Synergies among Electron, X-ray and Neutron Scattering for New Science at the Nanoscale

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ORNL will soon have a unique combination of facilities to address key issues in nanoscale science

- Center for Nanophase Materials Sciences (CNMS)
  - World-class facilities and staff for nanoscale synthesis and characterization in targeted areas of science
- Spallation Neutron Source (SNS)
- High Flux Isotope Reaction (HFIR)
  - World-leading neutron scattering facilities – both pulsed and steady-state
- National Leadership Computing
  - World-leading computing facility for scientific inquiry
- Shared Research Equipment (SHaRE) User Program
- High Temperature Materials Laboratory (HTML)
- Condensed Material Sciences (CMS) dedicated STEM R&D program
  - World-leading electron scattering and atom probe microcharacterization facilities and expertise

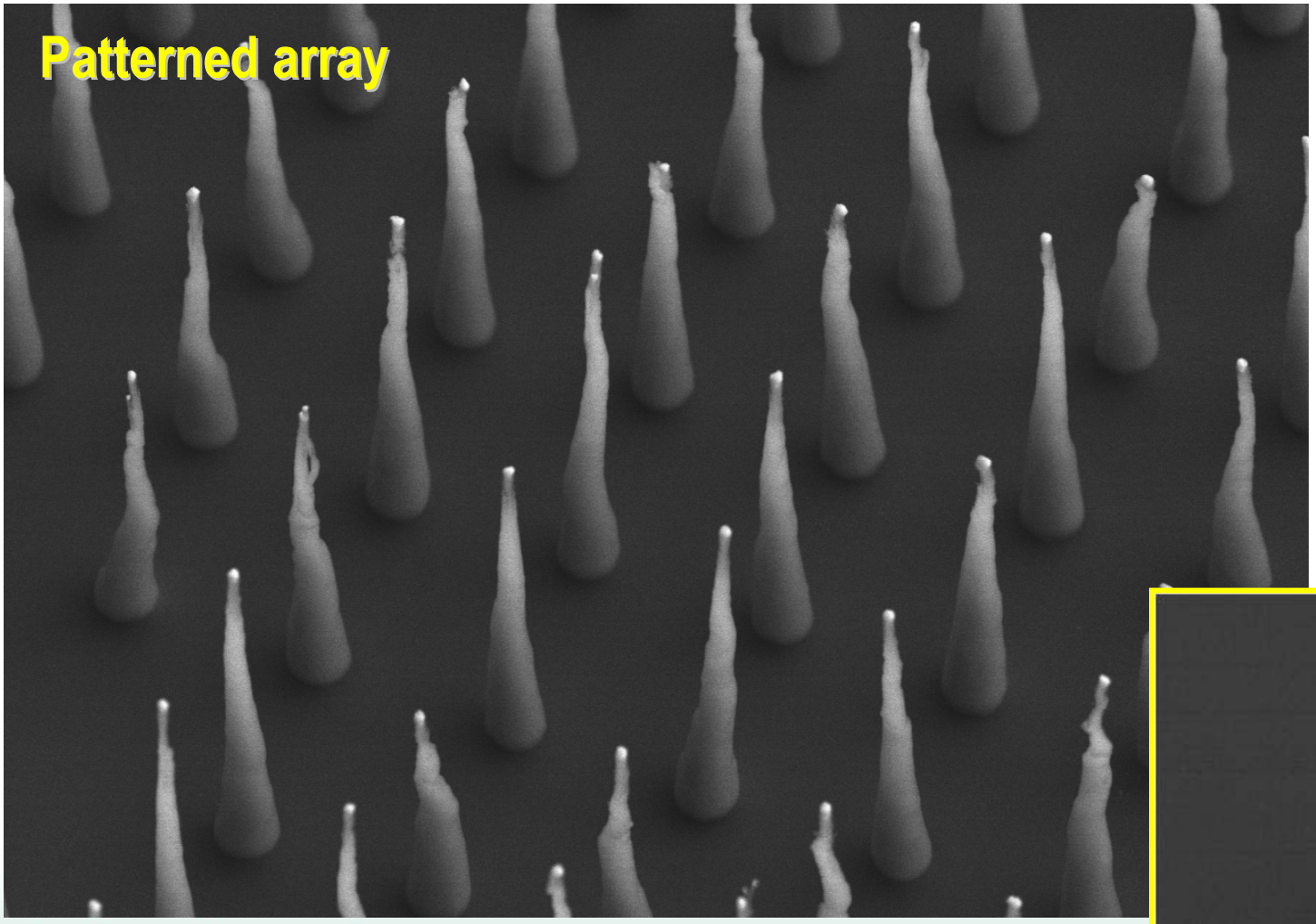
Electron and neutron scattering provide complementary capabilities for probing matter

