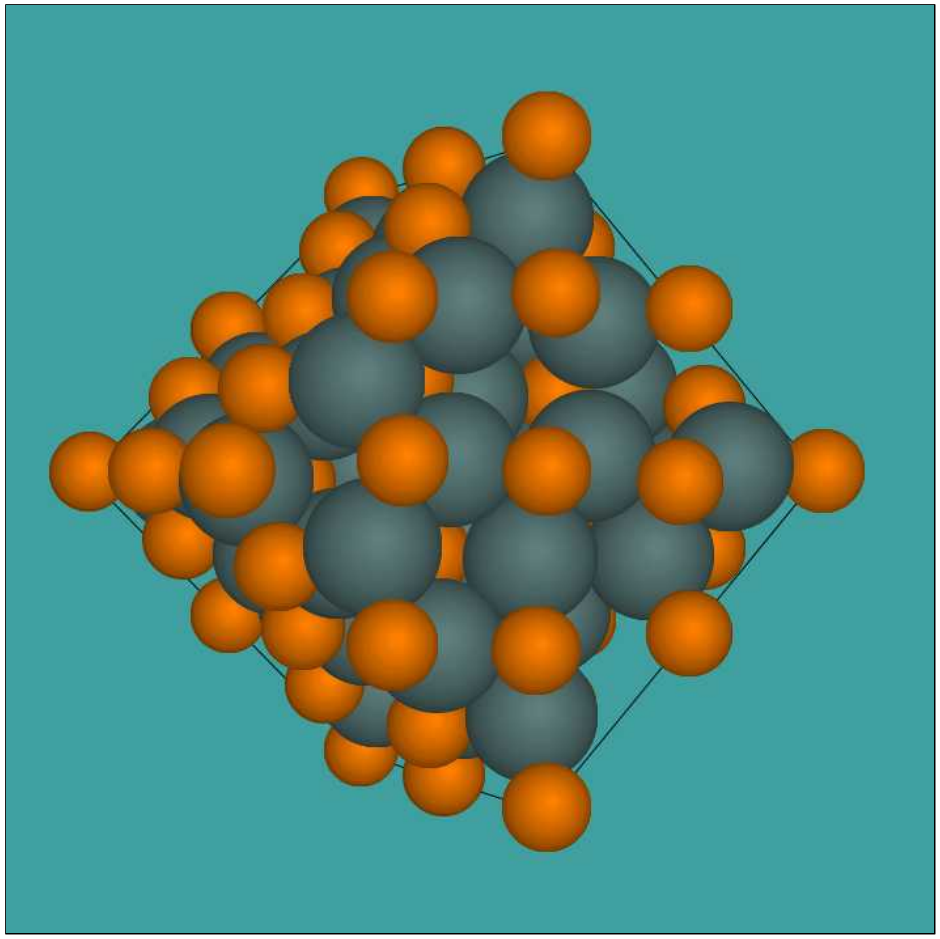
Oxygen Incorporation in Erbium Dihydride Thin Films

SAND2008-6412P



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Materials Science & Engineering

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Neutron Generators

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UNT University of North Texas
Discover the power of ideas.

Acknowledgements:
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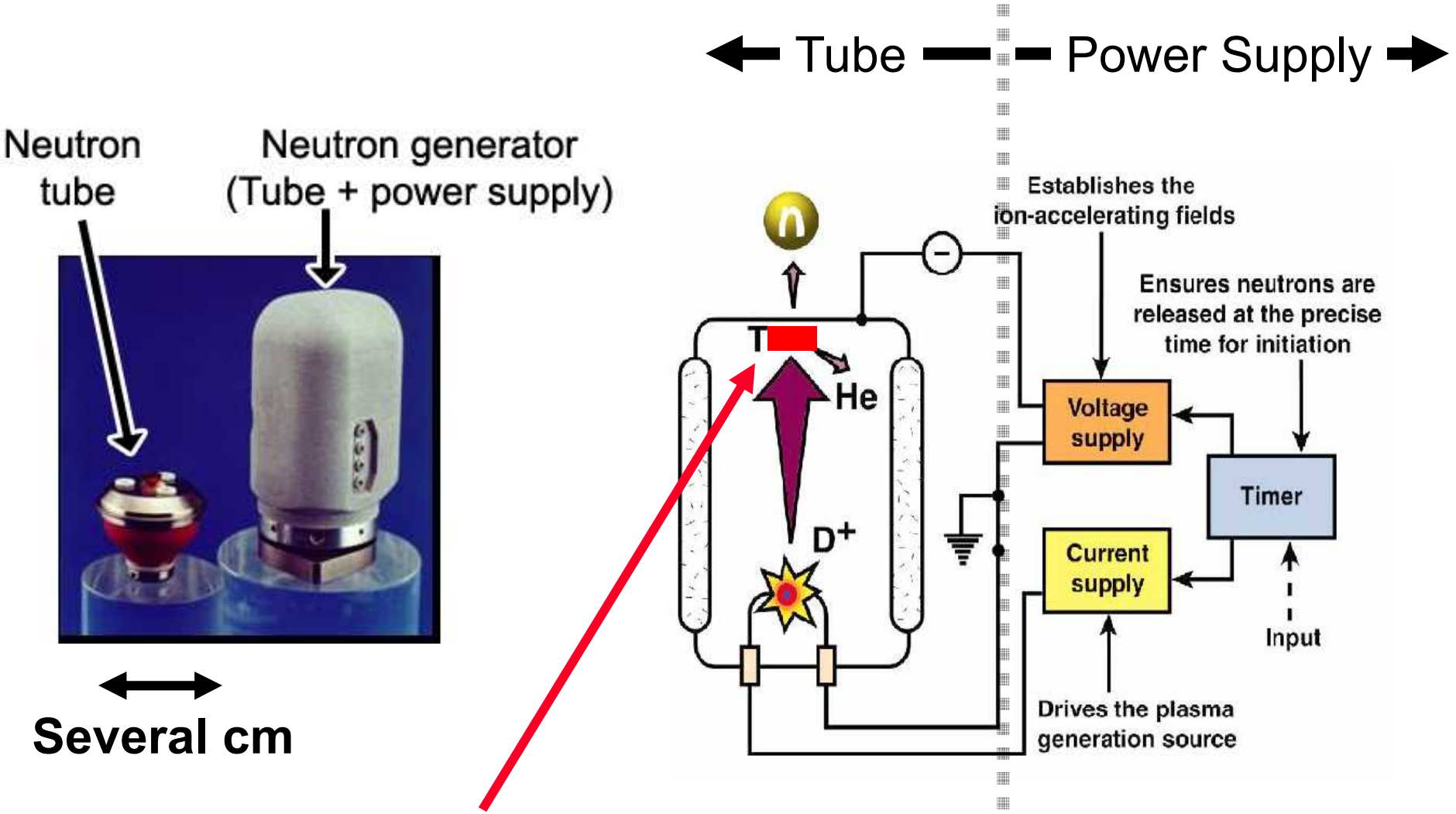
National Nuclear Security Administration

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.

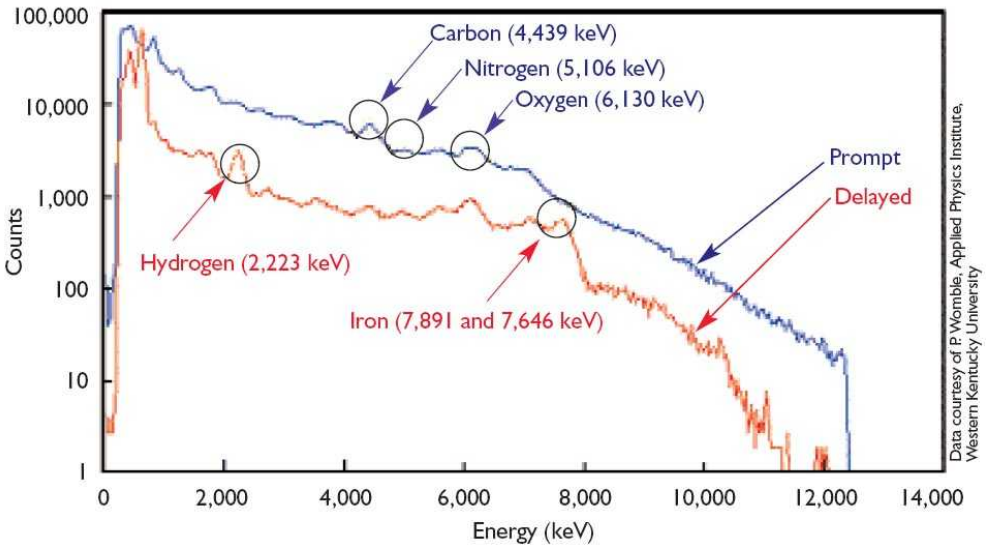
Neutron generators are compact sources for energetic neutrons



