Observation and stability of one-dimensional ionic BN and CsI chains in electron microscope

H. Komsa[1] A. V. Krasheninnikov[2]

[1]COMP, Department of Applied Physics, Aalto University, Finland
[2]Department of Applied Physics, Aalto University, Finland

Single atom thick one-dimensional chains have been previously observed when consisting of a single element such as carbon or gold. Chains consisting of two or more different atoms, and in particular chains of ionic character, have not been previously reported. The first scanning tunneling electron microscope observation of two such chains, consisting of BN and CsI ions, were recently reported [1,2].

Boron nitride chains were constructed via electron beam etching from two-dimensional (few layer) h-BN sheets. The chains were found to behave rather similarly to the carbon chains created from graphene, and thus completes the analogy between various boron nitride and carbon polymorphs. In the case of CsI chains, the chains were stabilized through encapsulation inside carbon nanotubes. In order to find out if such sensitive structures can remain stable in the conditions prevailing inside the electron microscope, we performed density functional theory (DFT) calculations to study the equilibrium energetics of the chains and DFT molecular dynamics calculations to study their thermal stability and ability to withstand knock-on events.

In both cases, dynamical effects were found to complicate characterization and identification of the observed features. Suspended BN chains were found to break easily, while BN chains supported on a BN sheet were rather stable, but were also found to vibrate strongly. In the case of CsI, I ions are located at the center of the tube, whereas Cs atoms are attracted to nanotube wall and undergo rapid circular motion along the wall. Finally, the electronic properties of the chains were found to retain the insulating properties of their bulk counterparts.

[1] R. Senga, H.-P. Komsa, Z. Liu, K. Hirose-Takai, A. V. Krasheninnikov, and K. Suenaga, *Nature Materials* **13**, 1050 (2014).
[2] O. Cretu, H.-P. Komsa, O. Lehtinen, G. Algara-Siller, U. Kaiser, K. Suenaga, and A. V. Krasheninnikov, *ACS Nano* **8**, 11950 (2014).