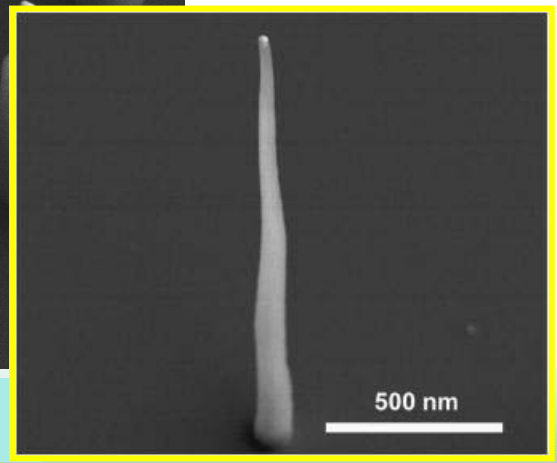
- **Electrons are well suited for the atomic-scale characterization of individual nanometer-scale structures**
  - **Coulomb potential provides strong electrostatic interaction with matter**
  - **Characteristic mean free paths of ~10 – 100 nm for elastic, phonon, and plasmon scattering**
  - **Probes variability of nanoscale structures within sample**

- **Neutrons are well suited for the atomic-scale characterization of ensembles of nanometer-scale structures**
  - **Characteristic mean free paths of ~1 mm**
  - **Measurement of average properties (structure, dynamics, etc.) with high precision**
  - **Explore synthesis during growth!**

We wish to correlate the individual and ensemble behaviors, and correlate with nanostructure synthesis!

