Determining the Arrangement of sub-Surface Dopants in a Silicon Quantum Device Platform

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Recently, efforts to realize a silicon-based, CMOS-compatible quantum computer have been intensifying. Central to its development are so-called Si:P δ-layers: i.e., ultra-sharp layers of phosphorus atoms placed beneath the silicon surface [1]. Until recently, one key property has remained elusive: the arrangement of the P dopants within the δ-layer. The answer to this question is of crucial importance, as the dopant arrangement will directly impact the energy separation (i.e., valley-splitting) of the supported quantum well states [2].

In this talk, we will demonstrate how the local neighborhood around encapsulated dopants in a bulk semiconductor can be directly probed using X-ray photoelectron diffraction (XPD). By utilizing subtle core level energy shifts that are concomitant with the coordination of a dopant, chemically specific diffractive images can be formed [3]. Through comparison with XPD simulations that are derived from models of the local atomic environment around the dopants, the true dopant atom placement can be ascertained. Typically, XPD is only used as a probe of surface structure [4]. We demonstrate here that – under the right conditions, it also can be used to determine the local arrangement of sub-surface atoms. Therefore, XPD is well suited for solving the long-standing mystery of the Si:P δ-layer structure.

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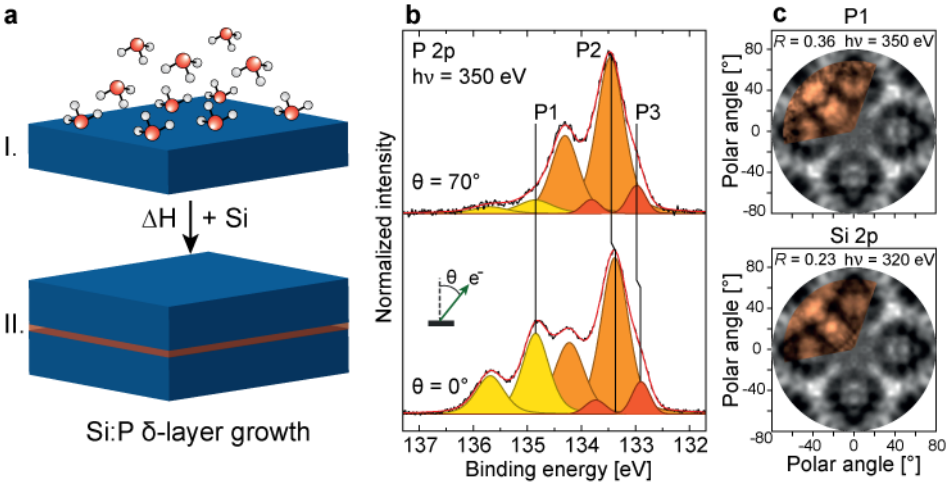

Figure 1 **a**: δ-layer growth. **b**: Angle-dependent XPS of P 2p from the finished structure. **c**: Measured (orange) and simulated (grey) XPD from sub-surface dopants (P1), compared to the measured and simulated XPD from bulk Si 2p.

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