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

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

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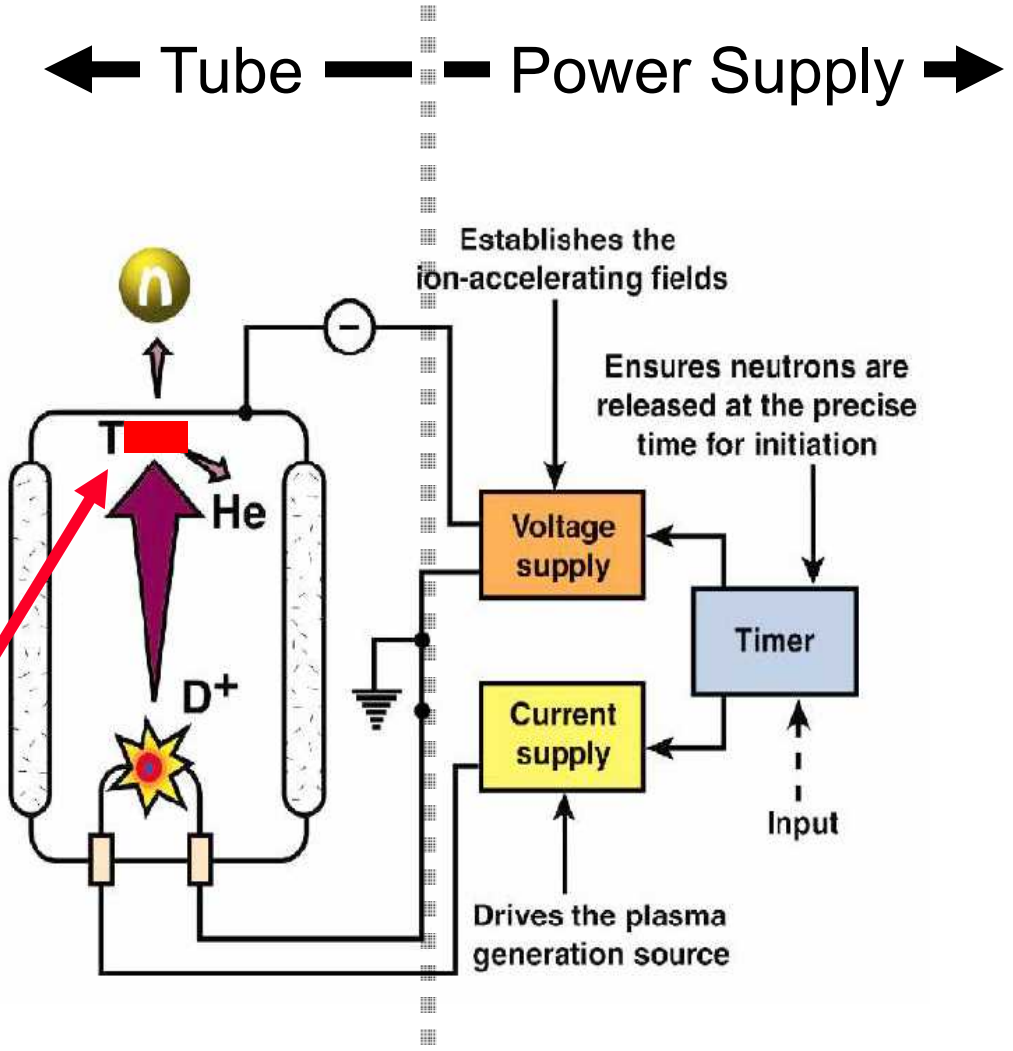
Neutron generators: 50 years of hydrogen storage

Much contemporary research focus on hydrogen storage

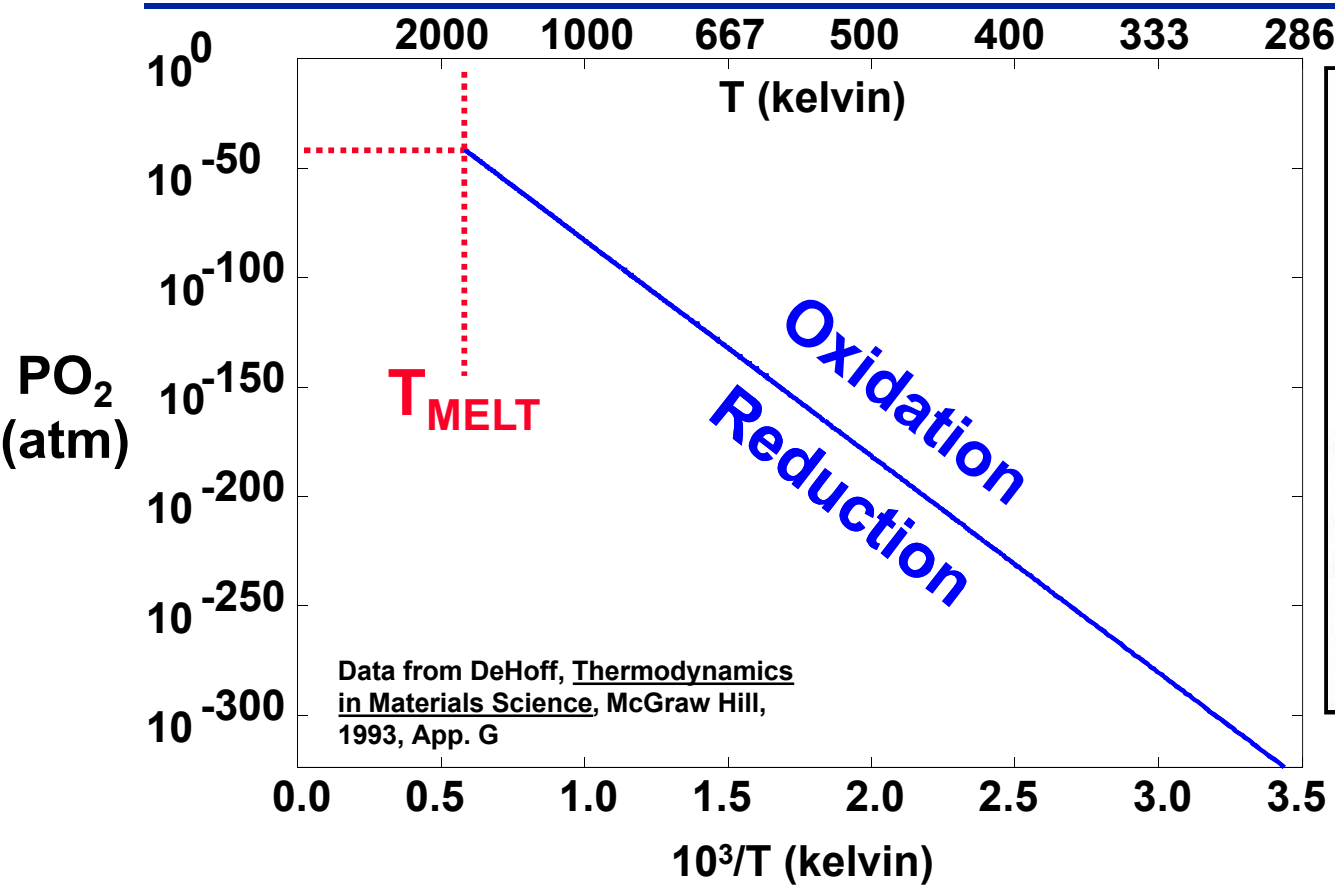
NGs have used solid-state storage of hydrogen since the early Cold War