Example application: plasma-enhanced CVD catalytic grown of carbon nanofibers

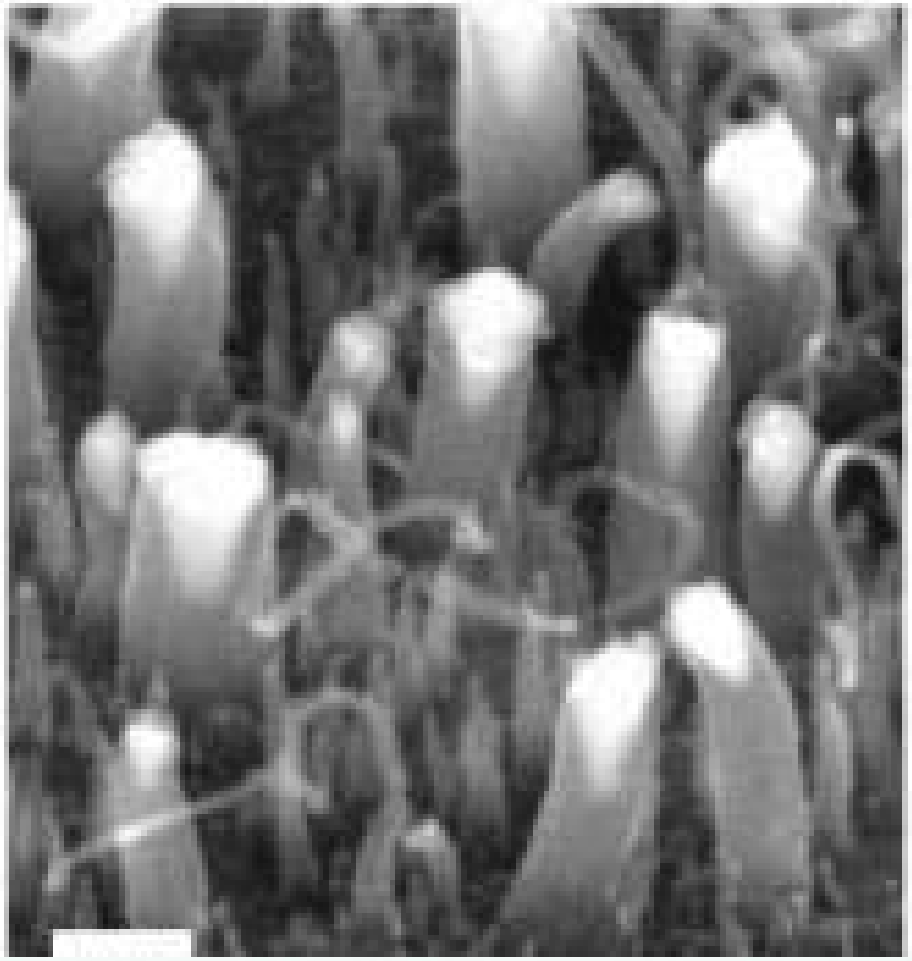




CNMS project:
T. Leventouri;
