Structure of Defects at the GaAs(100)-c(8x2) studied by DFT, LEED and STM simulations.

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The structure of the Ga terminated GaAs(100)-c(8x2) surface has been a topic under debate during the last decade. A complex model involving strong reconstructions was recently proposed after extensive Total Energy calculation[1], and was also confirmed by Low Energy Electron Diffraction (LEED) dynamical calculations[1]. Further studies, based on X-ray Diffraction techniques (SXRD), basically corroborate this model[2,3], although it was pointed out the need to introduce partial occupations for certain atoms in the unit cell, stressing the relevance of defects on this surface.

In this contribution we try to clarify the local structure of the defects by combining Total energy calculations, STM simulations and LEED I-V calculations. Based on the XRD results, we have considered 4 types of defected cells (see Figure 1). The structure of each cell is first optimised by DFT calculations. Next, we have performed a LEED I-V analysis considering all possible combinations for these four defected cells, optimising both the atomic coordinates and the relative weights of each cell. The R-factor analysis provides a considerably better fit to the experiment than when only the non-defected case is considered (Figure 2), with values close to the XRD results. However, accurate values for the weights of each cell cannot be obtained due to the large error bars.

Finally, STM simulations for these cells are compared against previously reported experimental images in order to further discriminate the actual type of defects present in this surface.

References

[1] S.H. Lee, W. Moritz and M. Scheffler, Phys. Rev Lett. 85, 3890 (2000)
[2] C.Kumpf,D. Smilgies, E. Landemark, M. Nielsen, and R. Feidenhans, Phys. Rev. B 64 075307 (2000)
[3]D.Paget, Y Garreau, M.Sauvage, P. Chiaradia, R. Pinchaux, and W.G. Schmidt, Phys. Rev. B 64 161305 (2000)

Figures

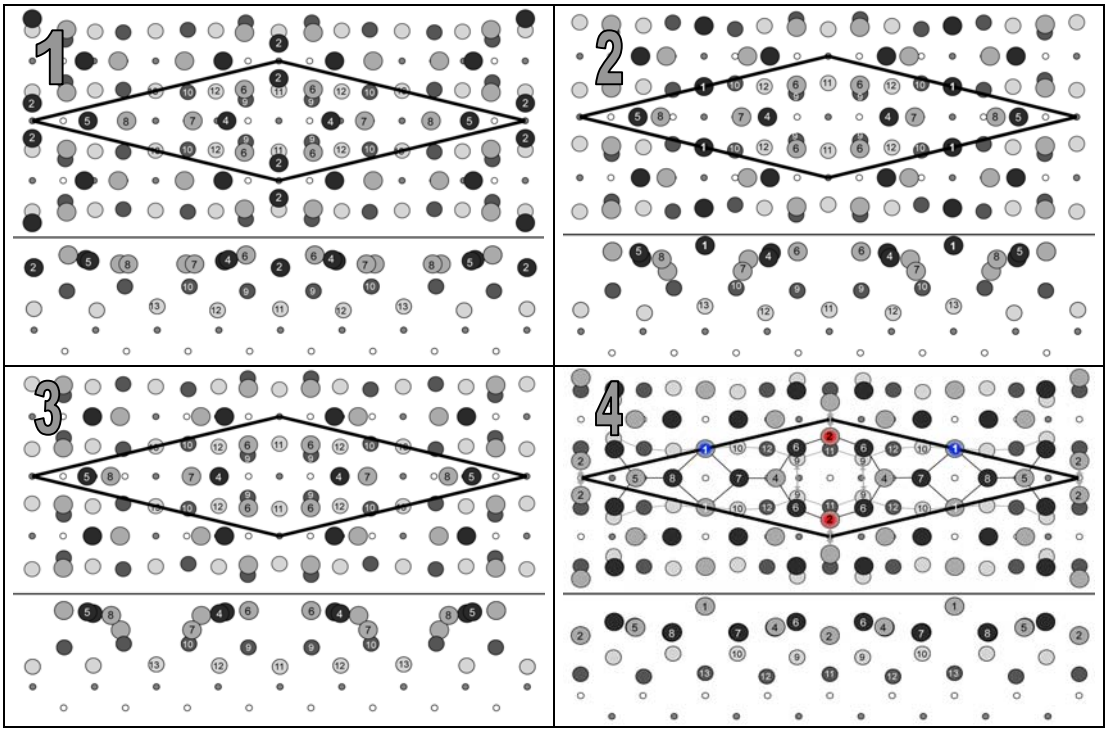

Figure 1. The four c(4x2) unit cells considered in this work.

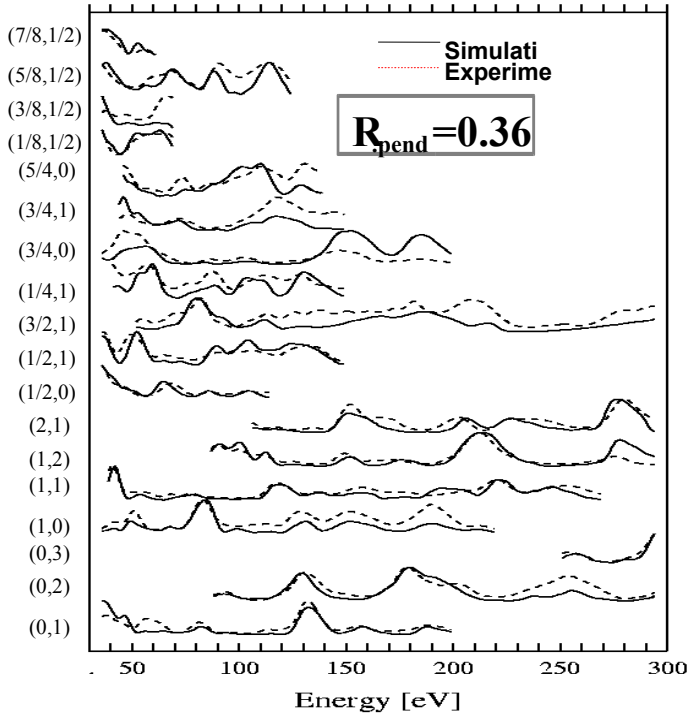

Figure 2. Experiment-theory LEED IV spectra comparison corresponding to an R-factor R=0.36, and consisting of 50% of model 1, 15% of model 2, 20% of model 3 and 20% of model 4.