STRUCTURAL DETERMINATION OF YTTRIUM SILICIDE FILMS EPITAXIALLY GROWN ON Si (111) BY LEED I-V ANALYSIS.

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Thin films of heavy rare-earth (RE) silicides epitaxially grown on n-type Si(111) are extremely interesting from a technological point of view as a consequence of unusual Schottky barrier height low values, very small lattice mismatch at the metal-semiconductor interface, and the abruptness of the silicide-vacuum interface. However, in spite of their technological relevance an important issue remains open: which is the atomic structure of the silicide surface?

Thin RE silicides epitaxially grown on Si(111) present several reconstructions as a function of the coverage. For RE coverage of around 1ML, these silicides present a two-dimensional (2D) metallic structure, exhibiting a p(1x1) periodicity [1]. At higher coverage, a $(\sqrt{3}x\sqrt{3})R30°$ LEED pattern is shown and a three-dimensional (3D) metallic silicide is formed. This 3D silicide consists of stacked hexagonal rare-earth planes and graphite-like Si planes with an ordered arrangement of Si vacancies. The ordered net of Si vacancies found in the interior planes is responsible for the lateral relaxations of the surrounding Si and RE atoms. The topmost layer does not present a graphite-like structure and forms a buckled Si layer with no vacancies. Two different structural models have been proposed based on the atomic resolution Scanning Tunneling Microscopy (STM) images of the surface of $ErSi_{1.7}$ epitaxially grown on Si(111). The first geometry was proposed by Roge et al.. The authors observed in their STM images that one of the three topmost Si atoms (Si_{up}) of the buckled layer seems to be lower than the other two. This observation led them to propose a geometry where one Si_{up} atom is sited just on top of the vacancy and, in consequence, it seems to be lower than the other two [2]. The second model, proposed by Martin-Gago et al. [3], is based on the observation of an association of the three Si_{up} atoms forming triangles. These groupings were interpreted as lateral relaxation of the topmost Si atoms. The three atoms move towards the Si_{down} atom situated just on top of the vacancy in the layer below. One open question is, therefore, the determination of the position of the vacancies w. r. t. the Si atoms in the bilayer because previous works could not determine whether the vacancies are below the Si_{up} or below the Si_{down}.

We have explored the atomic configuration of the last silicide layers based on quantitative Low Energy Electron Diffraction (LEED) experiments performed on the surface of the $YSi_{1.7}$ epitaxially grown on Si(111) [4]. To find the surface geometry we search for a global minimum of the Pendry R-factor. This standard procedure allows us to determine the values for structural and non-structural parameters. We find that the topmost plane is a buckled Si overlayer with no vacancies and presenting a slightly vertical relaxation of the Si_{down} atom, which is sited over the vacancy position in the last graphite-like Si plane. The atoms in this bilayer occupy the ideal hexagonal position whereas the Si atoms in the interior planes are laterally relaxed in order to homogenize the Si-Si bonds. As a consequence of this movement the Y atoms are also laterally displaced but in the opposite direction. In Fig.1 an schematic representation of this surface structure is shown.
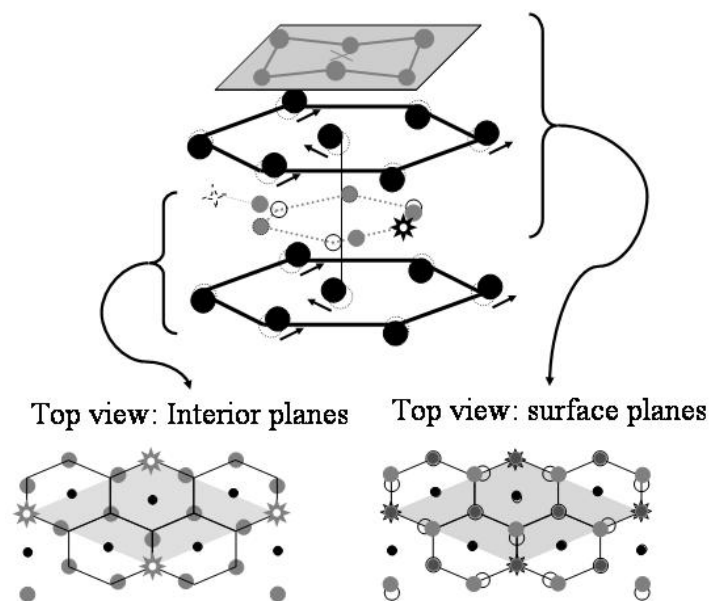
Fg.1 Proposed structure of the YSi$_{1.7}$ indicating the lateral and vertical relaxations.

References
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