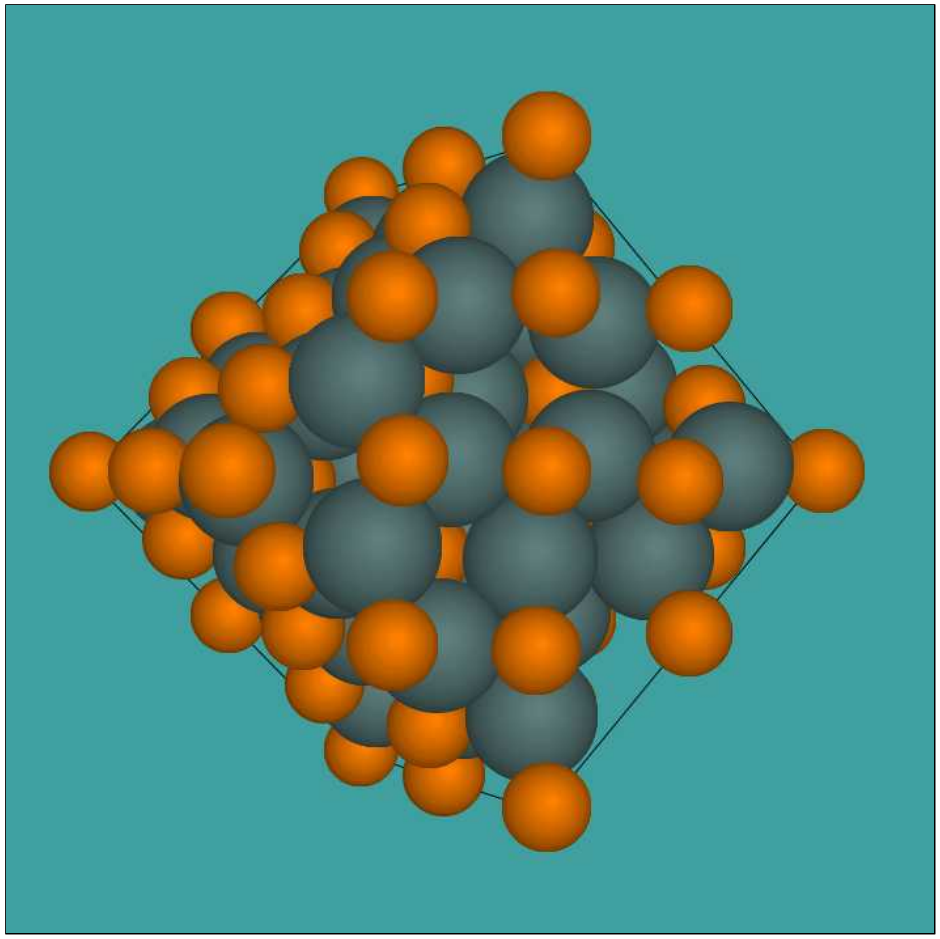
Oxygen Incorporation in Erbium Dihydride Thin Films

SAND2008-4827P



Chad Parish
Luke Brewer
Materials Science & Engineering

Sandia National Laboratories

Clark Snow
Neutron Generators

In collaboration with:
Brian Gorman
University of North Texas

UNT UNIVERSITY OF NORTH TEXAS Discover the power of ideas.

Acknowledgements:
Garry Bryant, Paul Kotula, Michael Rye

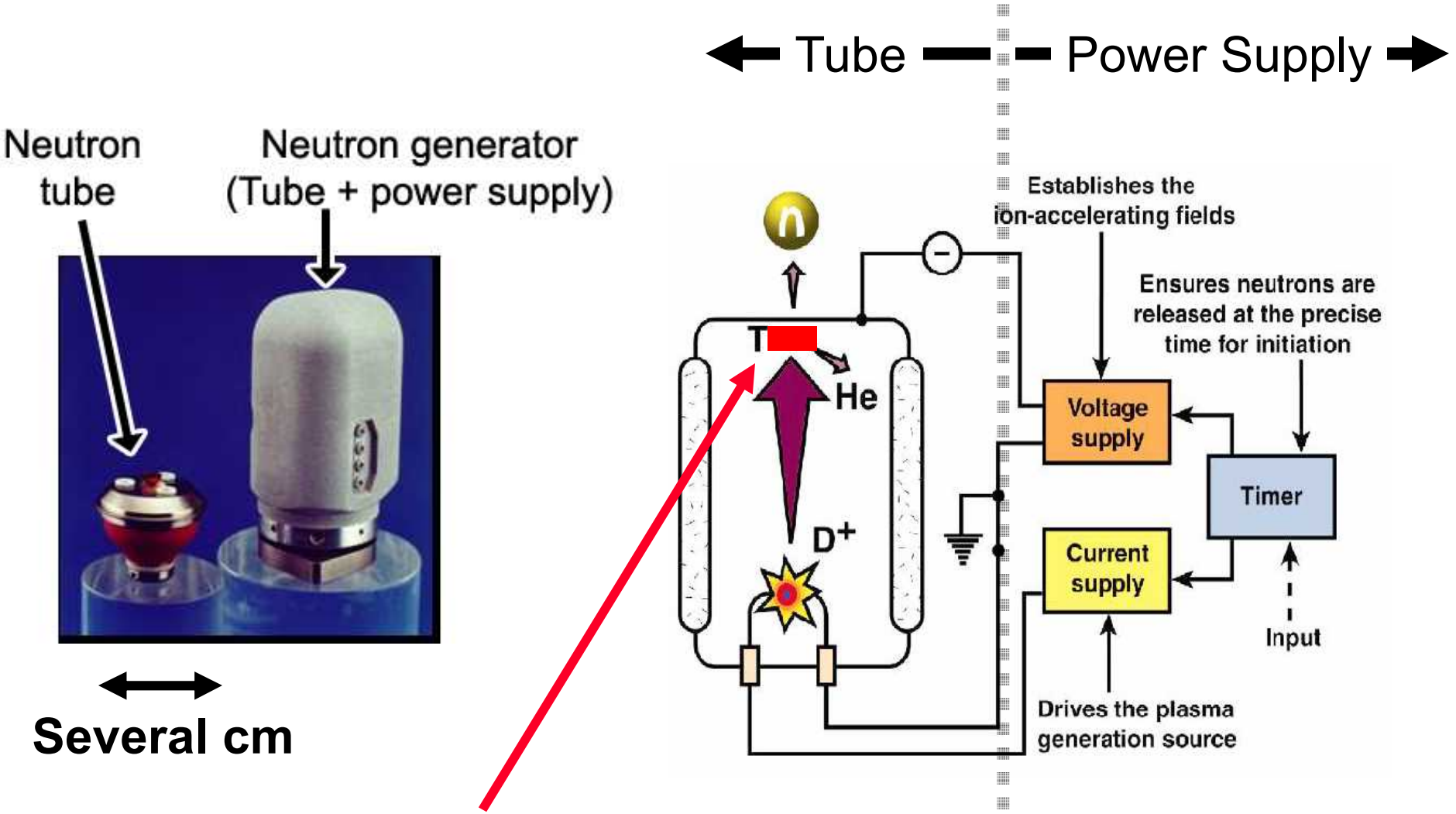
Sandia National Laboratories

Contact: cmparis@sandia.gov

National Nuclear Security Administration

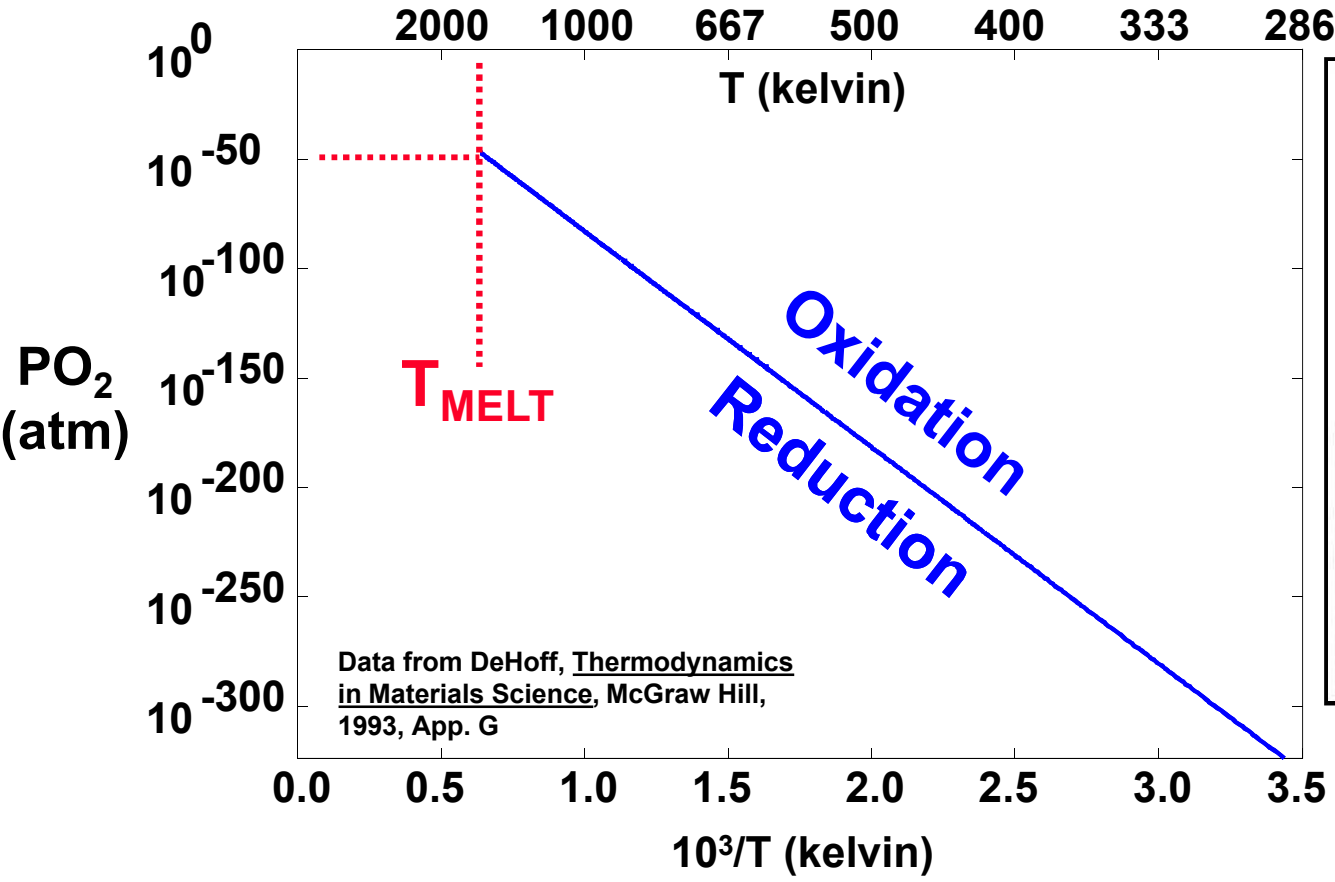
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