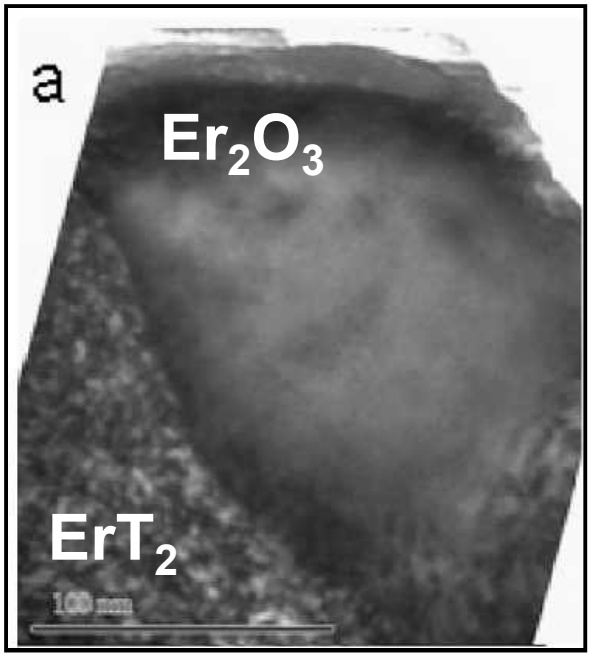


Metal tritide film

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

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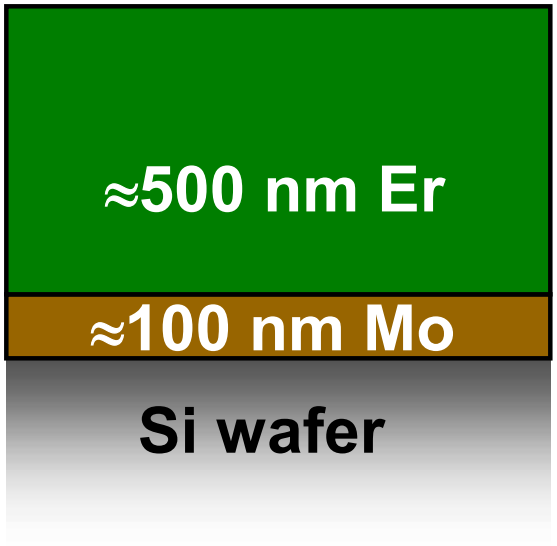
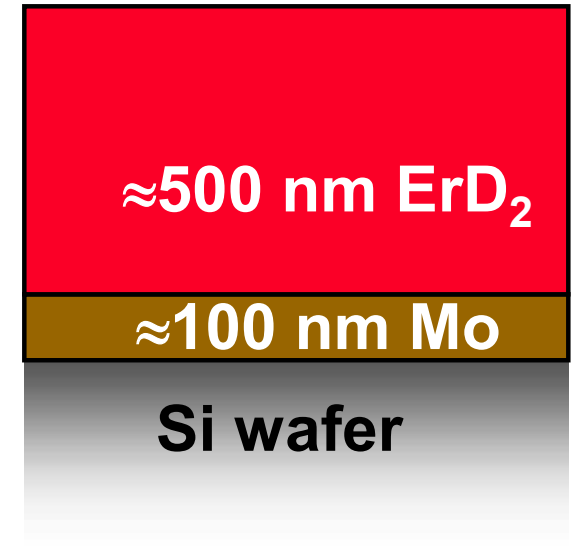
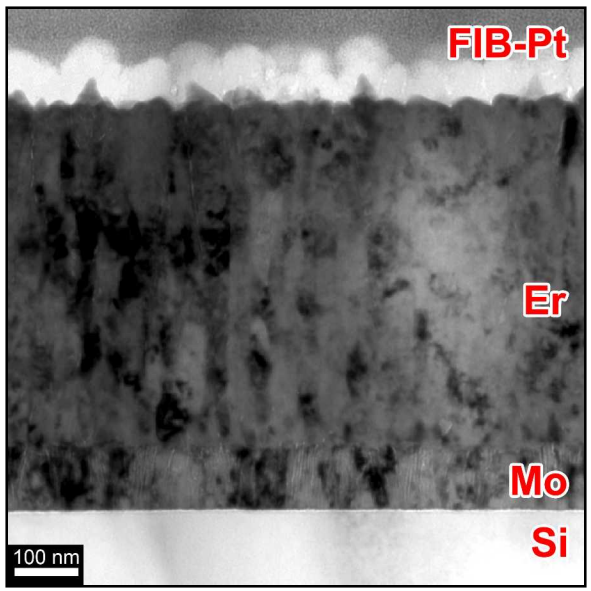
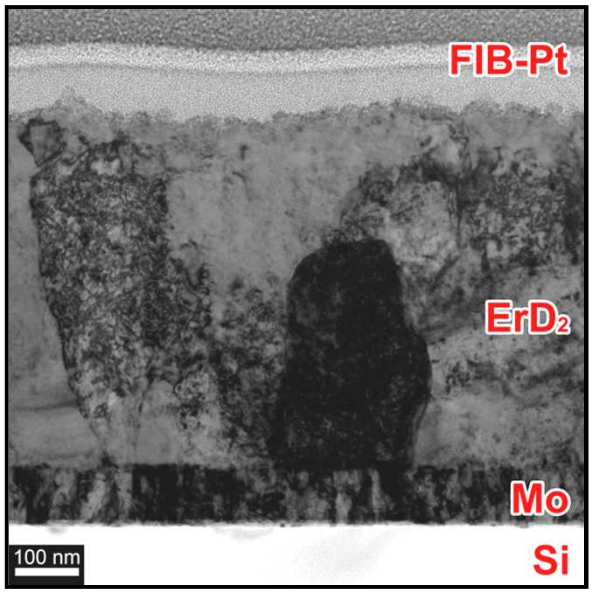
Samples are ErD_2 thin films on Mo // Si



