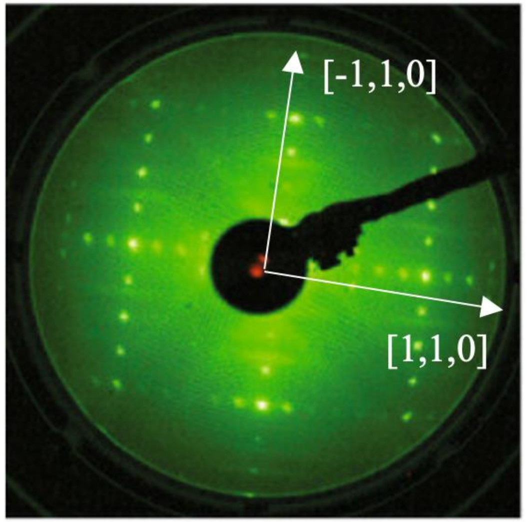
7. 4 Superstructures and expected LEED patterns - Solution





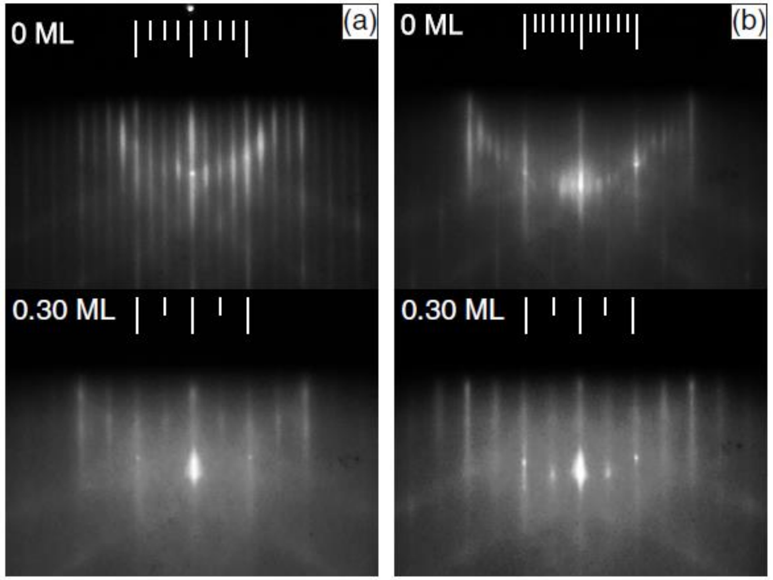
7.5 The GaAs(001) surface

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?



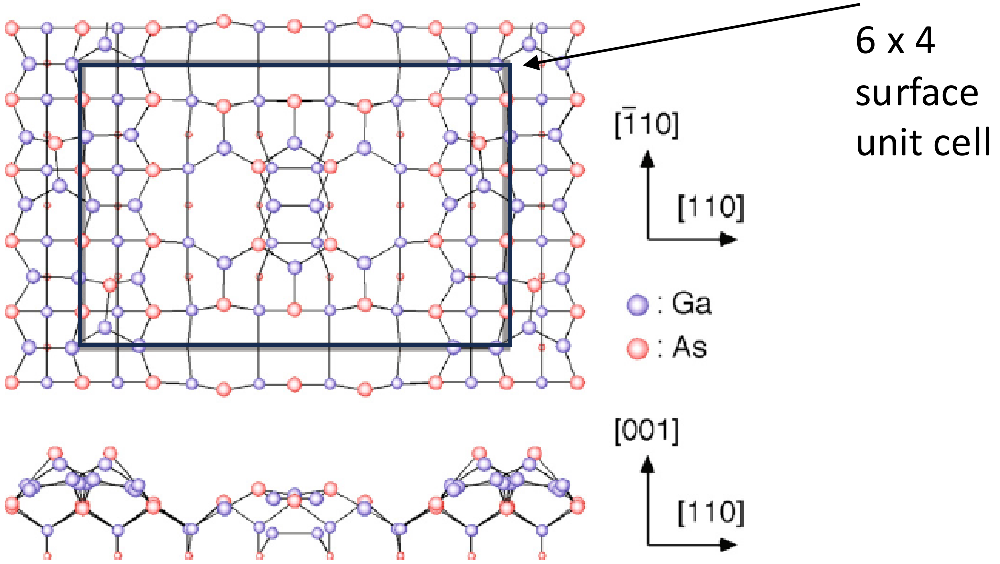
3) After these measurements, 0.3 ML of Mn are deposited on the surface and then the RHEED patterns are measured again (a and b, bottom panels). Does the surface reconstruction remain the same or does it change?