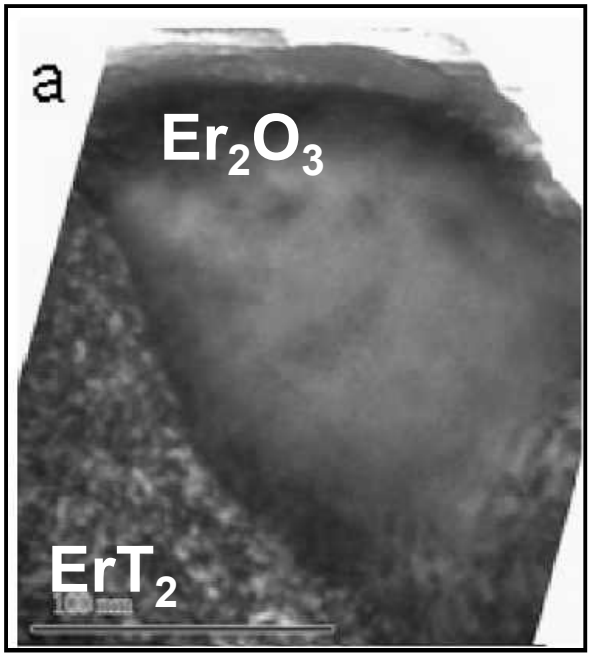
Neutron generators are compact sources for energetic neutrons



C. R. Loeber, Building the Bombs, Sandia National Labs, 2002

Major problem: Er oxidizes easily





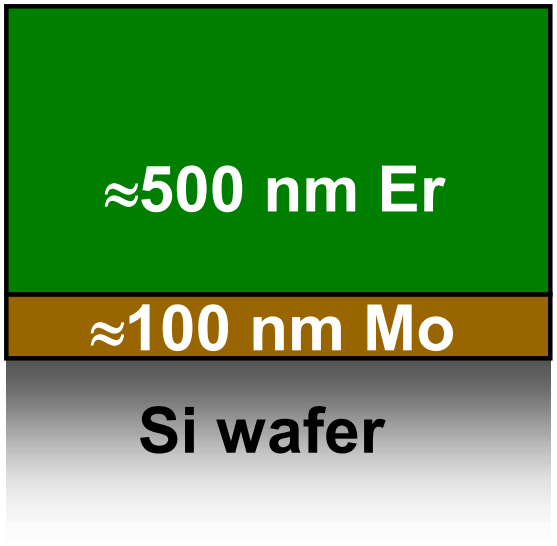
Snow et al., J Nuc Mater V374 (2008), P.147

ErD_2 used as non-radioactive analogue to ErT_2

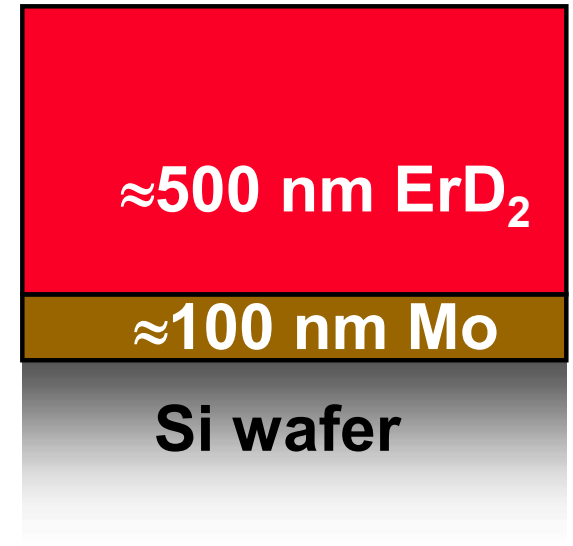
→Our hot TEM has fewer capabilities than the TEMs used in this study

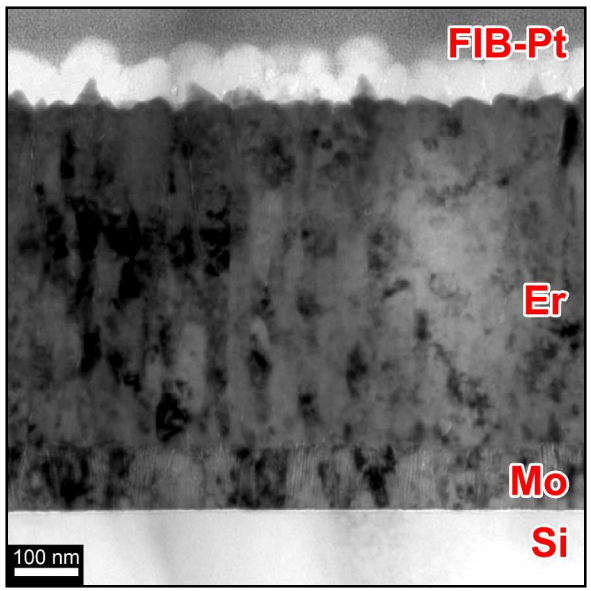
Sandia National Laboratories

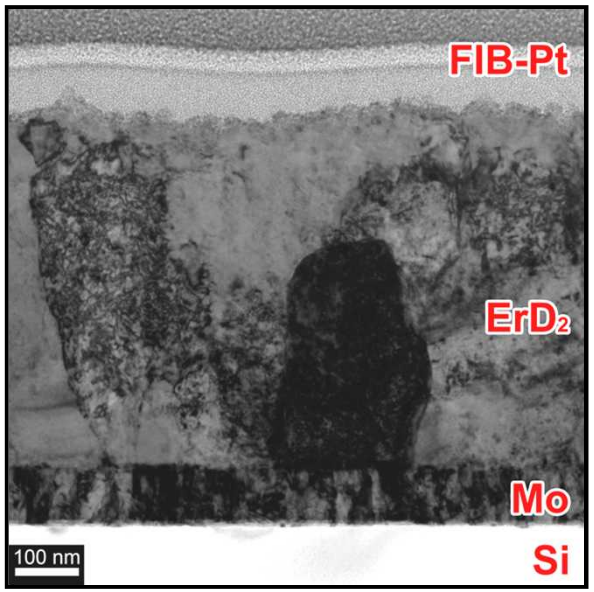
Samples are ErD_2 thin films on Mo // Si



