Electron microscopy provides atom-by-atom knowledge of doped graphene and carbon nanotubes

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A thread of research pursued in a pan-European collaboration lead by Aalto University Department of Applied Physics scientists has yielded prominent results for the electron microscopy of nitrogen-doped graphene and carbon nanotubes.

A paper published in September in the journal *ACS Nano* provides a detailed atomistic description of the electron-beam-induced damage in these important structures by combining advanced computational methods with state-of-the-art electron microscopy.

Toma Susi, postdoctoral researcher in Aalto University Department of Applied Physics, began studying the system in 2010 together with current University of Vienna researcher Jani Kotakoski.

"Our work began as a chance meeting during a workshop poster session. I had questions that Jani could answer by computational modelling. The collaboration eventually grew to include 11 authors from five European countries," recounts Toma Susi.

Susi and his colleagues investigated how the energetic electron beams used in transmission electron microscopes affect carbon-based nanomaterials doped with nitrogen atoms.

"The microscopes basically operate by the same principle as optical

microscopes, but they use electron waves instead of light for the imaging. The materials are interesting because they have exciting prospects for nanoelectronics, metal-free electrocatalysis and gas sensing."

The exact atomic bonding of the dopants greatly affects the resulting modification of host properties. Recent cutting-edge developments in instrumentation have enabled atom-by-atom analysis and even direct imaging of nitrogen sites in graphene. However, since electrons carry momentum, inelastic collisions can lead to the ejection of atoms from the target material, potentially leading to misidentification of the unmodified dopant structures.

"Most excitingly, we could directly image the ejection of carbon atoms next to the dopants and never the dopants themselves – exactly as the simulations predicted, explains Susi."

Besides providing an improved understanding of the irradiation stability of these structures, the results show that structural changes cannot be neglected in characterisation using high-energy electrons. This notion will increase in importance as the devices become more powerful.

"The significant scientific results notwithstanding, the story of our article illustrates well how scientific collaboration works. I gave a talk at the fifth ScienceSLAM Helsinki event about the story of the article and followed up with a blog post including an analysis of the 720 emails exchanged amongst the co-authors. Since the research was not directly related to any particular project work, it also goes to show to what a bit of academic freedom and quite modest resources can at best lead. I am grateful to our group leader Professor Esko Kauppinen for supporting our line of work."

More information: Susi, T. et al. Atomistic Description of Electron Beam Damage in Nitrogen-Doped Graphene and Single-Walled Carbon Nanotubes, *ACS Nano* online. dx.doi.org/10.1021/nn303944f

Toma Susi's blog post describing the process

Provided by Aalto University