A.V. Melechko,
K.L. Klein,
I.M.Anderson

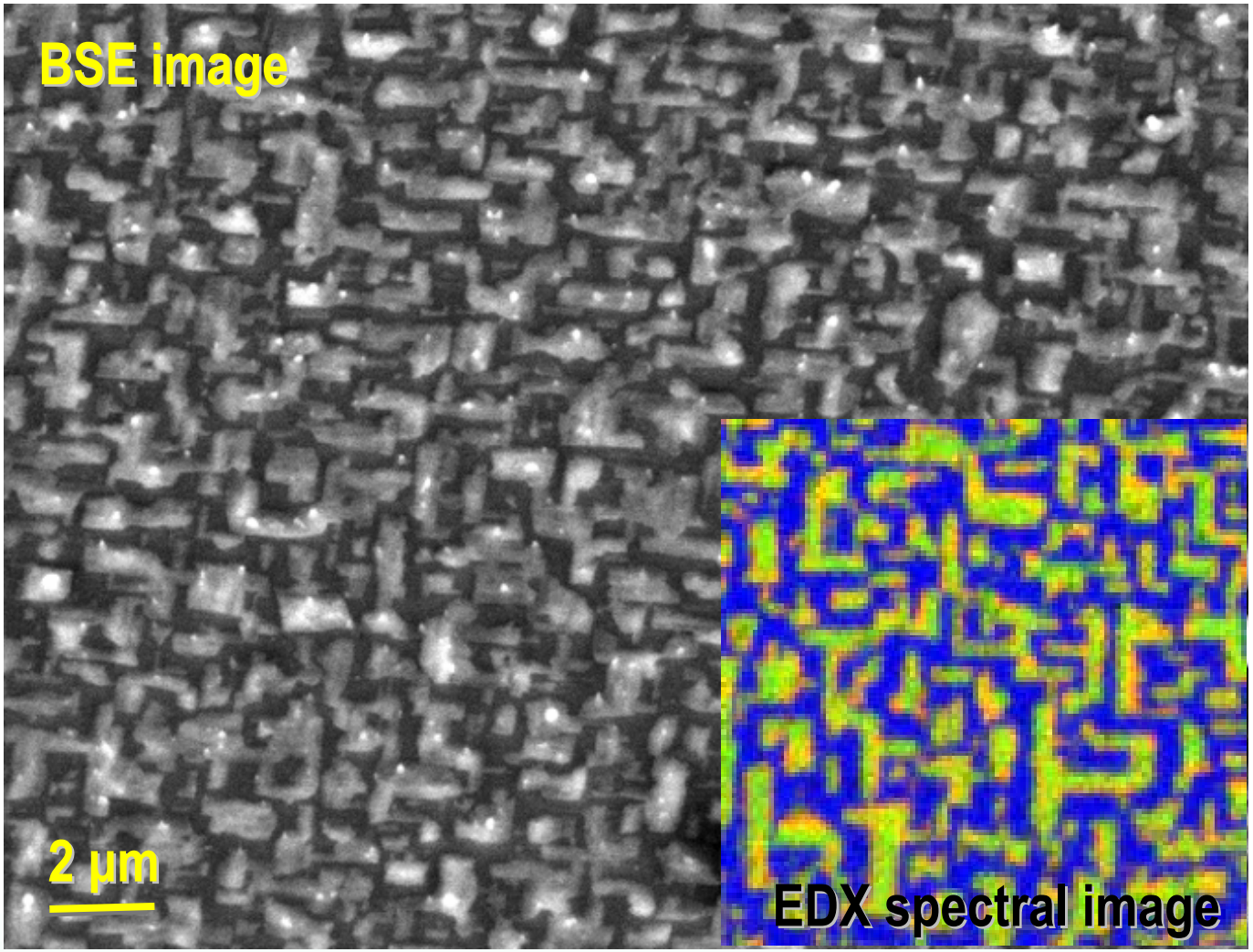
A.V. Melechko et al. J. Appl. Phys. **97**, 041301-39 (2005).