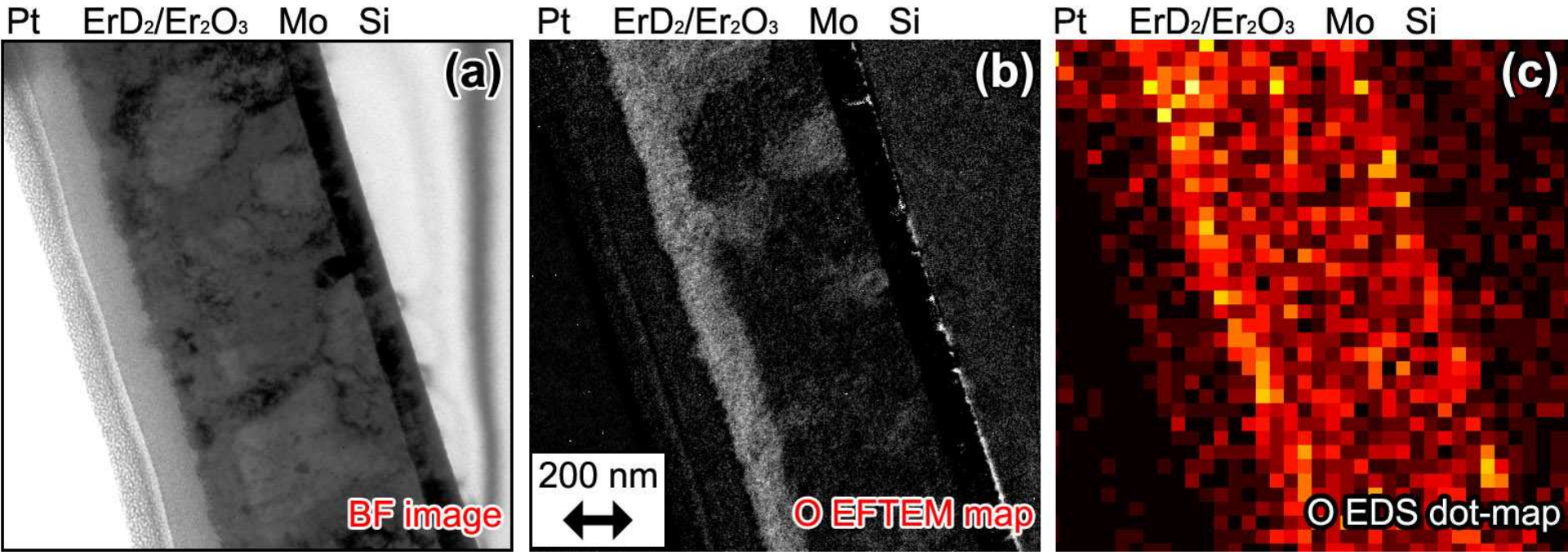
Hydriding





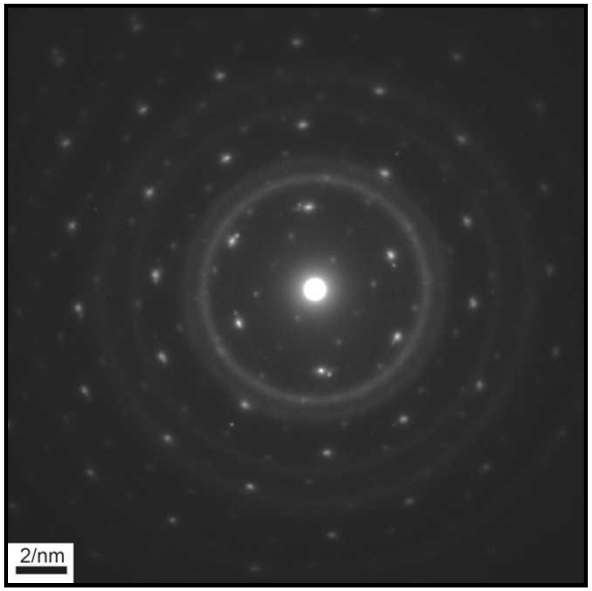


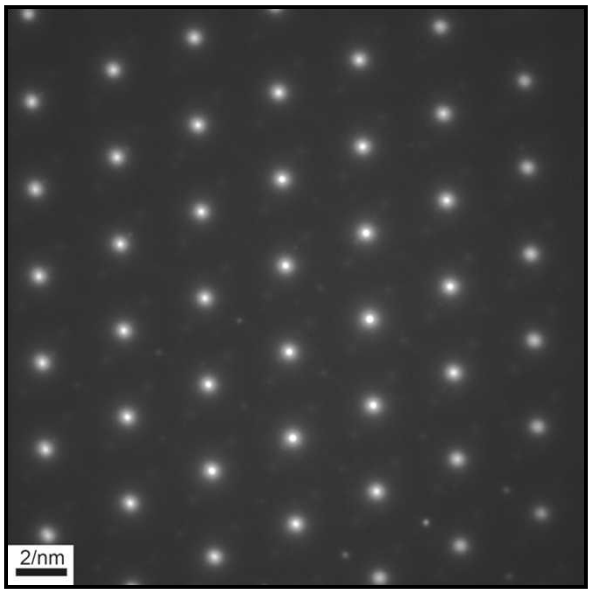
>100 nm of oxide observed via EFTEM



Sandia National Laboratories

We can use diffraction to verify crystallography of the layers

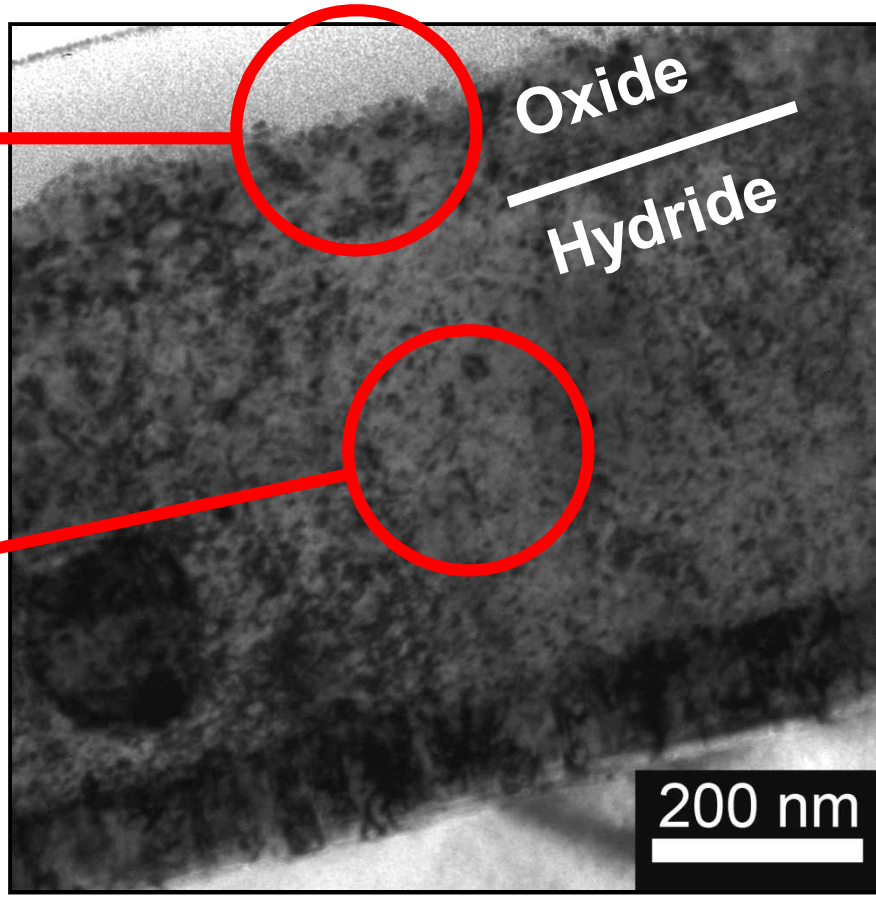




Surface

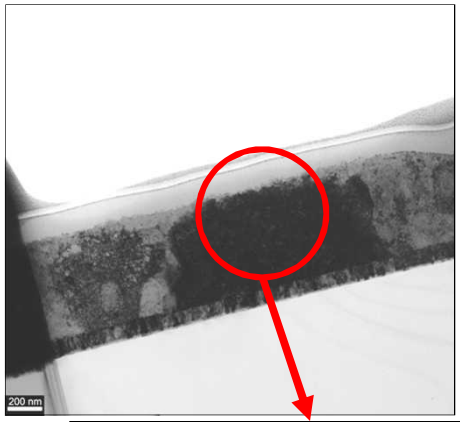
oxide

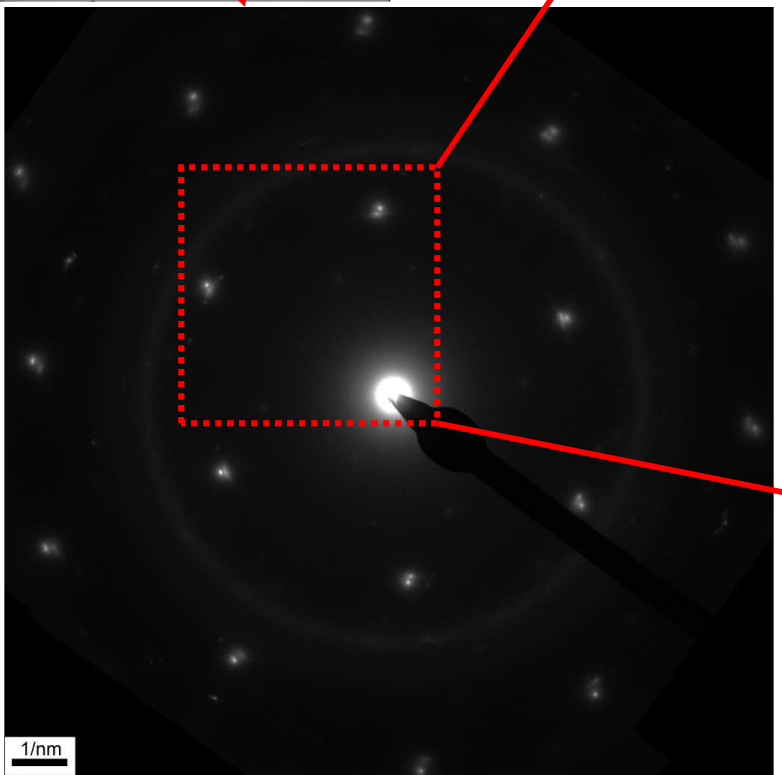
Hydride

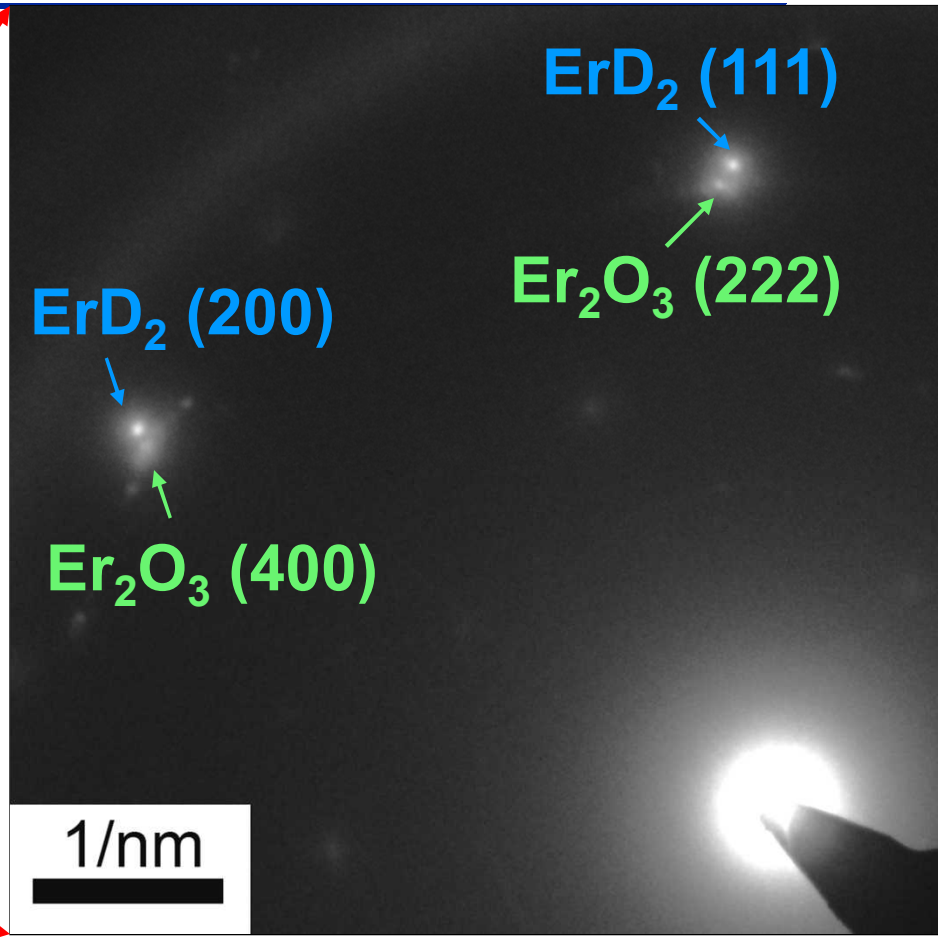


Sandia National Laboratories

