

"Ultra-Atomic Resolution Electron Microscopy Project" Seminar Series

"Revealing the role of individual molecules and strain in nanostructured materials using advanced and *in situ* electron microscopy"

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The understanding of the structure-property relation of individual nanostructures is of critical importance for the advancement of materials. The methods of advanced and in situ electron microscopy are well suited for characterizing these relationships since the enable site-specific and direct correlation between atomic structure, electronic structure, mechanical behaviour, electrical transport and photoresponse. The results provide information for a basic understanding of the properties of these nanostructures and for tailoring device performances.

By in situ transmission electron microscopy (TEM), a direct correlation between mechanical and charge transport properties was determined for InAs nanowires [1]. A uniaxial tensile stress was applied to individual nanowires and strain mapping was performed by using 4D scanning TEM (4D STEM), while electrical measurements were carried out simultaneously. A significant reduction of resistivity and enhanced piezoresistive response of the nanowires, compared to bulk InAs, were observed with increasing strain. Individual GaAs nanowires were also studied using the same in situ TEM approach [2]. Evidence for hole mobility modification by uniaxial strain was found. For bending deformation, the current-voltage (I-V) characteristics of the nanowires change from linear to nonlinear [3].

For individual GaAs nanowires with build-in radial p-i-n junctions, being equivalent to individual nanoscale solar cells, the photovoltaic properties, i.e., photocurrent and I-V characteristics, were investigated using an in situ scanning tunnelling microscope – scanning electron microscope (STM-SEM) setup [4,5]. A uniaxial tensile strain of 3% resulted in an increase of photocurrent by more than a factor of 4 during near-infrared (NIR) illumination. This increase is attributed to a decrease of 0.2 eV in nanowire bandgap energy, thus reflecting the effect of tensile strain on light absorption. The quality of the electrical contacts is crucial when performing in situ biasing studies [5]. The contacts are also of utmost importance in electronic devices and therefore currently attracts significant attention in the development in devices based on two dimensional materials [6].

Molecular dopant species are used to improve and optimize the properties of organic semiconductors. A higher dopant concentration may result in a higher electrical conductivity but the details of the spatial distribution of the dopant molecules, clustering and cluster morphology are equally important [7]. The charge transfer between the dopants and the surrounding polymer is promoted by a short distance between the dopant and the polymer. The dopant cluster morphology determines if each dopant molecule is in direct contact with the polymer or if a portion of the dopants are instead imbedded and parted from the polymer. Here, electron tomography was used to reveal the three dimensional (3D) distribution of individual dopants and dopant clusters.

This talk will show how advanced and in situ electron microscopy studies enable a quantitative understanding of the intriguing interplay between atomic structure, electronic structure, charge transport and photocurrent. It will also discuss crucial aspects of the studies and illustrate the importance of control experiments to ensure that the in situ experiments provide representative information of the correlation between atomic structure and properties.

References: [1] L. Zeng et al, Nano Lett. **18**, 4949 (2018), [2] L. Zeng et al., Nano Lett. **21** 3894 (2021), [3] L. Zeng et al., Phys Status Solidi., **13**, 1900134 (2019). [4] J. Holmér et al., Nano Energy **53**, 175 (2018). [5] J. Holmér et al., Nano Lett. **21**, 9038 (2021). [6] N. Shetty et al., ACS Appl. Nano Mat. **6**, 6292 (2023). [7] G. Persson et al., Nanoscale **14**, 15404-15413 (2022).

Main meeting room at Institute of Engineering Innovation, Faculty of Engineering, Bldg. 9, 1F, 22 March 2024 (Fri.) 16:40~18:10