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ALTERNATIVE METHODS FOR LEED IVSURFACE STRUCTURAL DETERMINATION: DIRECT METHODS AND ANALYSIS OF OFF-NORMAL INCIDENCE CURVES.

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Low-energy electron diffraction takes advantage of strong interactions between electrons and atoms to achieve highly sensitive and accurate surface structural determinations. The prize to pay for that sensitivity is that an appropriated analysis should include costly multiple scattering calculations. Dynamical LEED-IV calculations based on a trial and error procedure, present some limitations for obtaining the atomic structure of the surfaces. For example, when you do not have any hint for the surface geometry, the number and range of the parameters that one has to explore is very high. Moreover, the minimization procedure of the R factor involved in the trial and error method could lead to several occurrences of minima in the R factor. In order to solve the two abovementioned limitations, we introduce two alternative procedures, both based on recording LEED-IV curves at non-normal incident angles.

To improve the search of the correct geometrical arrangement, we propose the use of a direct inversion procedure. We explore the use of the Patterson function formalism to directly invert the experimental IV curves measured at different angles between the surface normal and the incident electron beam. This idea was recently demonstrated in the literature by Wu and Tong using theoretically simulated IV curves [1]. Computationally, this method is simpler and faster than the standard trial and error procedure. The space parameters can be reduced significatively, and subsequent dynamical LEED-IV determination can be performed with great accuracy. We introduce a suitable R factor for the Patterson function to make the structural discrimination as objective as possible [2]. In Fig.1 we show a typical Patterson Function map the two dimensional yttrium silicide, YSi_2 p(1x1) epitaxially grown on Si(111). The black spots correspond to the interatomic distances between two atoms in the structure.

We also demonstrate how the analysis of the LEED-IV curves recorded at different incidence angles can help to discriminate spurious local minima on YSi_2 p(1x1) epitaxially grown on Si(111). A careful consideration of the R-factor behaviour for each set of IV-curves makes possible a clear discrimination because, the R factor value of the spurious minima increase for higher incident angles whereas the real minimum remains unchanged [3]. As a way of example, in Fig.2 we show the variation of the Pendry R factor as a function of two interplanar distances for YSi_2 p(1x1)/Si(111). Two sets of experimental IV curves recorded at normal incidence (left) and 14º out of normal incidence (right) are shown. On the left we clearly observe the multiple occurrence of local minima, whereas on the right only one minimum shows up.

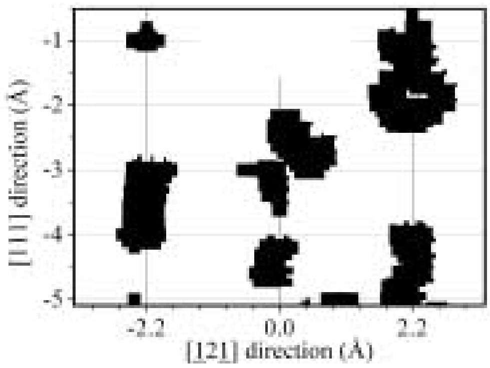

Fig.1 Patterson function map of the YSi_2 p(1x1) epitaxially grown on Si(111). Black spots correspond to the interatomic distance between two atoms in the structure.

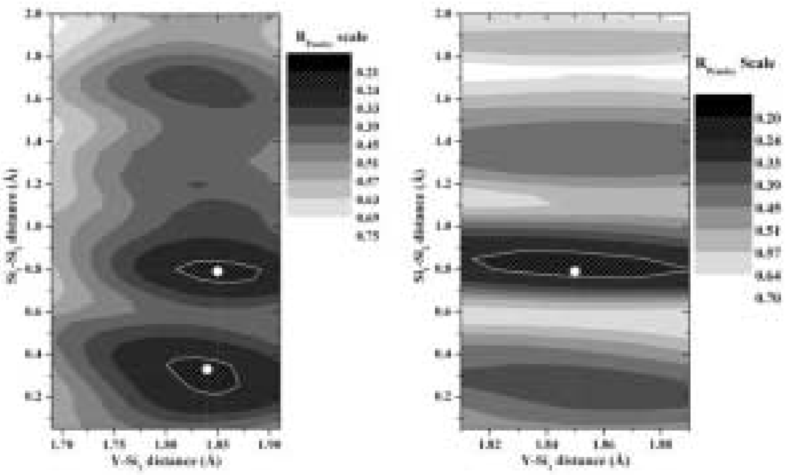

Fig.2 Variation of the Pendry R factor as a function of two interplanar distances in the determination of the atomic position of the YSi_2 p(1x1) epitaxially grown on Si(111) for two set of experimental IV curves recorded at normal incidence (left) and 14º out of normal incidence (right).

References

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[3] C. Rogero, C. Polop , L.. Magaud, J.L. Sacedón, P.L. de Andrés and J.A. Martín-Gago Phys.Rev. B 66, 235421 (2002)