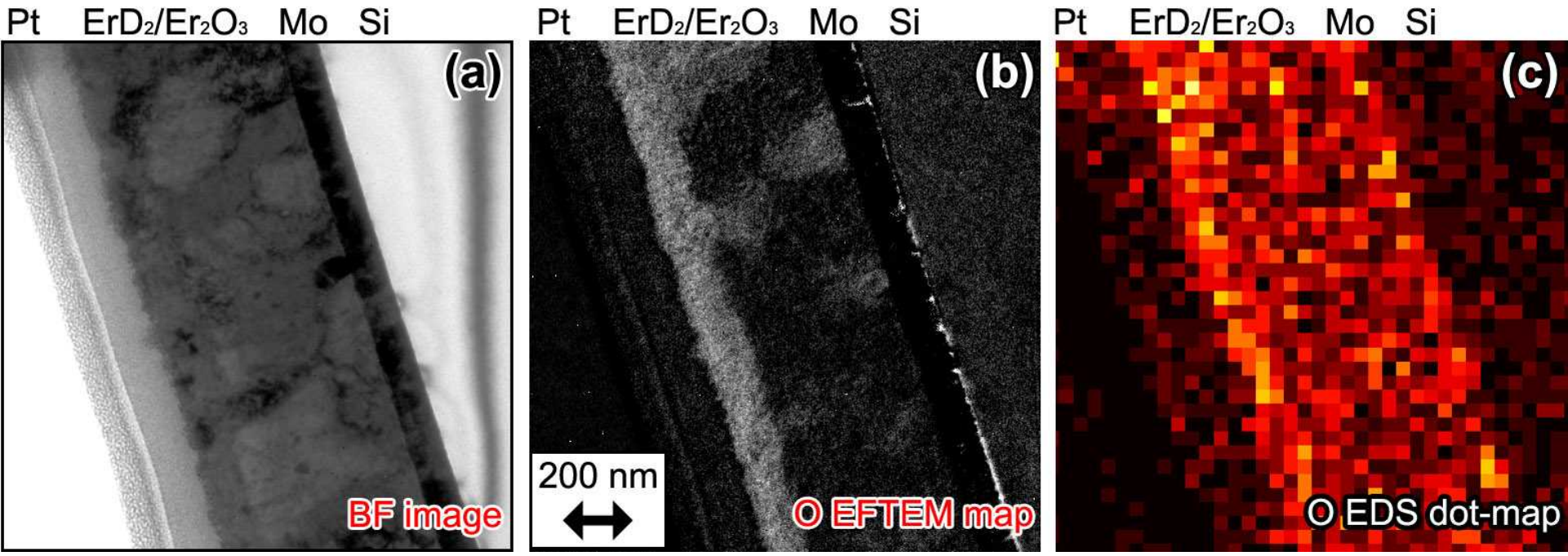
Hydriding







>100 nm of oxide observed via EFTEM



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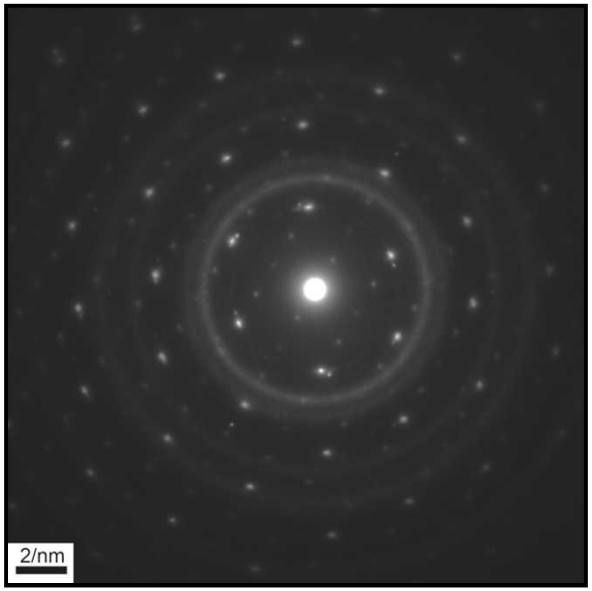
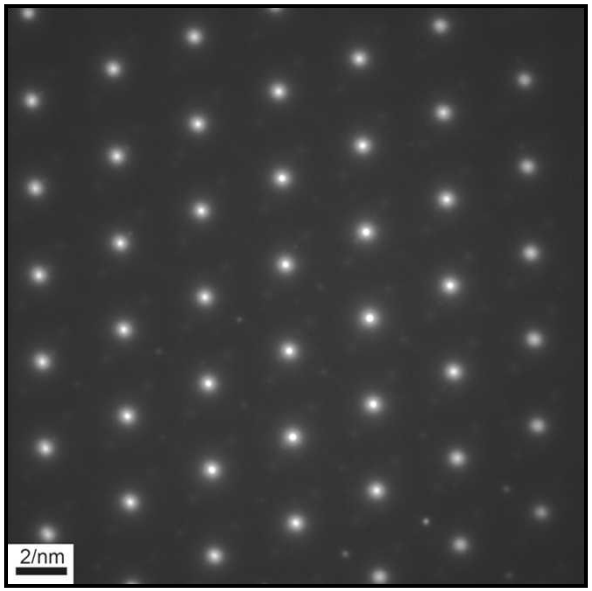
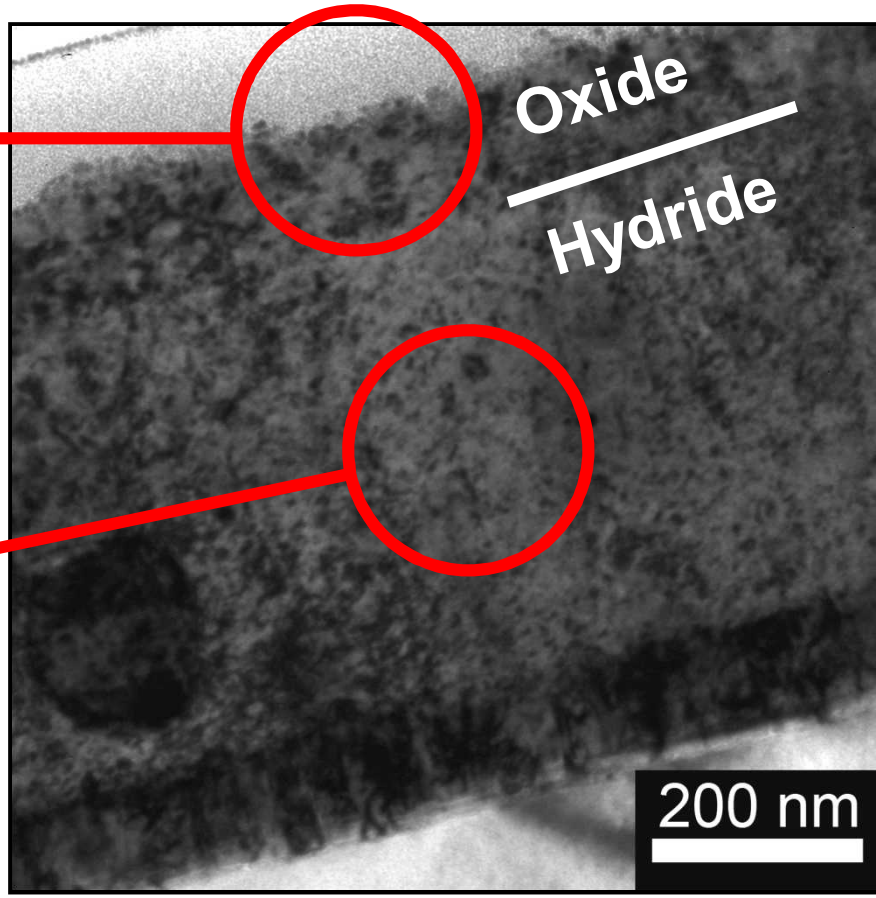
We can use diffraction to verify the layers' crystallography





Surface Oxide (Er_2O_3)

Hydride



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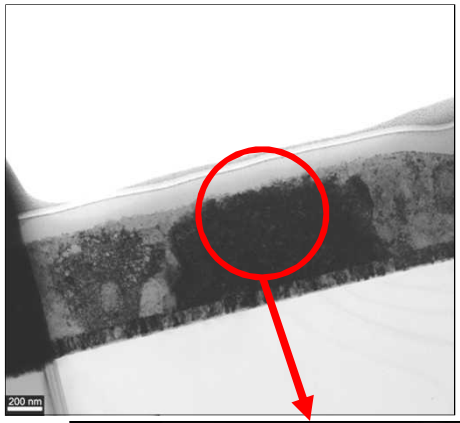
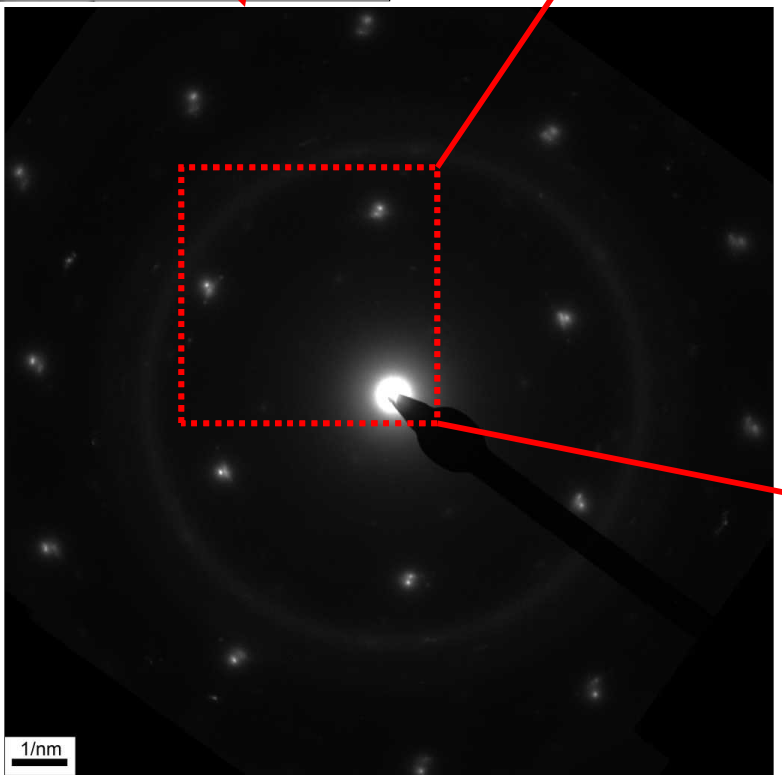
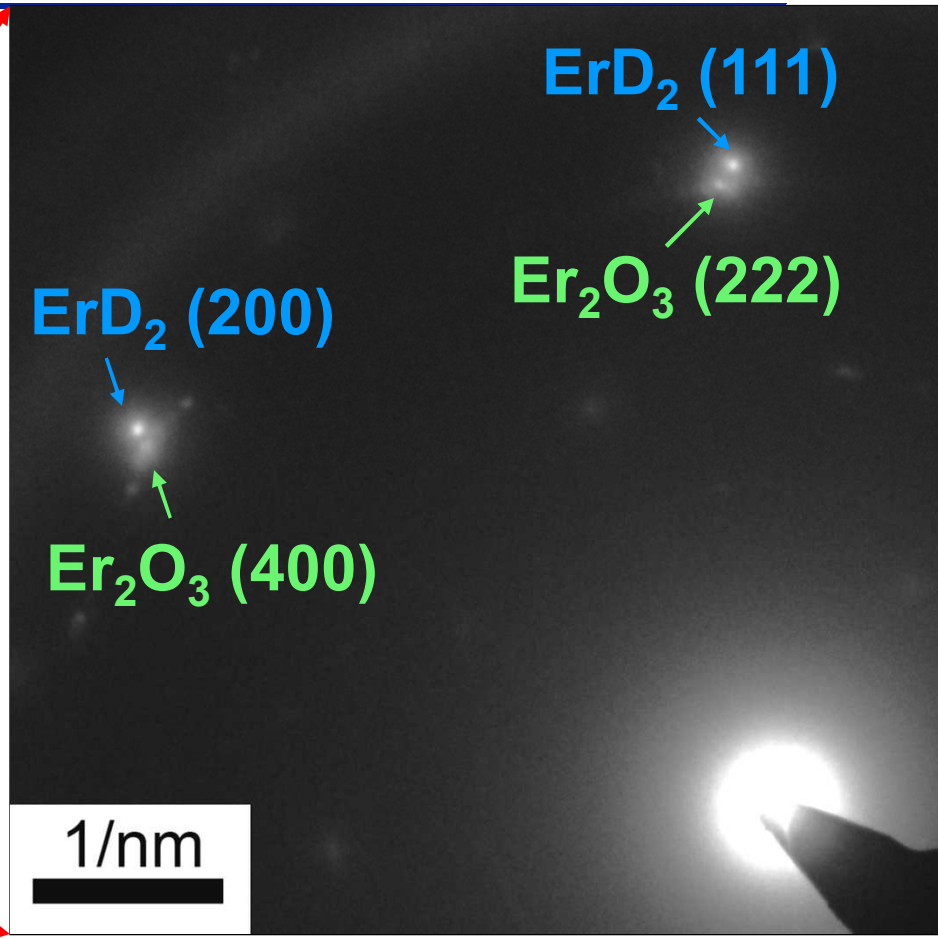
Diffraction shows hydride and oxide have epitaxial orientation







