Accessing Atomic-scale Phosphorus Dopant Distribution in Precise Silicon Devices by Advanced STEM Imaging and Spectroscopy

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The structural and chemical characterization at the atomic-scale plays a critical role in understanding the structure-property relationship in precise electrical devices such as those produced by atomic-precision advanced manufacturing (APAM). APAM [1,2], utilizing hydrogen lithography in a scanning tunneling microscope, offers a potential pathway to ultra-efficient transistors, and has been developed to produce phosphorus (P)-based donor devices integrated into bare Si substrates. Structural characterization of the buried, Si with P dopant (Si:P) delta-layer in the devices by scanning transmission electron microscopy (STEM), however, is a challenge due to similar atomic number and low concentration of the P dopants. Here we describe several efforts of utilizing advanced STEM imagining and spectroscopic techniques to quantify the Si:P delta-layers. STEM imaging combining low-angle and high-angle annular dark-field (LAADF, HAADF) detectors [3] as well as atomic-scale elemental mapping using energy-dispersive X-ray spectroscopy (EDS) [4,5] are used to reveal the P and defect distribution across the delta-layer processed under various thermal conditions.

Fig. 1a shows a typical cross-sectional STEM HAADF image of an embedded Si:P delta-layer produced by APAM. The HAADF image contrast for the delta layer is slightly darker than the background despite the higher atomic number of P than that of Si, indicating the contrast is likely due to the presence of strain and/or vacancies. High-resolution STEM HAADF image in Fig.1b shows width of the delta layer is about 10 monolayers of Si or about 2.5 Si unit cells. The EDS mapping (Fig.1c) displays the P K x-ray map, indicating the presence of P at the layer position. By modeling and removing background counts using the counts at an area away from the P delta layer position, the P concentration can be quantified. The result corresponds to about 0.25 monolayer of P atoms across the entire delta layer, and an average atomic concentration of about 2.5 at% for the sample shown in Fig.1. The line-profiles of the HAADF image, Si K, and P K x-ray maps (Fig.1d) at the atomic-scale also show the consistent results. The measurements on several samples processed under different and controlled conditions indicate the P layer concentration and width of the delta layer are strongly impacted by how the P layer is placed, as well as by the subsequent thermal processing condition used for growing the Si capping layer.

The efforts have also been applied to measure vacancy concentration in the delta layer by utilizing a combined LAADF and HAADF imaging technique [3]. The LAADF image taken at the low scattering angle is known to have more contribution due to thermal scattering, which is sensitive to the vacancy/defect concentration. By comparing the HAADF and LAADF images taken from same region, distribution of vacancy/defect in the Si:P delta-layer structure can be illustrated. The results of these studies will be collaborated and presented [6].
Figure 1. (a) STEM HAADF image, (b) high-resolution STEM HAADF image and (c) EDS map of P K x-rays, taken in cross-section of an embedded Si:P delta layer; (d) atomic-scale line-profiles of HAADF, Si K and P K x-rays across the Si:P delta layer.

References
2. D.R. Ward et al., Electronic Device Failure Analysis Mag. 22 4-10 (2020).
6. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. This work was supported by the Laboratory Directed Research and Development Program at Sandia National Laboratories and was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE, Office of Basic Energy Sciences user facility.