Propagation and stability of stacking faults in Ir(111) homoepitaxy

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Homoepitaxial growth is a basic playground for studying the kinetics of stacking faults (SFs) formation, as no SF should form relying on energetics. It is a first step towards understanding the practical issue of thin films microstructuration through SFs. It was recently successfully employed by two of the Authors, who discovered heterogeneous nucleation of SFs on monoatomic rows decorating the boundary between regular and SF areas in Ir(111).

We used X-ray surface diffraction to investigate *in situ* the propagation and stability of SFs during Ir(111) homoepitaxy, in ultra-high vacuum. Figure (a) shows the qualitative evolution of the integrated scattered intensity corresponding to the volume of (1) twinned crystallites, i.e. resulting from SFs along [111], (2) twinned crystallites resulting from SFs along an alternative <111> direction, and (3) crystallites twinned twice, corresponding to a SFs along [111] + another one along another <111> direction. The twinned signals are clearly identified on the crystal truncation rods (CTRs) by the presence of additional Bragg peaks. This is exemplified for the [01L] CTR [fig. (b)] where the regular fcc stacking peaks being only present in the case of the clean Ir(111) single crystal surface, are supplemented by twin peaks after the thin Ir film growth. While the defect type (1) was already observed by scanning tunneling microscopy (STM) by two of the Authors, defect types (2) and (3) were not identified up to now, and are now tentatively searched for in new STM measurements.

The monotonic increase of the various twin volumes directly points out the propagation of the SFs which was proposed following STM observations. The similar trends observed, whatever the type of twin, indicate similar processes are involved. Starting with no SFs, the growth is first layer by layer and then dominated by a roughness increase after a couple of nm, as a result of the proliferation of SFs, consistent with the STM observations. While defect type (1) exhibits high thermal stability (above 1500 K), defects types (2) and (3) are found to disappear at moderate temperatures around 750 K. Preliminary quantitative analysis of the CTRs yield a 50±10 % volumic fraction of twins; thorough analysis will yield the absolute volume fraction of twins during deposit. A comprehensive growth model is currently developed to interpret the presence of the new defect types (2) and (3), the distinctive thermal stability of the different defects, as well as the sharp signals evolving from growth and pointing at well-defined locations in reciprocal space, such as the one highlighted in fig. (b). This should provide a unified picture of Ir(111) homoepitaxy through STM and X-ray surface diffraction.

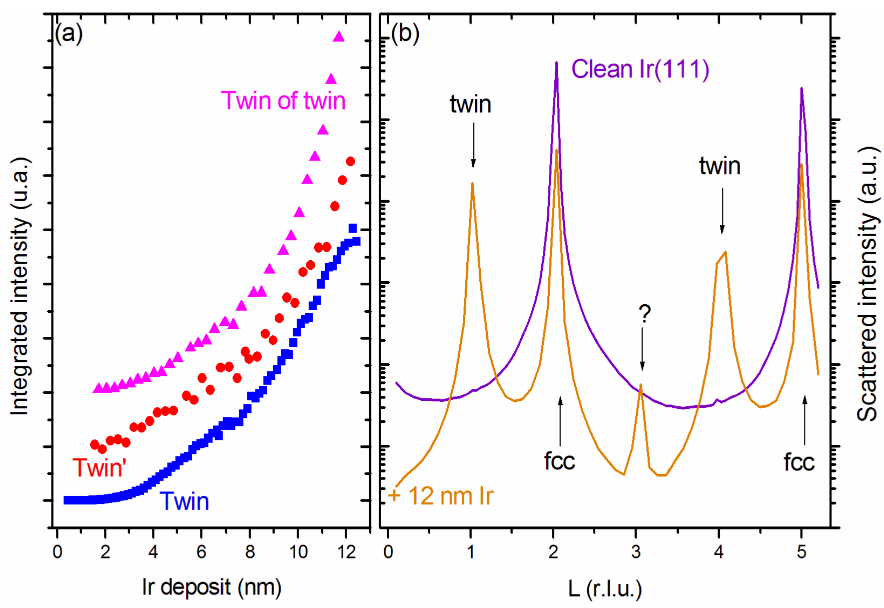

Figure: (a) Integrated intensity associated with the fraction of the crystal that are twinned with respect to (111) (blue), or another <111> plane (red), and twinned with respect to (111) + twinned with respect to another <111> plane (pink). Curves are vertically shifted for clarity and a scale factor of 10^3 has been applied to "Twin'" and "Twin of twin" (b) [01L] CTRs of the bare Ir(111) single crystal (violet) and after 12 nm of Ir have been grown (orange). "fcc" and "twin" denote the regular fcc and the twin stackings Bragg reflections. "?" remains unidentified.

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