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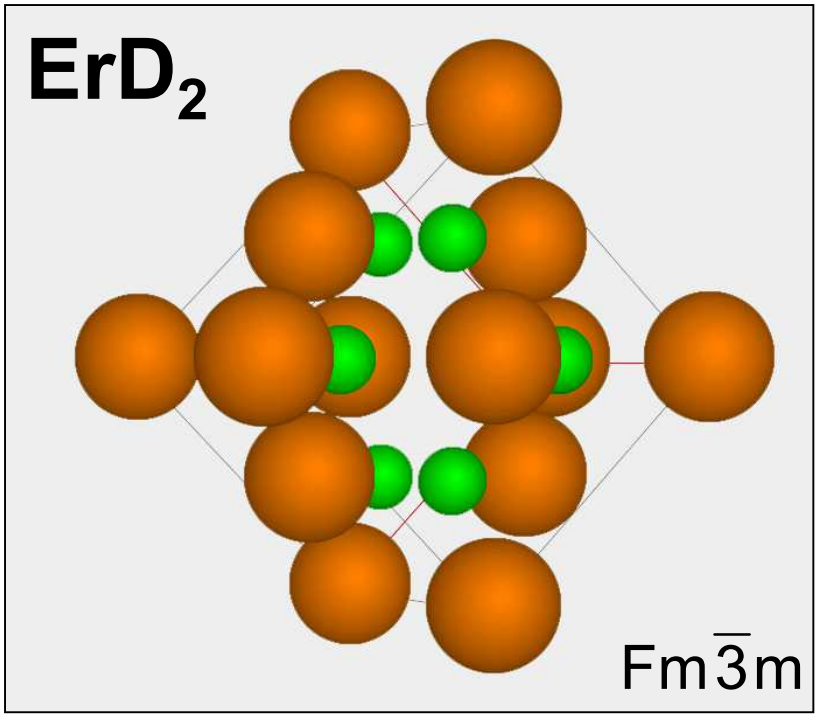
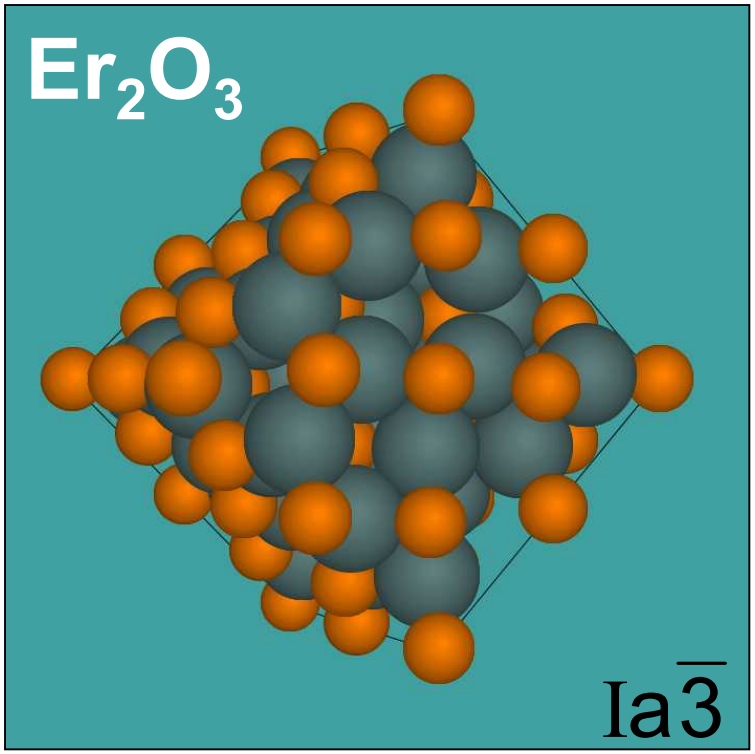
Near-integral lattice mismatch probable cause for epitaxy





a_{ErD2}=0.512 nm

a_{Er2O3}=1.054 nm

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

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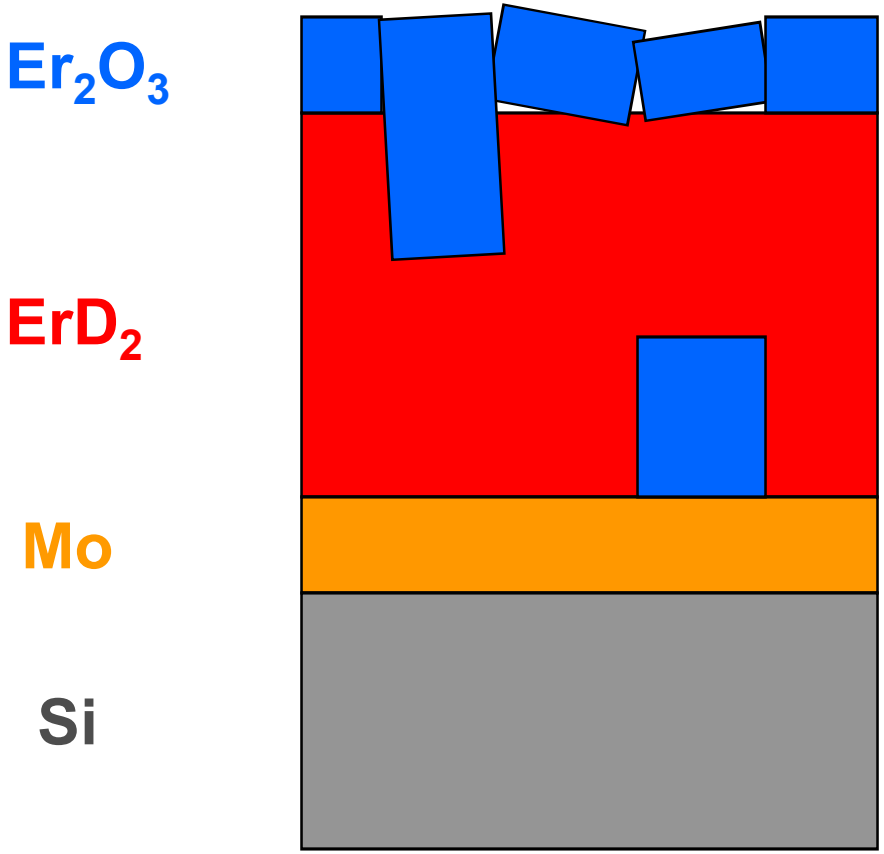
Oxides seen at the surface and penetrating within the film