Diffraction shows hydride and oxide have epitaxial orientation

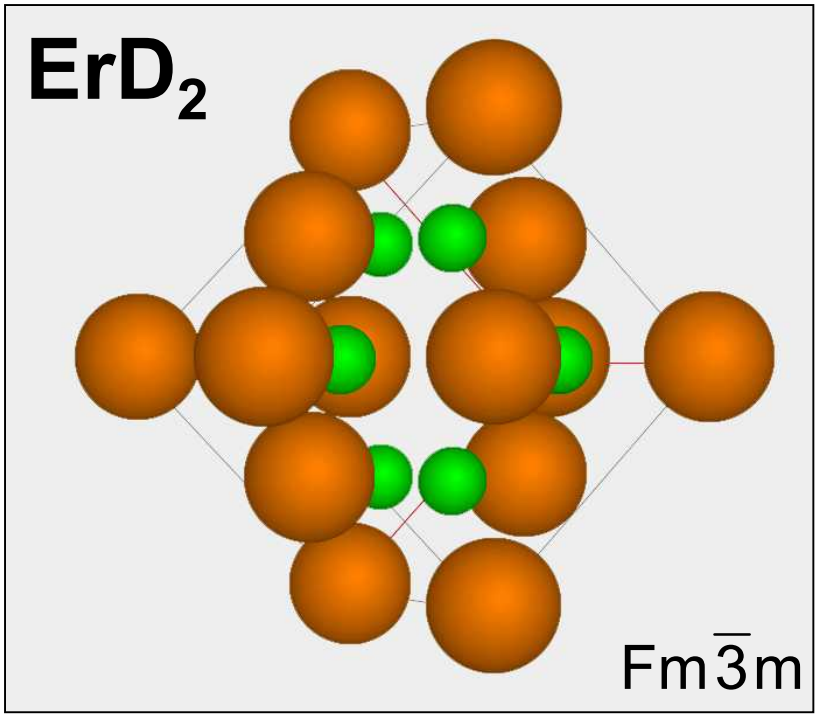


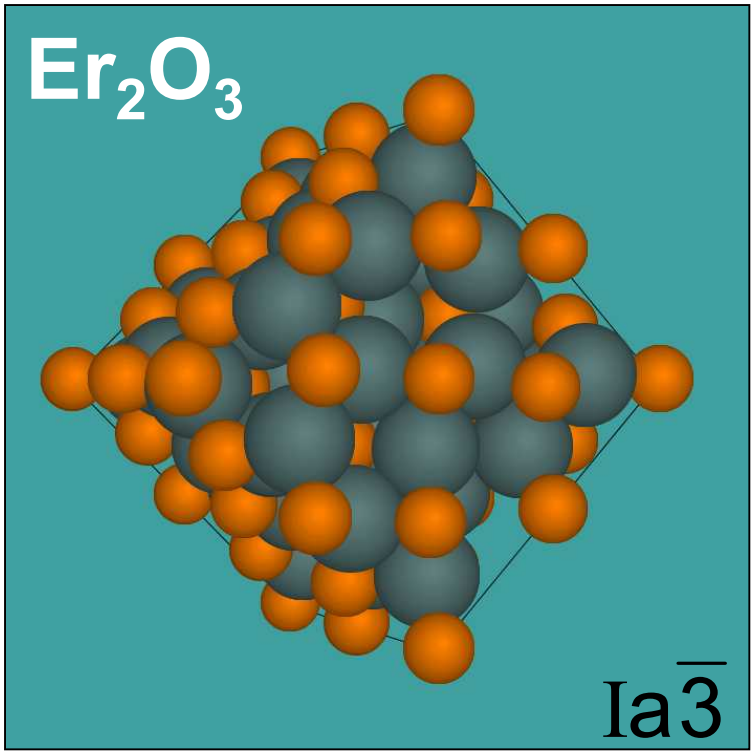




Sandia National Laboratories

Near-integral lattice mismatch probable cause for epitaxy





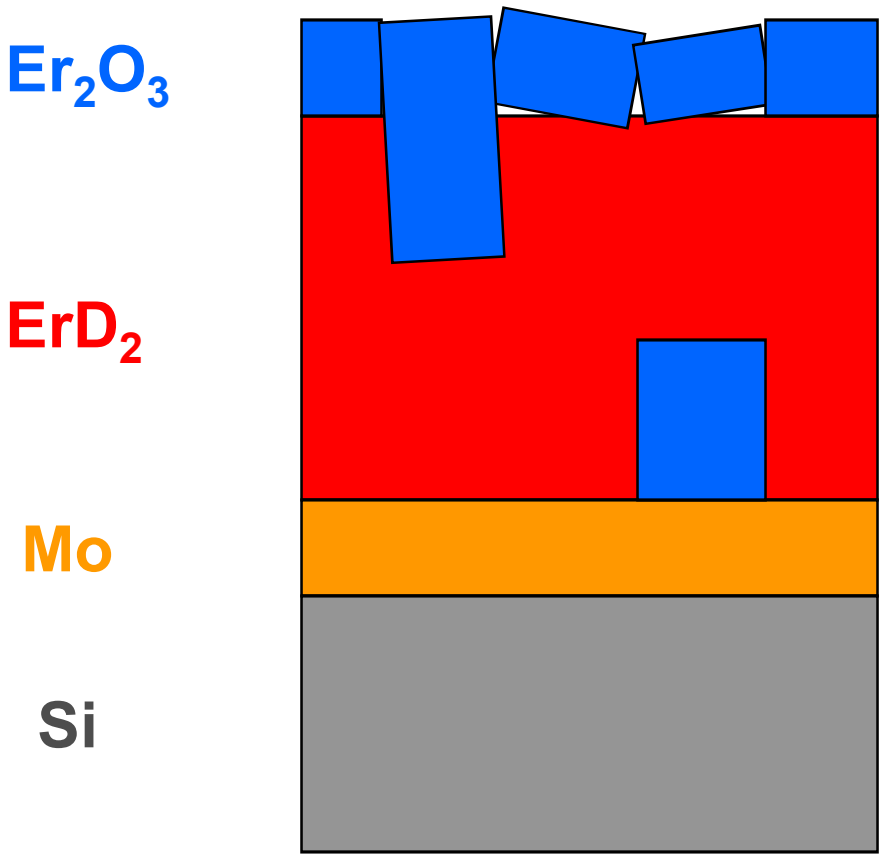
a_{ErD2}=0.512 nm

a_{Er2O3}=1.054 nm

$$a_{Er2O3} / a_{ErD2} \approx 2.06$$

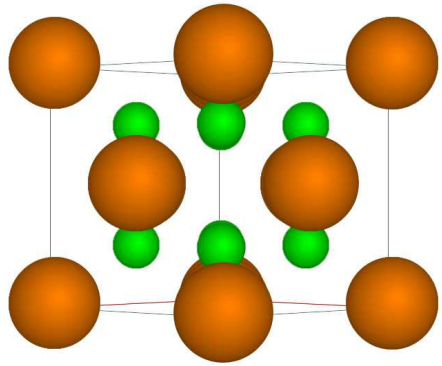
Sandia National Laboratories

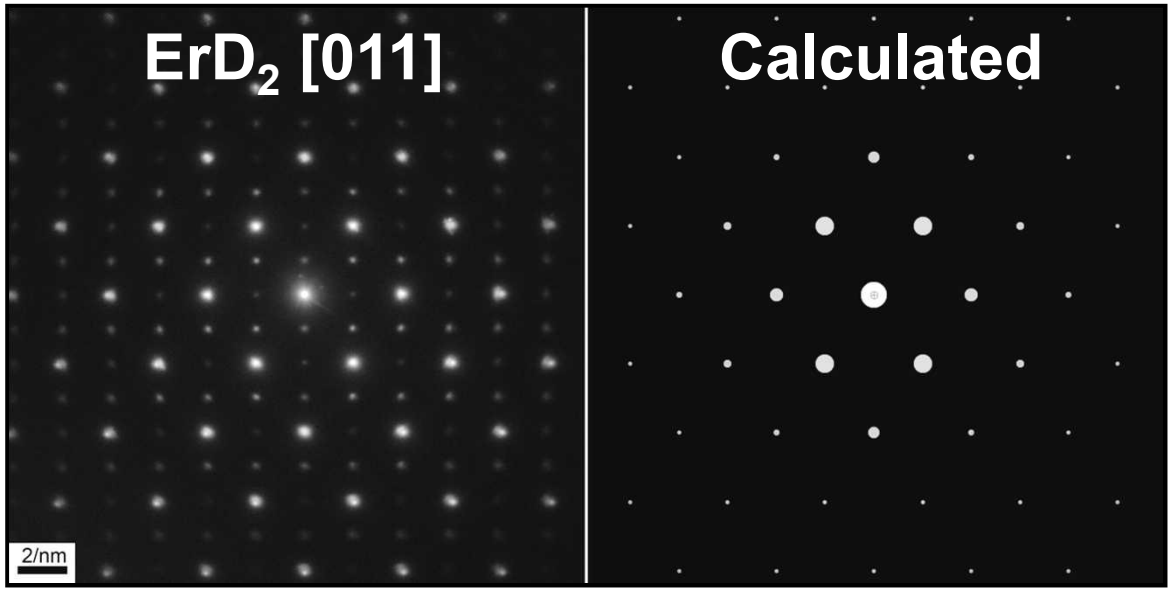
Oxides seen at the surface and penetrating within the film

