Measuring Local Electric Fields and Charge Densities using 4D STEM

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The recent development of ultrafast pixelated detectors has allowed the acquisition of so-called '4-dimensional' scanning transmission electron microscopy (4D STEM) datasets. For such datasets there is an associated convergent beam diffraction (CBED) pattern for each pixel recorded in a STEM image. Recent theoretical calculations have shown that the change in intensity distribution of a CBED during image acquisition can be quantitatively related to local electric fields and charge densities[1]. This has opened-up an exciting opportunity for our research on the integration of III/V-based electronic devices with Si substrates. Such structures would allow the possibility of seamlessly combining highly efficient solar cells and monolithic lasers[2] with current CMOS technology, and the development of high electron mobility transistors[3]. Materials which possess a small lattice mismatch to Si, such as GaP and AlP, can act as a buffer layer between the active III/V materials and the Si substrate. However, the polar nature of these materials can lead to significant charge build-up at the III/V-Si interface and at resulting defects such as anti-phase domains (APDs)[4]. This leads to degraded device performance. The ability to experimentally characterise the distribution of charge in such regions would therefore be highly desirable.

By combining a pixelated detector (PNDetector) with aberration-corrected STEM (JEOL 2200FS), we have been applying the recently established theory[1] for mapping electric fields and the build-up of charge at III/V-Si interfaces and at the local atomic level. Our recent measurements suggest the ability to detect the presence and sign of the charge build-up at the GaP/Si interface and APDs located in GaP. In addition, our results indicate that atomic electric fields and charged densities can be mapped to within sub-Angstrom resolution for the GaP/Si system, with the possibility of visually distinguishing atoms with different atomic charges from charge density maps. This appears to be possible for samples as thick as 25 nm, which exceeds theoretical expectations[1].

Future work will firstly aim to analyse the nature of charge build-up at the GaP interface and APDs in detail. Additional systems such as AlP/Si and III/V-based p-n junctions will also be characterized. Furthermore, atomic level measurements will be quantitatively analysed using density functional theory (DFT) calculations and multislice simulations using our in-house developed code[5]. The ability to measure local electric fields and charge densities at interfaces will allow us to explore the derivation of atomic scalar potentials and the measurement of band alignments using STEM.

[1]Müller, Knut, et al. *Ultramicroscopy* 178 (2017): 62-80.

[2]Kunert, B., et al. *physica status solidi (b)* 244.8 (2007): 2730-2739.

[3]Mukherjee, N., et al. *Electron Devices Meeting (IEDM), 2011 IEEE International*. IEEE, 2011.

[4]Beyer, A., et al. *Applied Physics Letters* 103.3 (2013): 032107.

[5]Oelerich, Jan Oliver, et al. *Ultramicroscopy* 177 (2017): 91-96.