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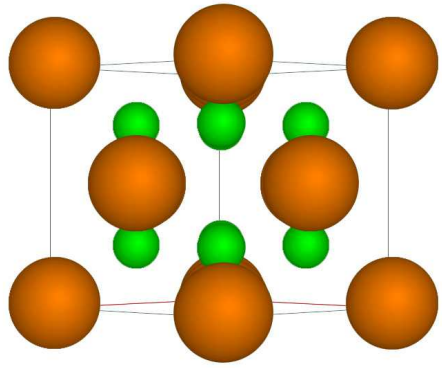
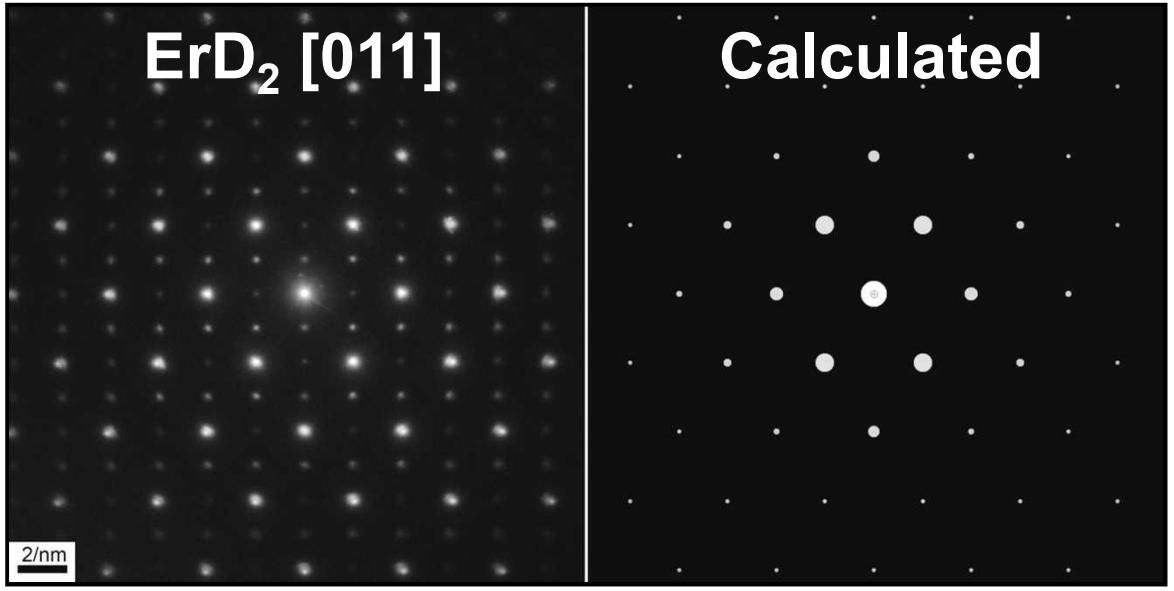
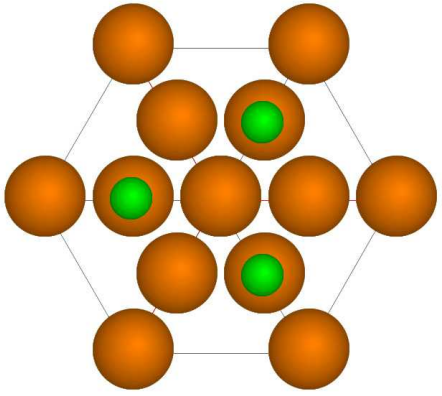
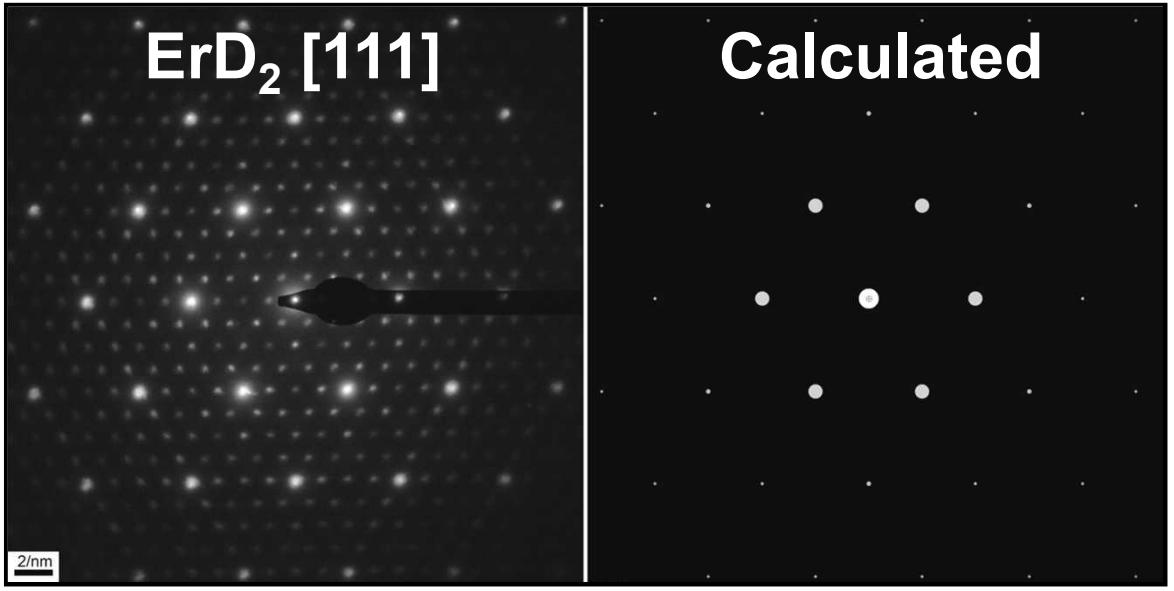
We observe satellite spots that are not predicted from the ErD_2 structure









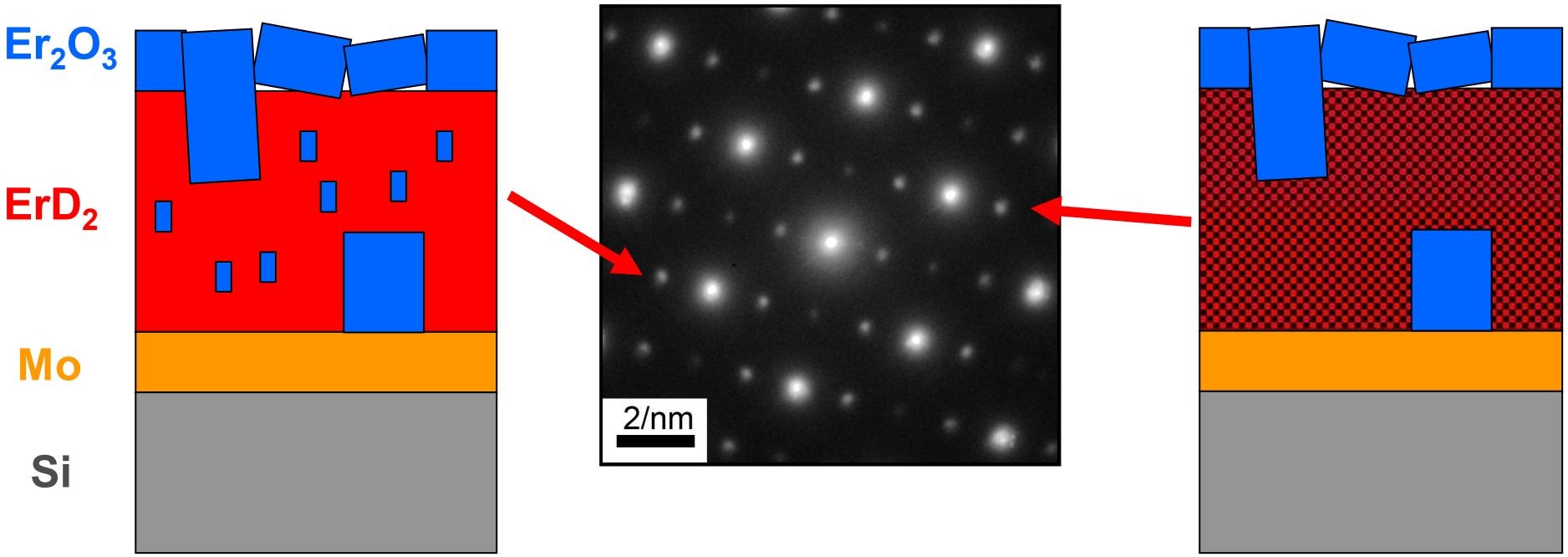
Two hypotheses for satellites: oxide inclusions or hydrogen ordering

Hypothesis 1:

Nano-oxide inclusions

Hypothesis 2:

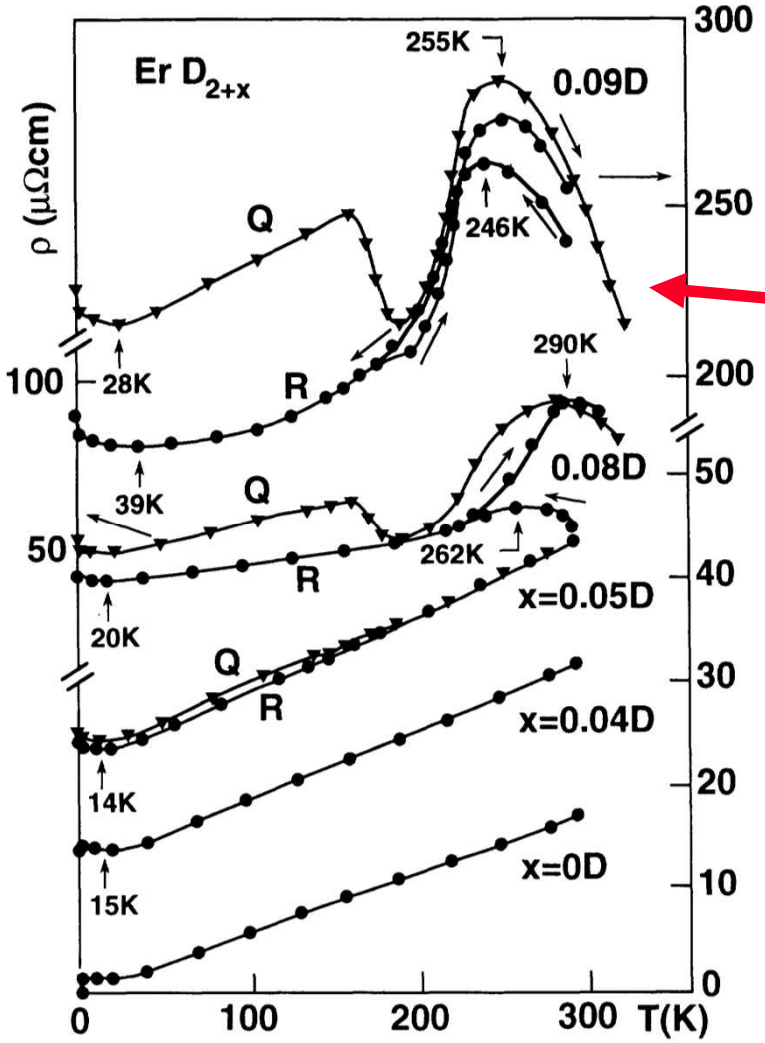
Ordering of D in ErD_{2+x}



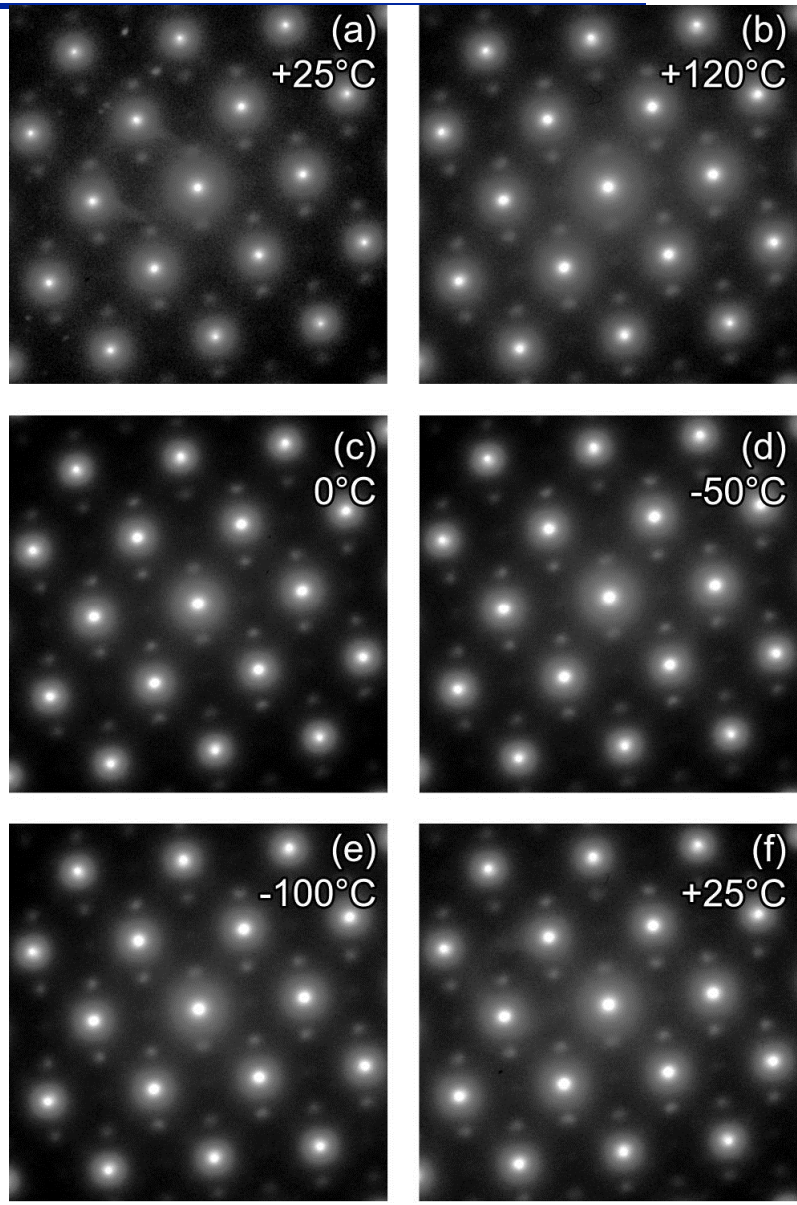
Snow et al., J Nuc Mater V374 (2008), P.147

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

Variable-temperature diffraction rules out hydrogen ordering

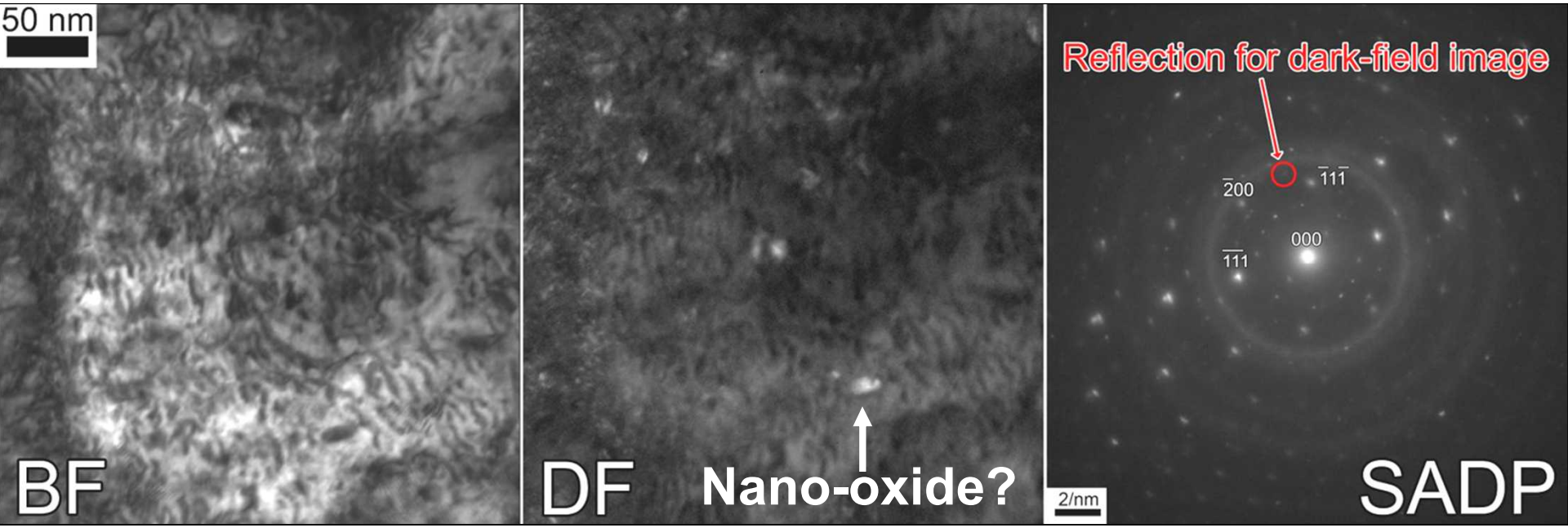


Ordering in $ErD_{2.09}$ disappears at < 25°C

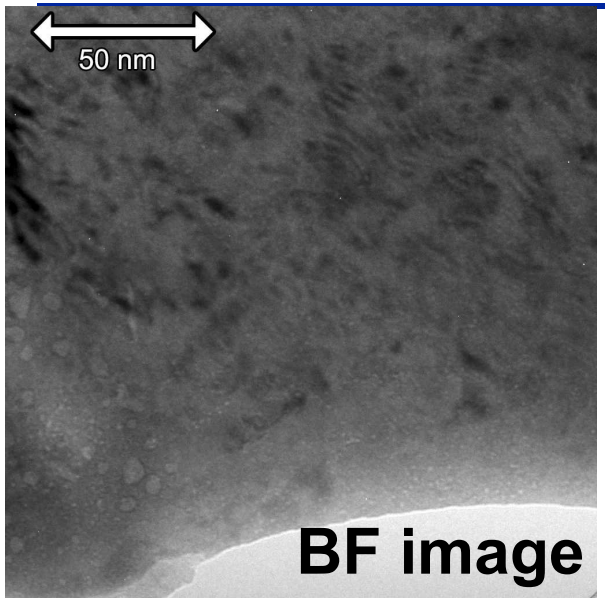


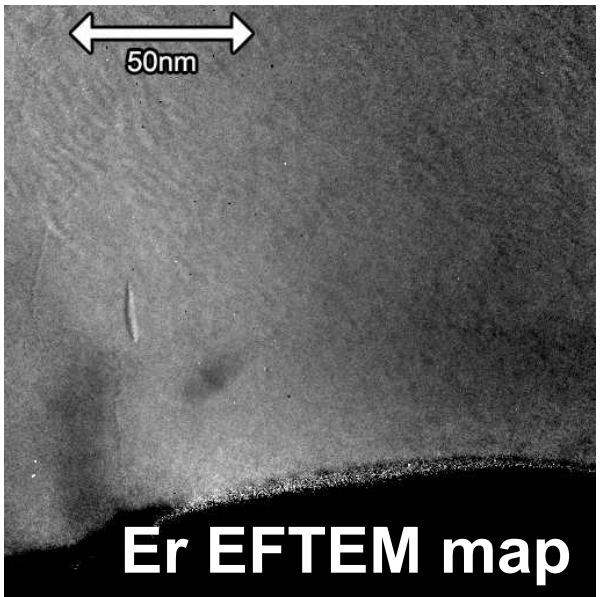
Vajda & Daou, Phys Rev B V49(5), P. 3275, 1994