“Forests” of carbon nanofibers can also be grown on self-assembling thin films

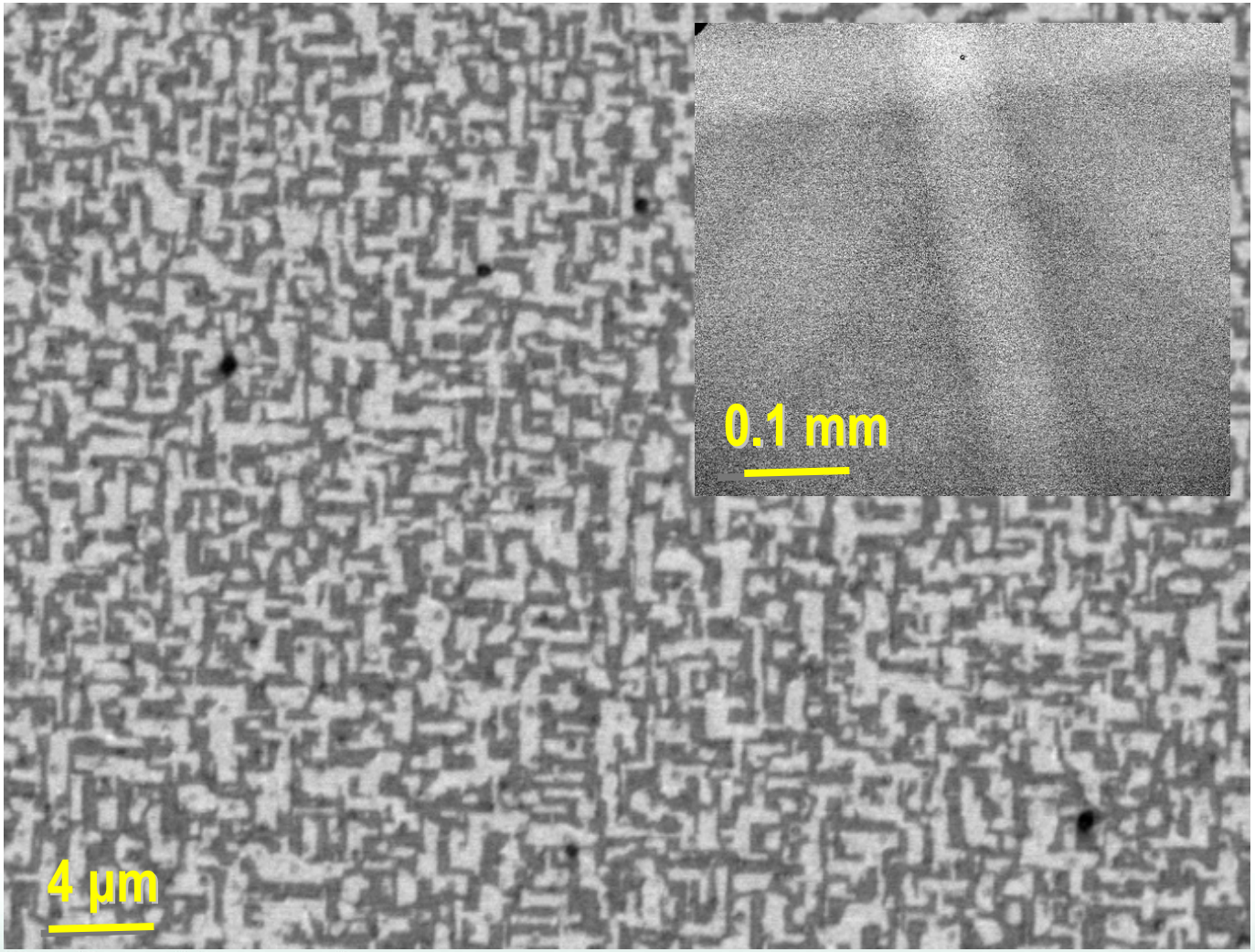


- Fe/Co catalyst particles form from heat treatment of thin films
- Carbon nanofibers grown catalytically in ammonia (NH_3) / acetylene (C_2H_2) plasma
- Synthesis questions:
  - What is thin film geometry (microstructure, texture) before initiation of growth?
  - What is the catalyst / nanofiber interface configuration?

Thin film microstructure at the onset of growth

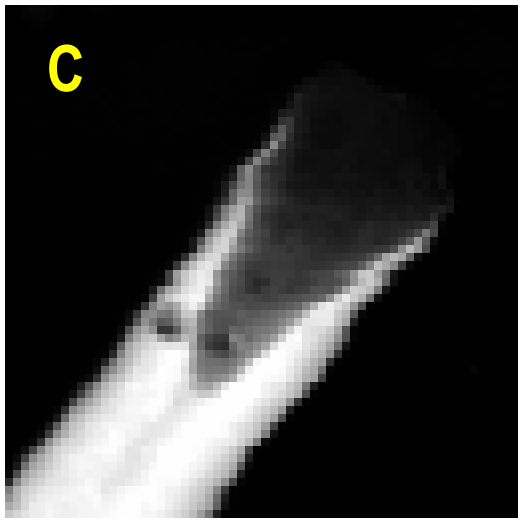


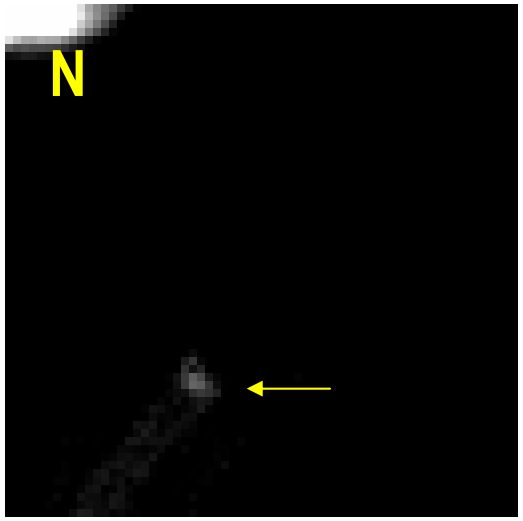
After annealing, FeCo thin film oriented with Si (001) substrate: texture, channeling pattern

