

## Atomic Structure of Single Walled Carbon Nanohornes

Gerd Duscher<sup>\*,\*\*</sup>, M.F. Chisholm<sup>\*\*</sup>, A. A. Puretzy<sup>\*\*,\*\*\*</sup>, C. M. Rouleau<sup>\*\*,\*\*\*</sup>, and D. B. Geohegan<sup>\*\*,\*\*\*</sup>

\* Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996-2200

\*\* Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

\*\* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Single walled carbon nanohorns (SWNH), are a novel form of nanostructured carbon with tunable pore sizes to optimize the storage of hydrogen and can serve as metal catalyst support in various applications. The shape and size of the individual nanohorns as well as their interstitial pore sizes in their aggregates can be changed by varying their synthesis conditions and by post-processing chemical treatments. Synthesis methods range from high temperature laser ablation to chemical vapor deposition processes with different catalytic nanoparticles [1].

The shape variations can easily be determined electron microscopy, but one needs atomic resolution at acceleration voltages below the kick-out threshold to observe the Moiré patterns locally at the SWNHs. With the NION dedicated scanning transmission electron microscope (STEM) UltraSTEM with 5<sup>th</sup> order corrector the atomic distances of carbon in graphitic materials can be resolved even at low voltages with Z-contrast imaging [2]. Therefore, changes of the Moiré pattern indicate grain boundaries and other defects. The Moiré pattern of a near defect free SWNH are shown in figure 1. The chirality of the SWNHs can be obtained through a simple Fourier transformation as shown in the inset of figure.

There are point defects and impurity atoms present in the process. Figure 1 shows such an impurity atom with a brighter than the carbon contrast. The approximate area of 4 by 4 nm where the beam was scanned while an EELS spectrum was taken is also indicated in the image. The volume of the single walled nanotube of this area contains 144 atoms, and the analysis of the EELS spectrum with a fitting method [3] shows that the Si/C ration is 0.7 atom %, which is about 1 atom in 144. Therefore, single atom sensitivity and resolution was obtained in this experiment.

Not only different shapes of the carbon nanohorns, but also carbon nanohorns and graphene sheets are found in the samples. The interfaces of the graphitic nanostructures with metallic nanoparticles will be shown, as well. With the new tools at hand the graphitic nanostructures are becoming a model system for materials science of point defects.

### References

1. A.A. Puretzy *et al. Appl. Phys. A* **93** (2008) 849.
2. O.L. Krivanek, *et al., Nature* **464** (2010) 571.
3. Gerd, D. *Quantifit. 2010*; Available from: <http://web.utk.edu/~gduscher/Quantifit/>.

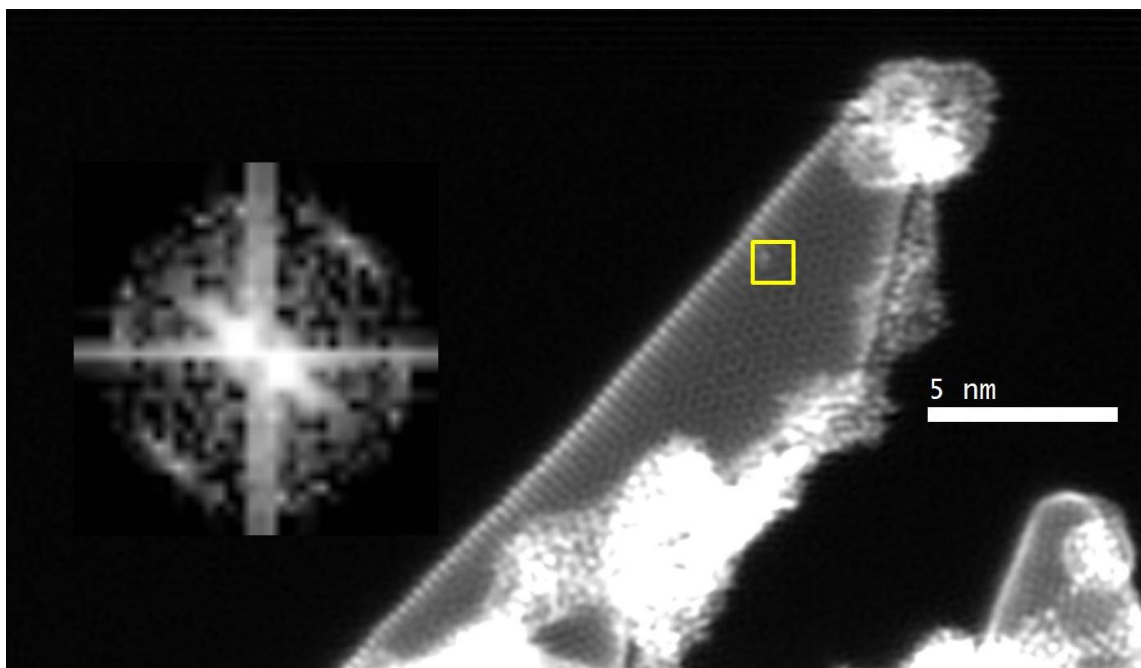


Figure 1: Z-contrast image of a carbon nanohorn with an impurity atom in the indicated box. The Fourier transformation in the inset is used to determine chirality.

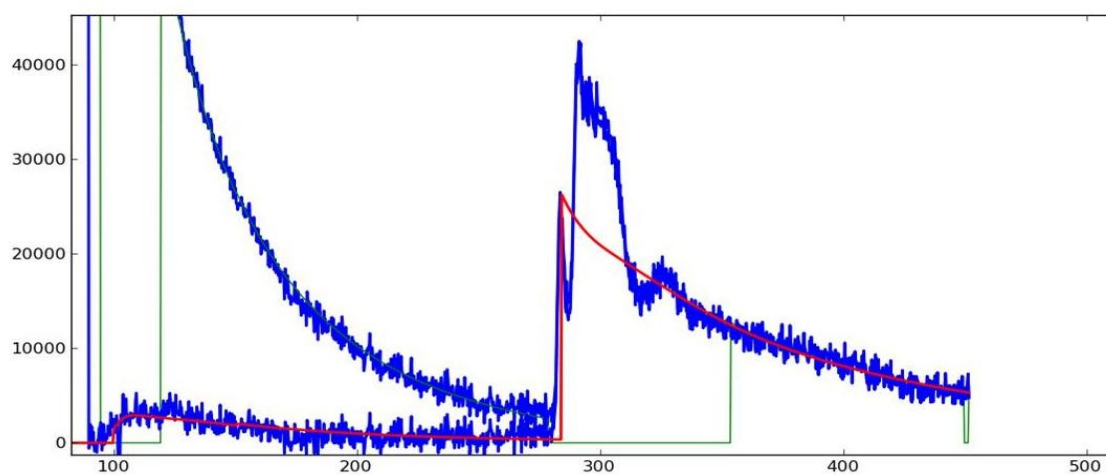


Figure 2: Electron energy-loss spectrum of the indicated area on the carbon nanohorn reveals a Si/C ratio of 0.7 atom%.