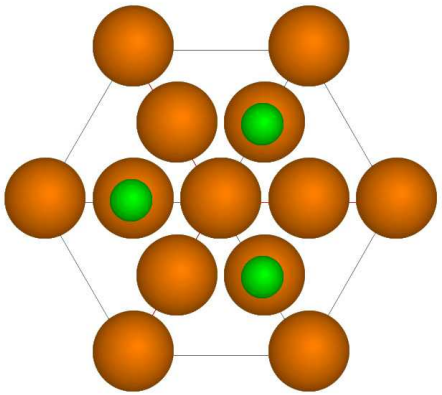


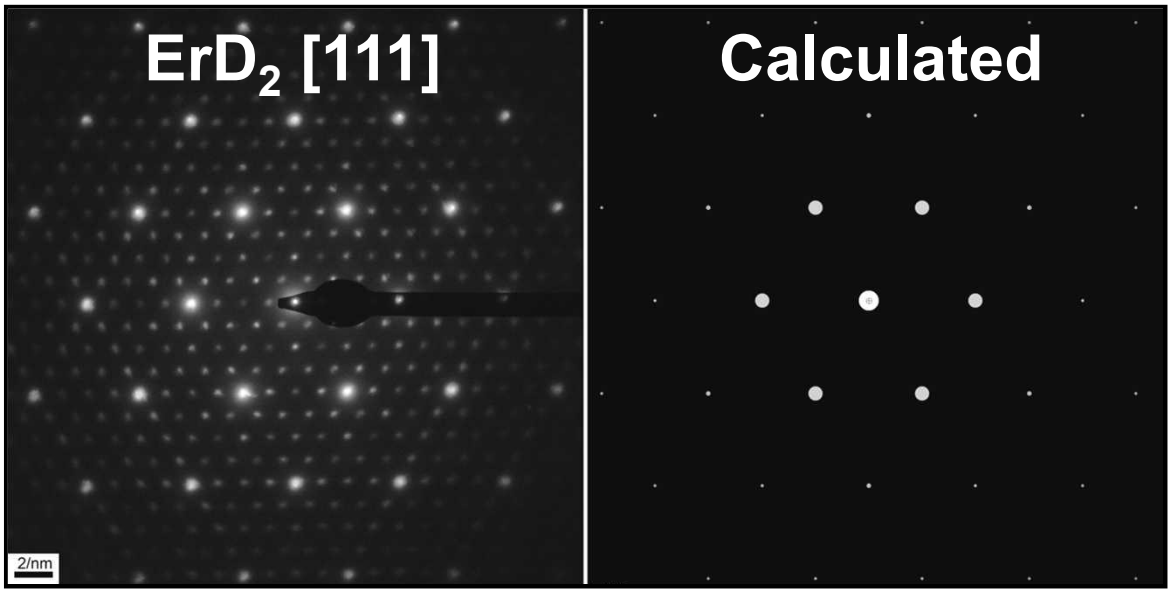
Sandia National Laboratories

We observe satellite spots that are not predicted from the ErD_2 structure









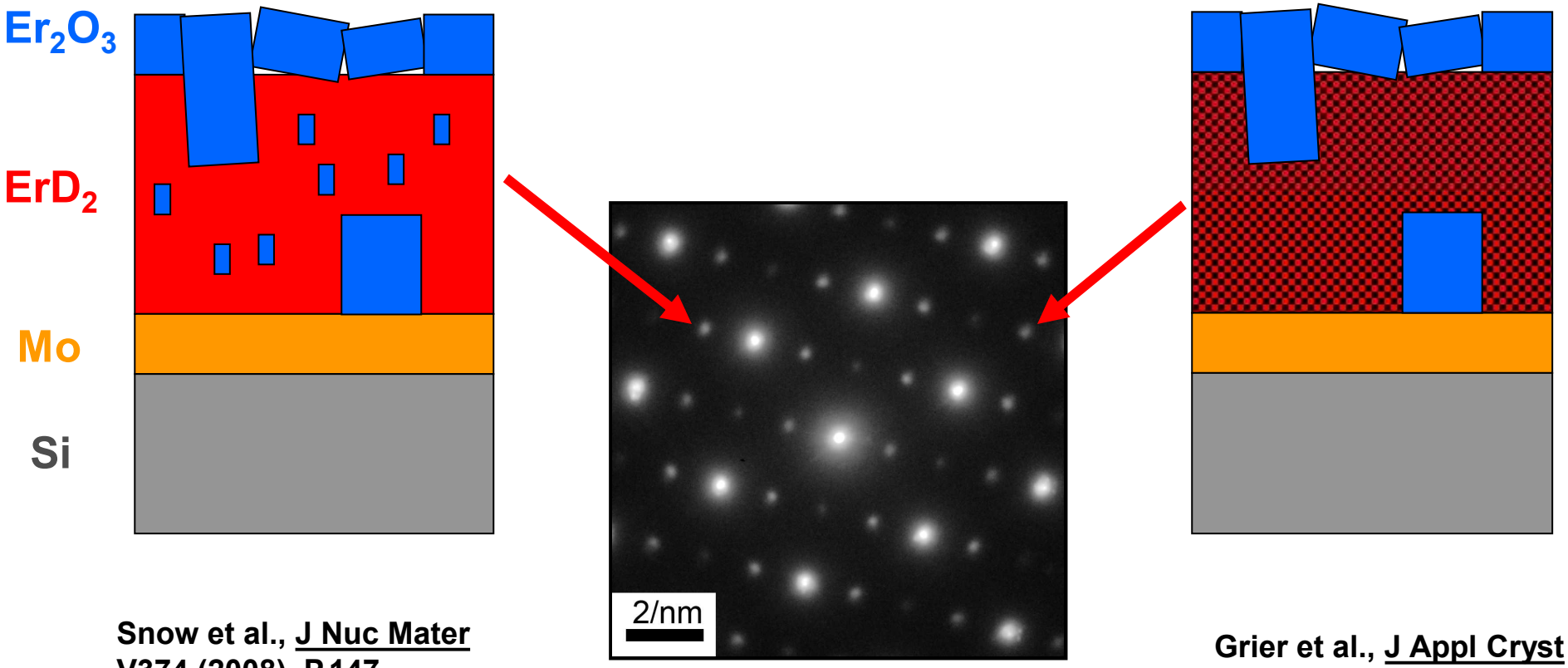
Two hypotheses for satellites: oxide inclusions or hydrogen ordering

Hypothesis 1:

Nano-oxide inclusions

Hypothesis 2:

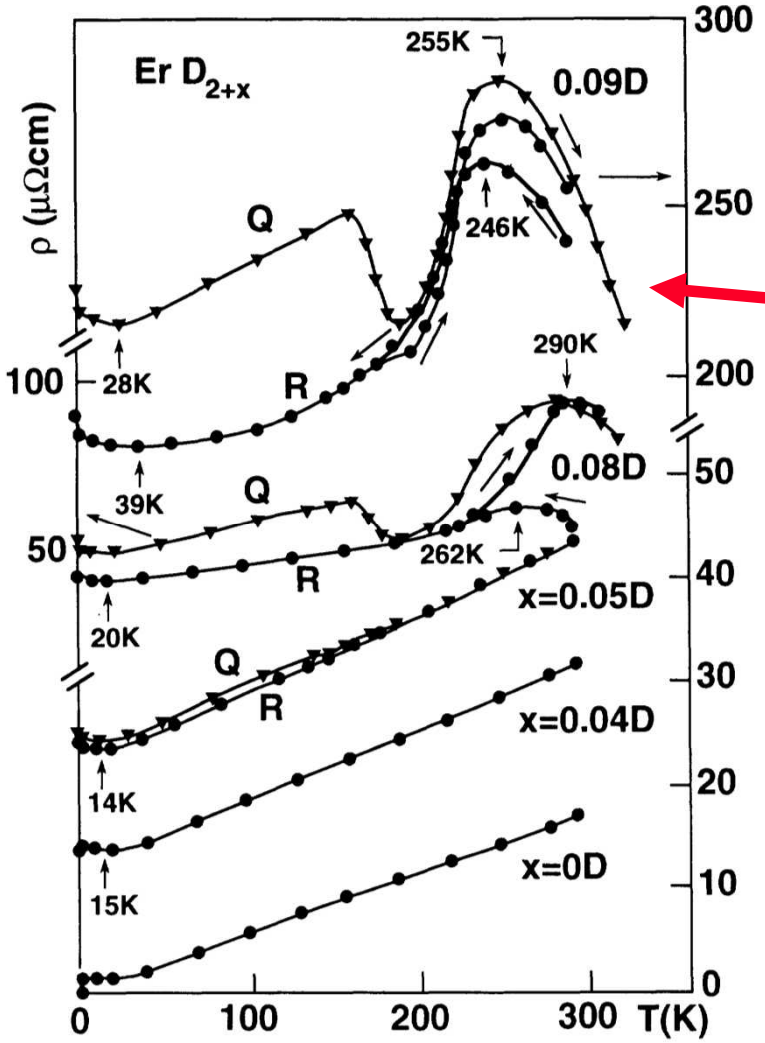
Ordering of D in ErD_{2+x}



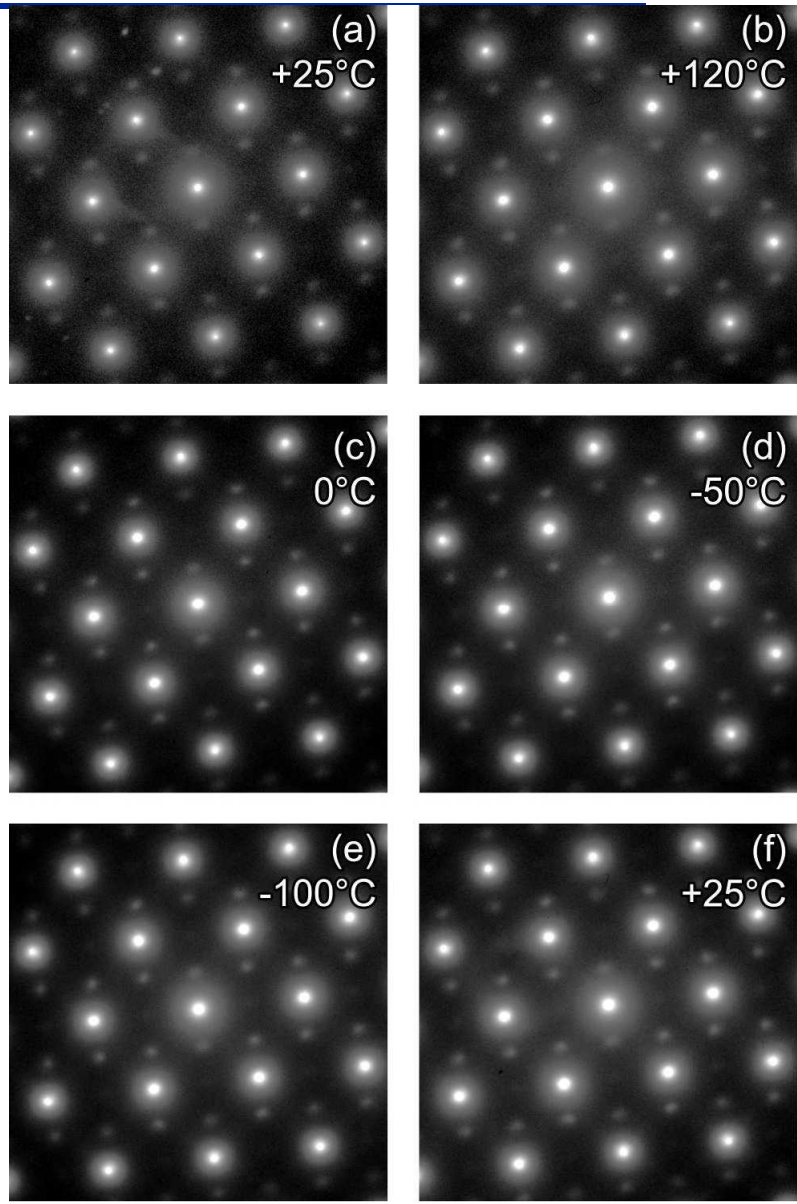
Snow et al., J Nuc Mater V374 (2008), P.147

Grier et al., J Appl Cryst V33, P. 1246, 2000

Variable-temperature diffraction rules out hydrogen ordering

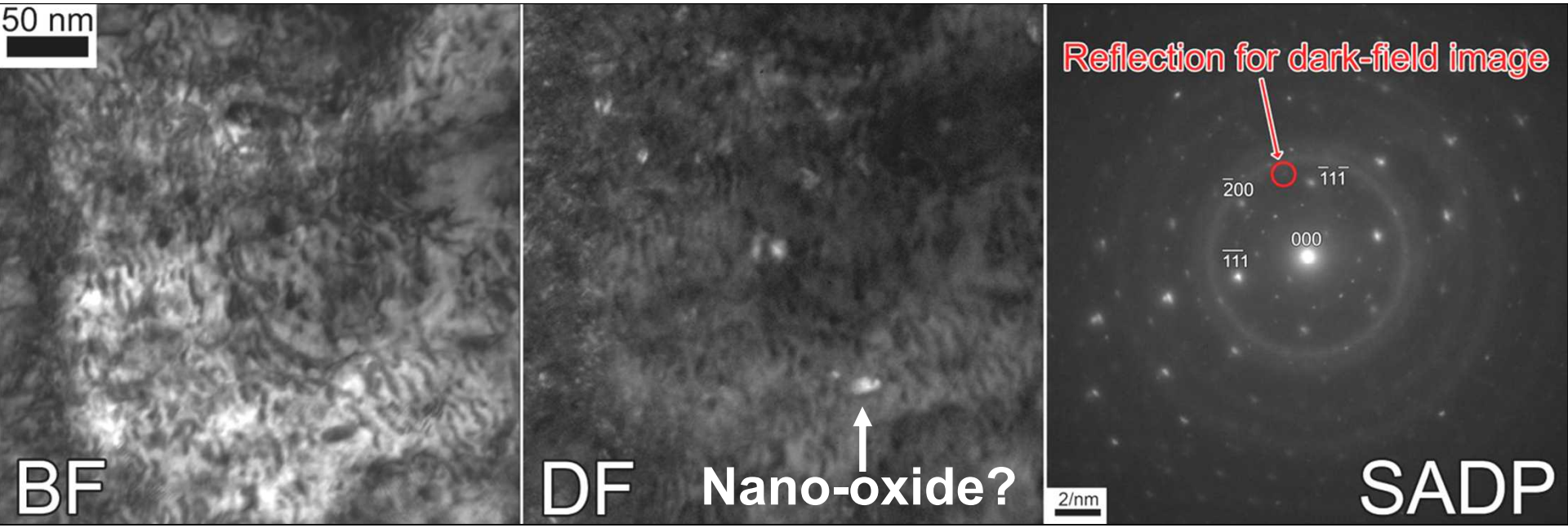


Ordering in $ErD_{2.09}$ disappears at < 25°C

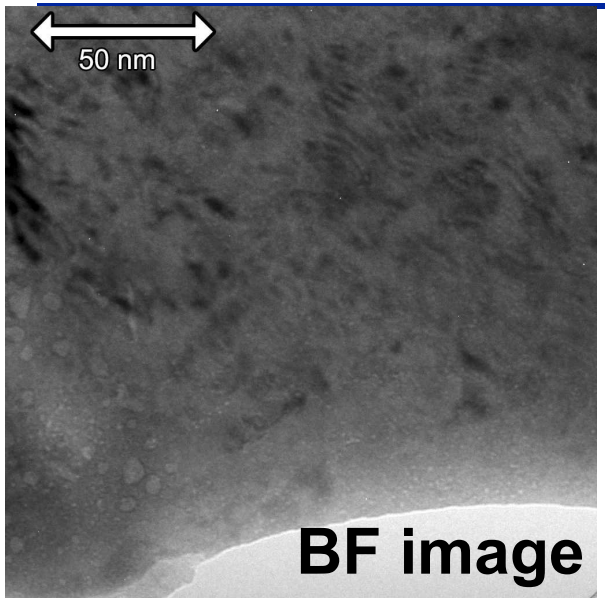


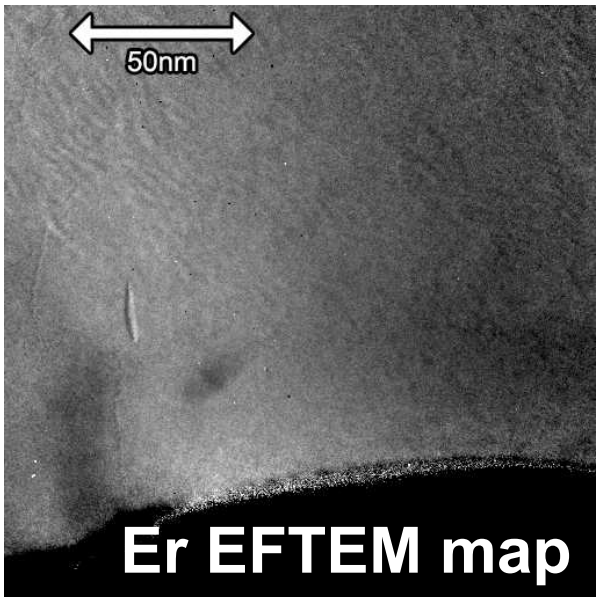
Vajda & Daou, Phys Rev B V49(5), P. 3275, 1994