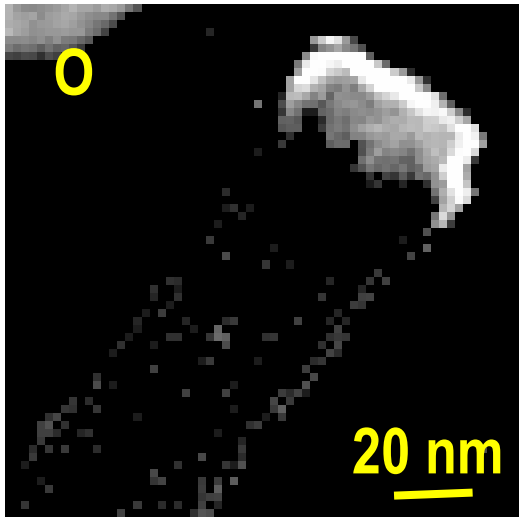


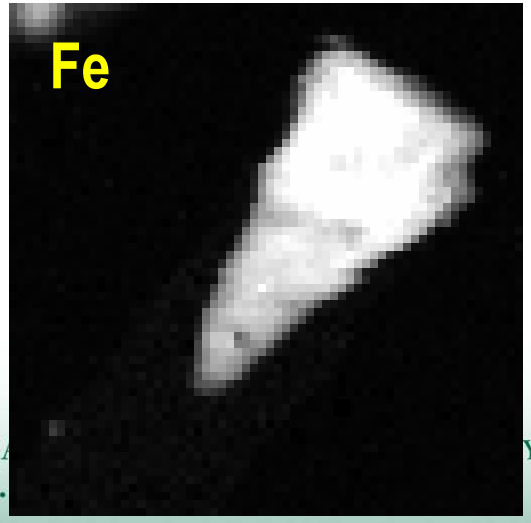
- FeCo islands show local facetting along substrate orientation
- Channeling pattern in low magnification image (inset): particles oriented over entire substrate

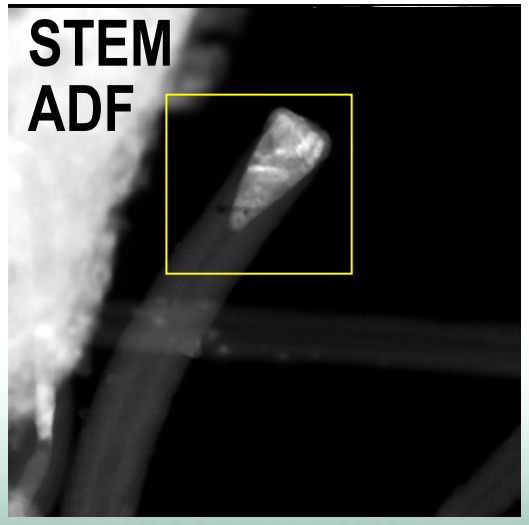
STEM-EELS spectral imaging reveals FeCo catalyst / carbon nanofiber interface structure

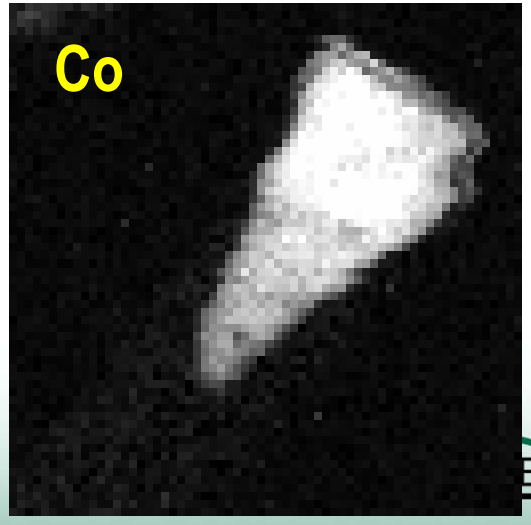












Neutron (or X-ray) scattering: seeing the other half of the picture!!

- Explore ensemble properties of thin films / catalyst particles / carbon nanofibers
- Monitor magnetic and structural properties of FeCo catalyst layer during synthesis
  - As deposited film
  - During process of annealing to form island structure
  - During growth of carbon nanofibers
- Monitor dynamics of synthesis process
- Isotope substitution to tailor scattering sensitivity (neutrons only)

Electron, X-ray, and neutron scattering complement one another to show the full story!!!