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

7.5 The GaAs(001) surface - Solution

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

Top and side view of the actual surface structure are shown in the figure



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.
In fact, in image a) 3 additional spots are visible, which means that the beam can probe the periodicity along the the [-1 1 0] direction (the [-1 1 0] direction is perpendicular to the beam).
In image b), 5 additional spots are visible, which means that the beam can probe the periodicity along the the [1 1 0] direction (the [1 1 0] direction is perpendicular to the beam).

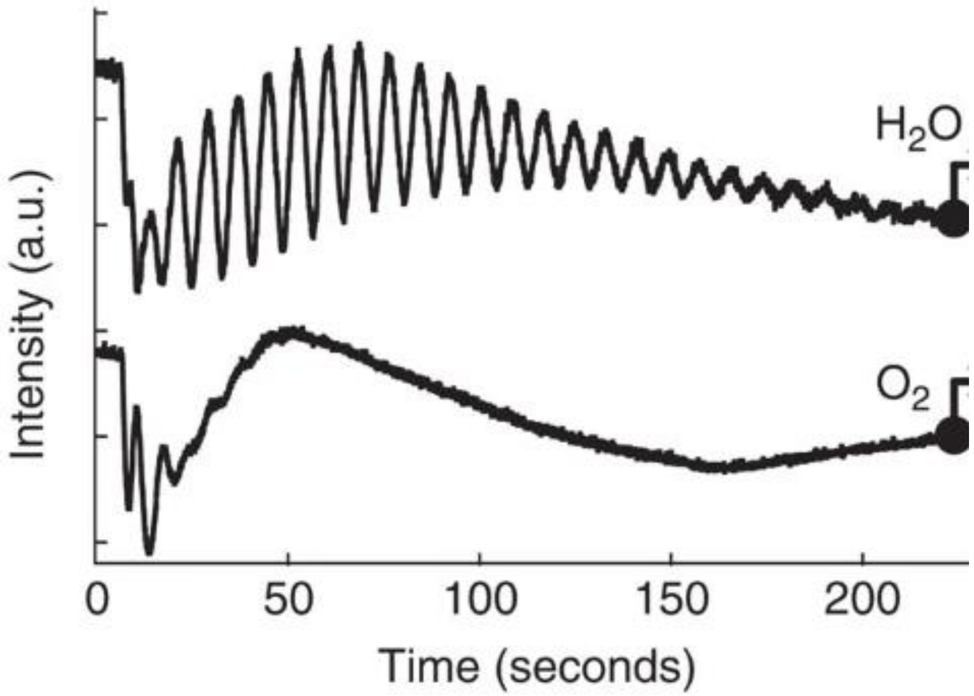
3) After Mn deposition the surface reconstructs into a (2 x 2) structure

Growth of calcium oxide (CaO) on a given substrate requires MBE deposition of Ca in an O rich atmosphere.

The figure 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? (approximatively)



doi.org/10.1038/ncomms1470

7.6 Growth of CaO on GaN - Solution

1) Depositing Ca in presence of H_2O results in a FM (layer-by-layer) growth mode. Deposition in O_2 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_2O allows to grow a flat film of about 15-20 atomic layers. Adding more CaO results in a very rough surface