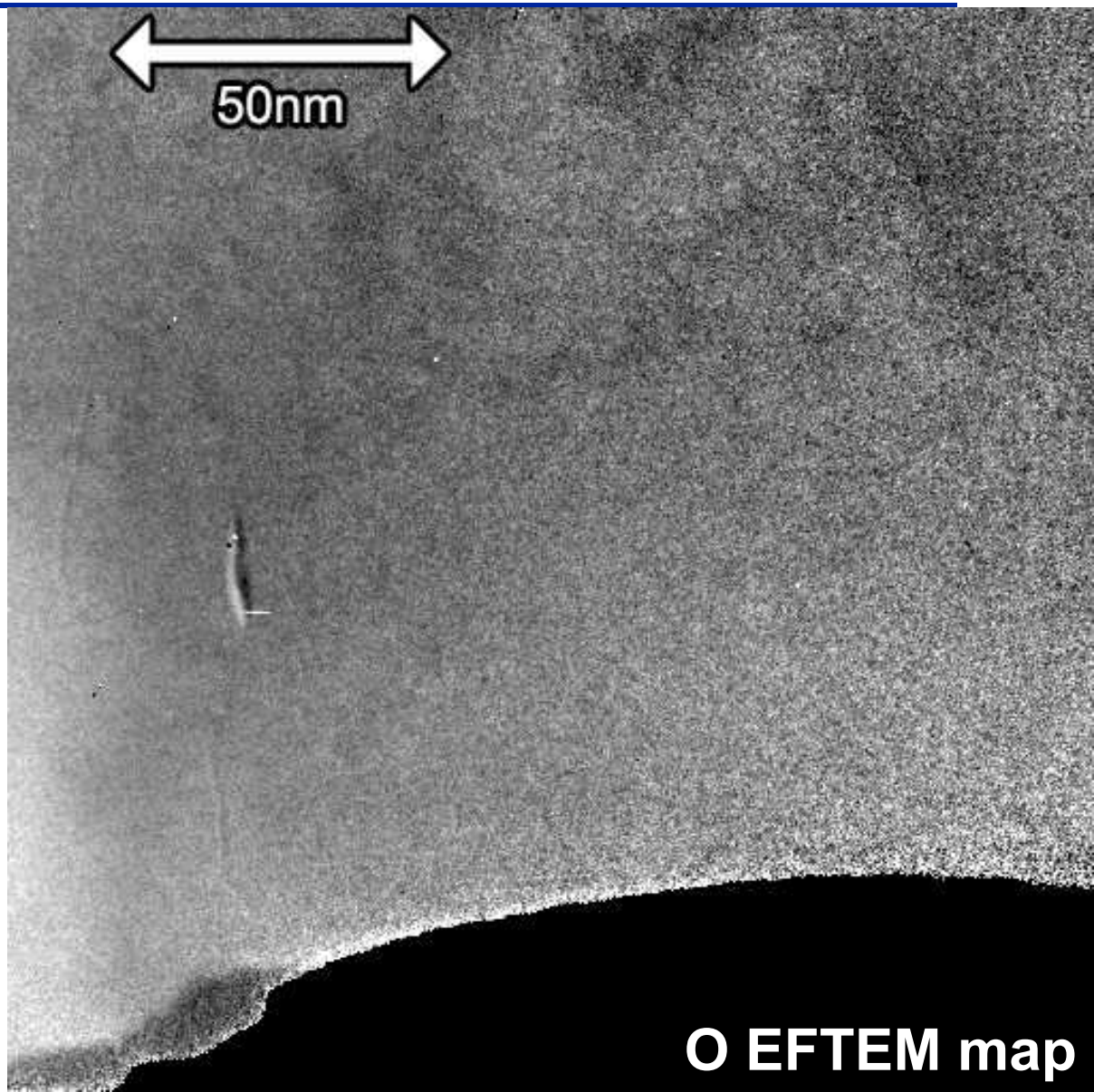
Nano-oxides difficult to observe in TEM



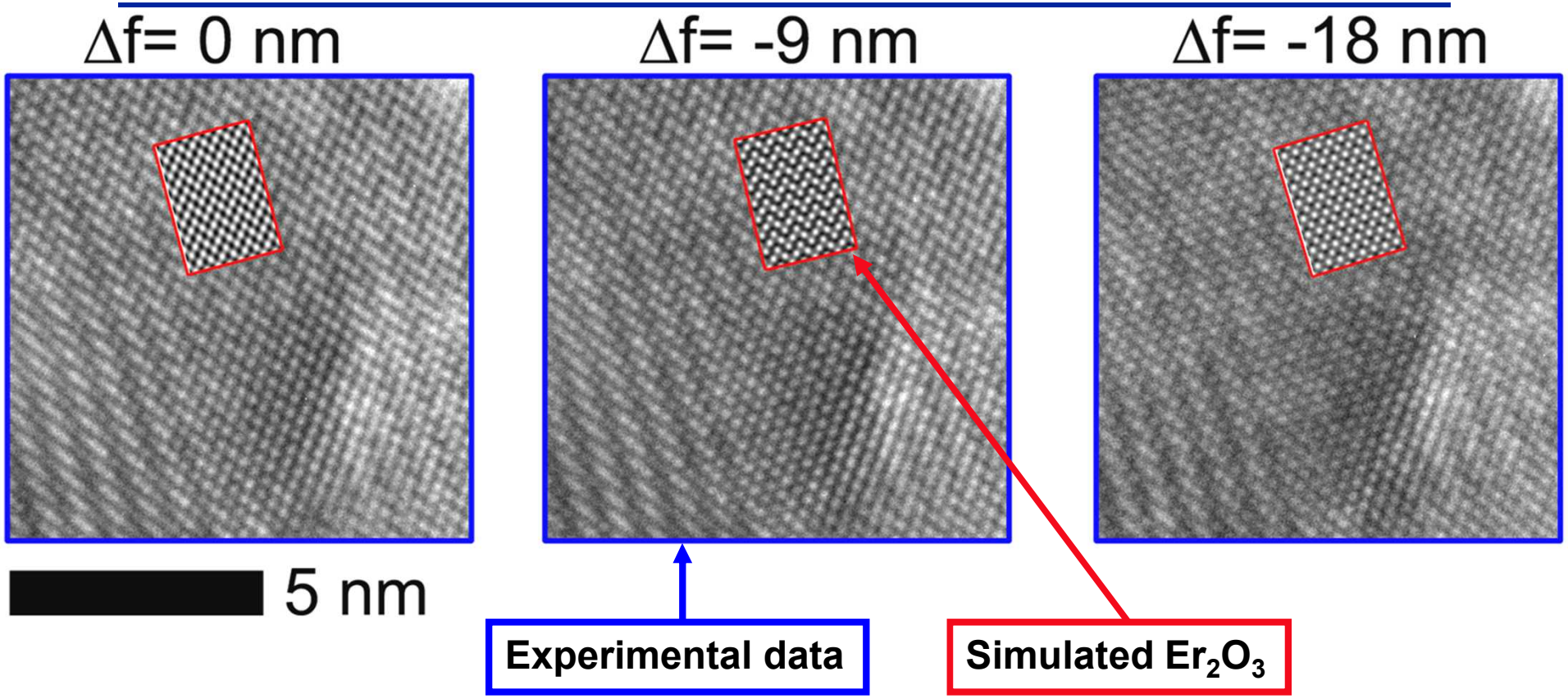
Higher-resolution EFTEM shows no obvious oxide particles







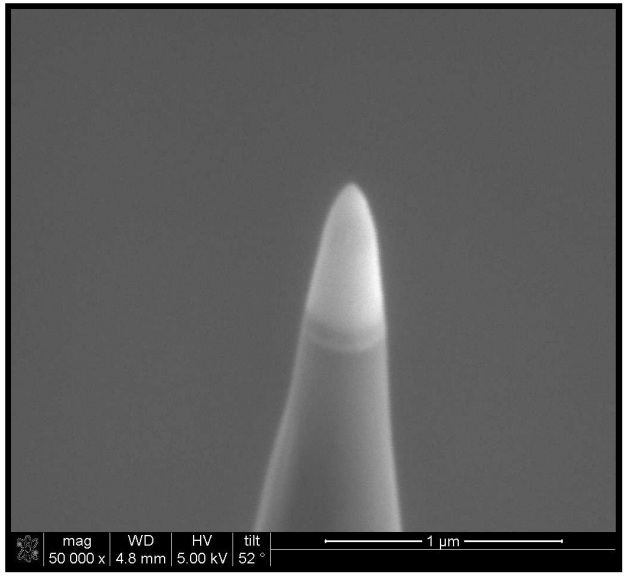
Lattice imaging matches some areas to oxide



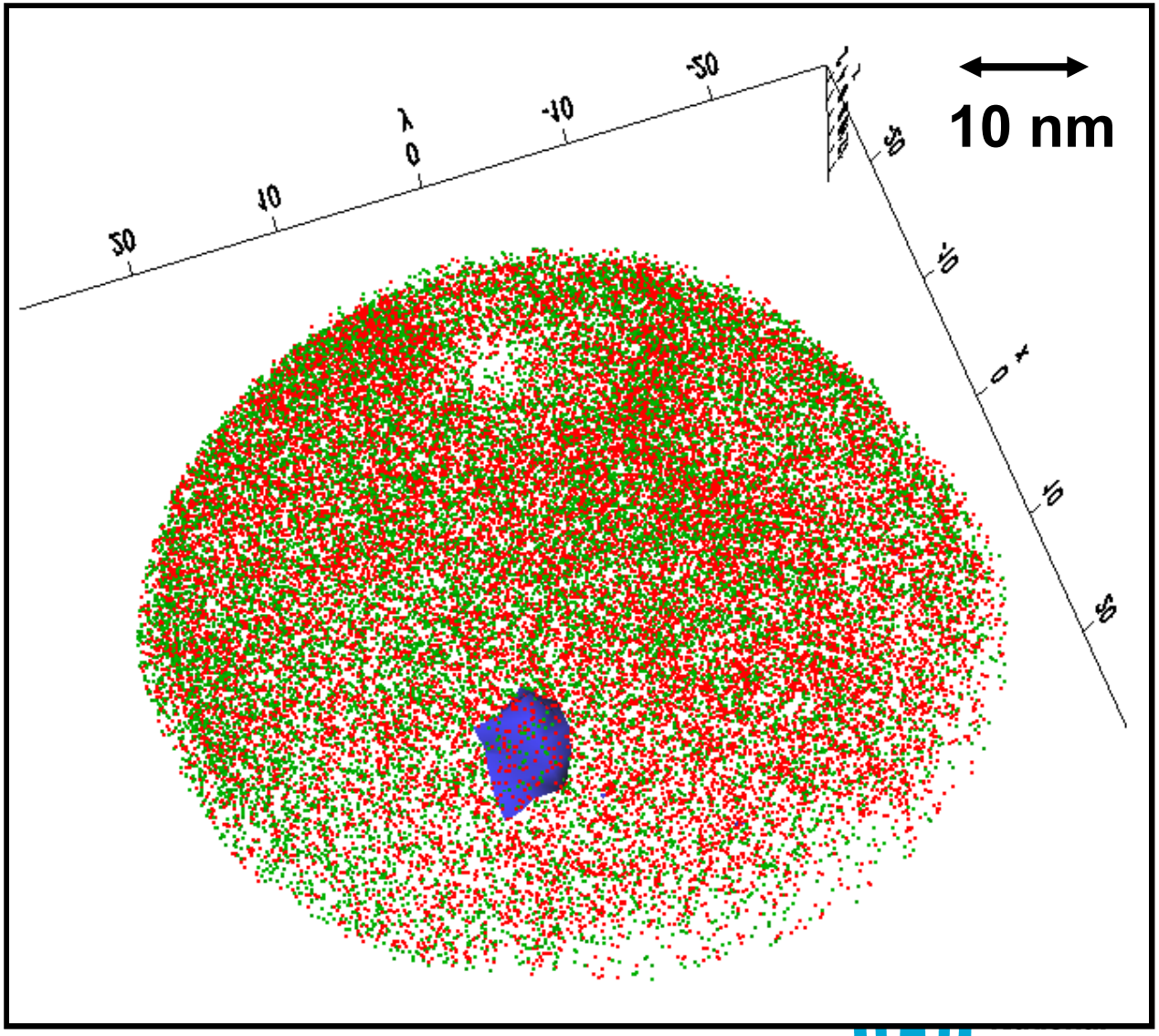
- Calculated images match some sample areas
- Some sample areas cannot be matched to ErD_2 or Er_2O_3

