Computational Transmission Electron Microscopy

Elena Bichoutskaia[1]

1. School of Chemistry, University of Nottingham, University Park, Nottingham NG7 2RD, UK

E-mail: Elena.Bichoutskaia@nottingham.ac.uk

Computer image simulations provide a crucial aid to high-resolution transmission electron microscopy (HRTEM) in gaining fundamental understanding of the structure of materials. Interpretation of HRTEM images is, however, complicated due to continuous structure deformation caused by the imaging electron beam. A computational methodology, *CompuTEM* [1,2], has been implemented that takes into account the effects of the electron beam on deformation of sample structure during observation and imaging in HRTEM. The evolution of the sample structure is described as a sequence of externally initiated discrete damage events with a frequency determined by the cross section, which depends on the energy of the electron beam. A series of images showing structure evolution with time is obtained by coupling molecular dynamics simulations with the image simulation. These simulation parts are linked by two experimental parameters: the energy of the electron beam and the electron dose rate. As the energy of the electron beam also determines resolution and contrast of the obtained HRTEM image, a careful selection of its value is required to achieve a fine balance between reduction of the sample damage caused by the electron beam and the quality of the acquired image.

CompuTEM has been used to simulate the observed process [3] of structural transformation of a small graphene flake into a fullerene cage. The simulated series of images showing the evolution of a graphene flake under the 80 keV electron beam closely reproduces experimental HRTEM images with regard to the structure evolution route, evolution rate, and signal-to-noise ratio. We show that under the increased electron beam energy of 200 keV a similar observation will be obscured by high damage rate or low signal-to-noise ratio.

Structural HRTEM characterisation of individual molecules is fundamentally limited by the element specific interactions of a sample with the e-beam. The principal cause of instability of organic molecules in TEM is the low atomic weight of hydrogen and its facile atomic displacement by the e-beam. We demonstrate [4] that the exchange of hydrogen for the heavier isotope, deuterium (doubling the atomic weight) can lead to a more than two-fold increase in stability of organic molecules in the e-beam. To demonstrate this, single-walled carbon nanotubes were filled with stacks of coronene and deuterated coronene, and the stability of the encapsulated molecules was compared under the 80 keV e-beam. The observed enhanced stability of deuterated molecules matches well our theoretical predictions and confirms the general principle that isotopic substitution of hydrogen for deuterium can significantly extend the lifetime of organic molecules in the e-beam. This makes a significant step towards ultimate structural analysis by AC-TEM at a single-molecule level.

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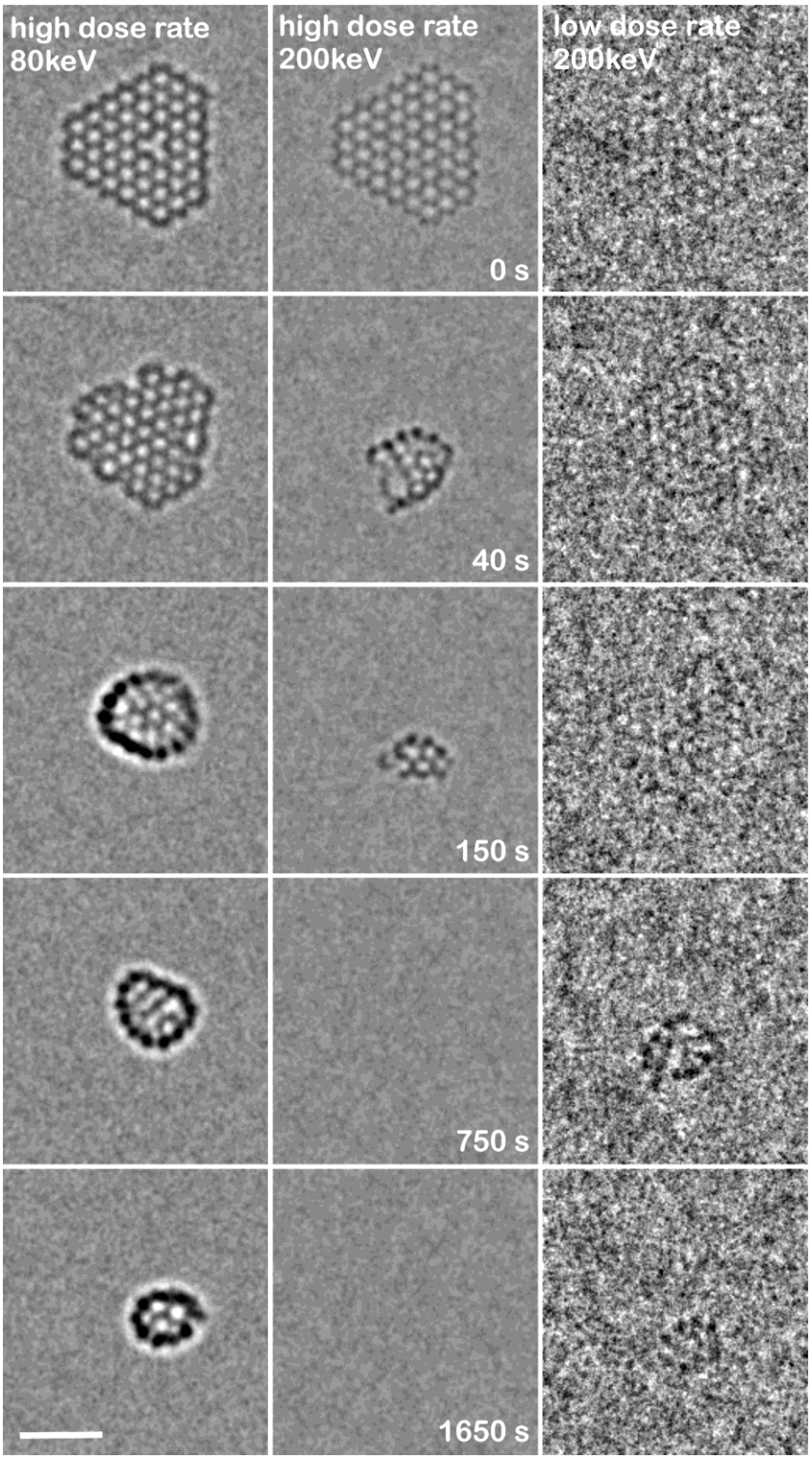

Fig. 1. *CompuTEM* simulations of the flake-to-fullerene transformation for three sets of experimental conditions in HRTEM. Left panel: accelerating voltage 80 keV and electron flux 4.1×10^6 electrons s^{-1} nm^{-2}; middle panel: accelerating voltage 200 keV and electron flux 4.1×10^6 electrons s^{-1} nm^{-2}; right panel: accelerating voltage 200 keV and electron flux 0.25×10^6 electrons s^{-1} nm^{-2}. The quality of the imaging system was considered to be the same. Scale bar = 1nm.