Sandia National Laboratories

Preliminary atom probe results: small oxides observed



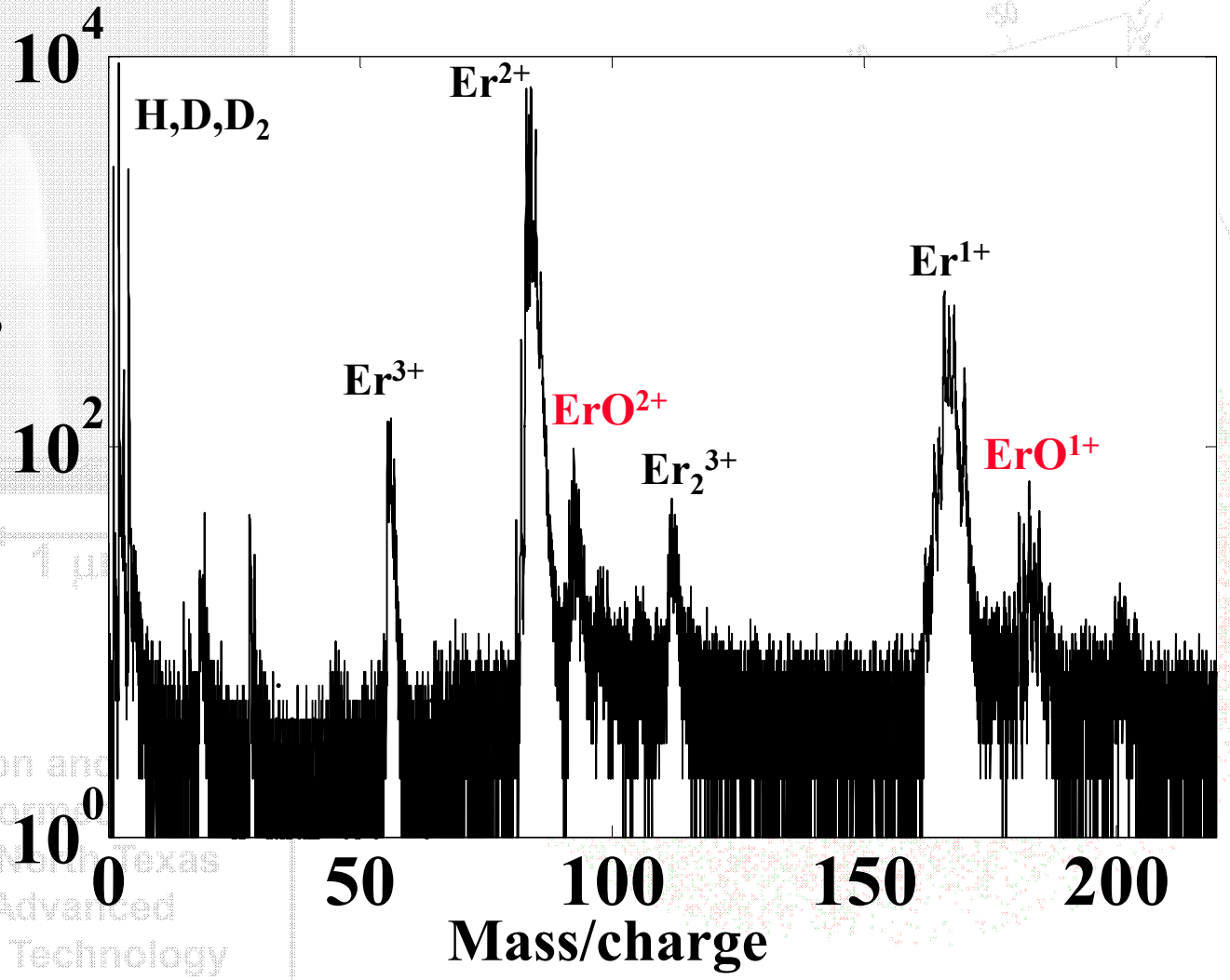
1 µm



FIB preparation and atom probe performed at University of North Texas Center for Advanced Research and Technology

Laboratories

Preliminary atom probe results: small oxides observed

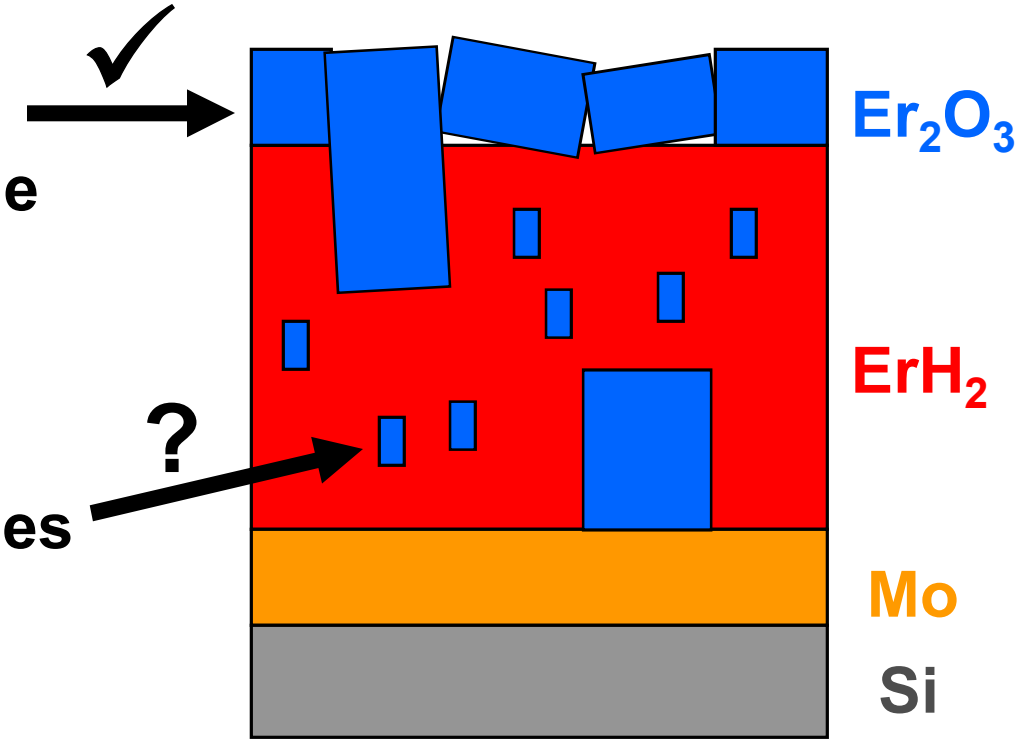


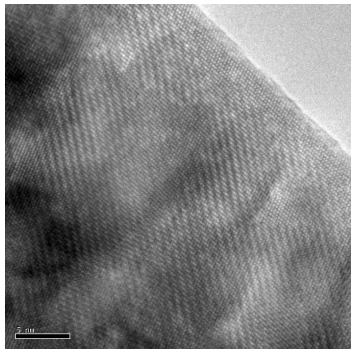
Oxides in ErD_2 grow epitaxially on the surface, and nano-oxides may exist in the matrix

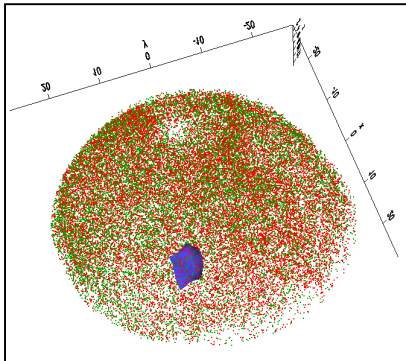
Imaging, EFTEM, and diffraction indicate oxide films formed on the sample surface

Satellite diffraction spots could be due to nano-oxides within the ErD_2 matrix

Additional experiments are underway to confirm or refute this nano-oxide hypothesis

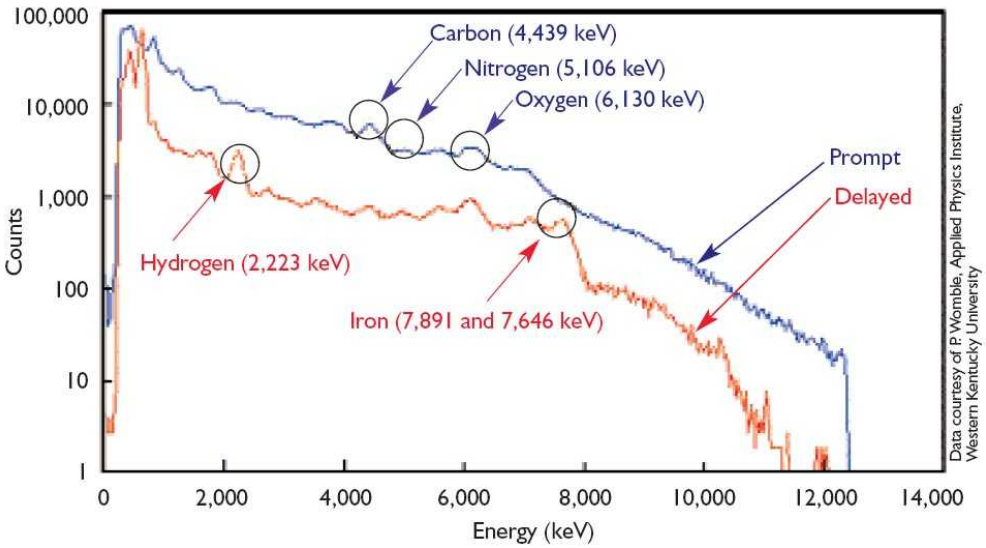






Neutron generators (NGs) have several applications

- **Oil-well down-hole characterization**
  - →Neutrons activate geological materials, allowing spectroscopic analysis
- **Homeland security**
  - →Neutrons activate materials to look for explosives, drugs, etc.
- **Laboratory benchtop source**
- **Nuclear weapons**
  - →Sandia produces NGs for the US deterrent



Chichester & Simpson, The Industrial Physicist, Dec.03/Jan.04, P.22

Sandia Labs