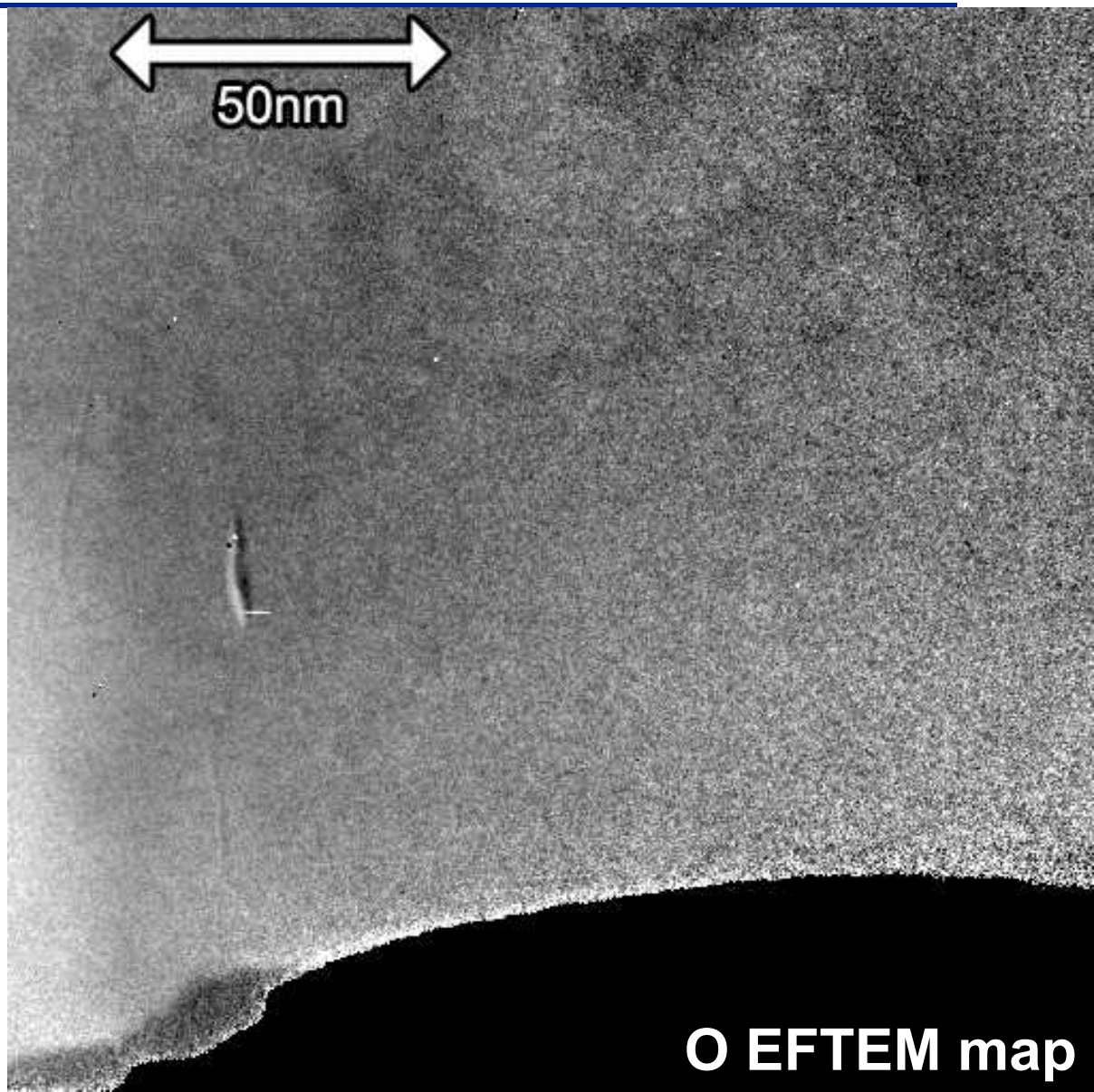
Nano-oxides difficult to observe in TEM



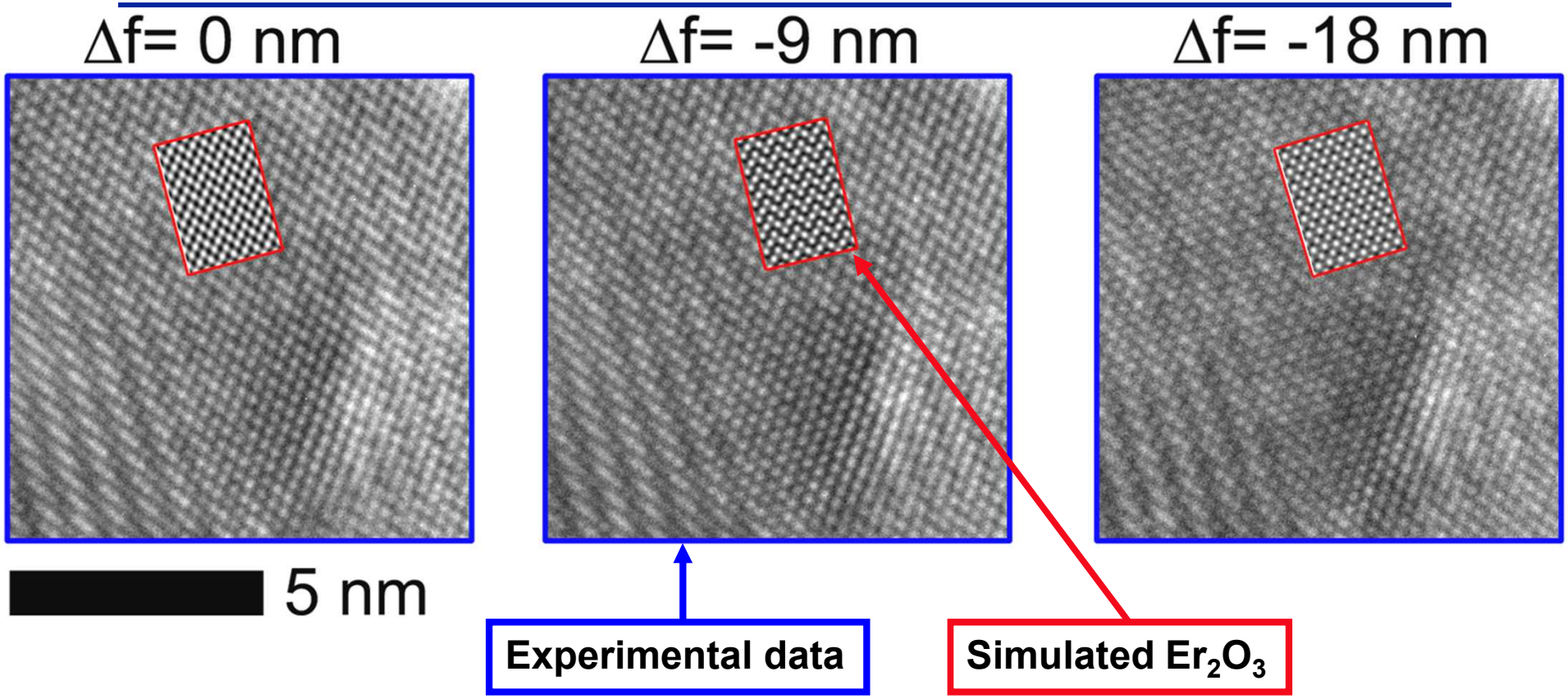
Higher-resolution EFTEM shows no obvious oxide particles







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

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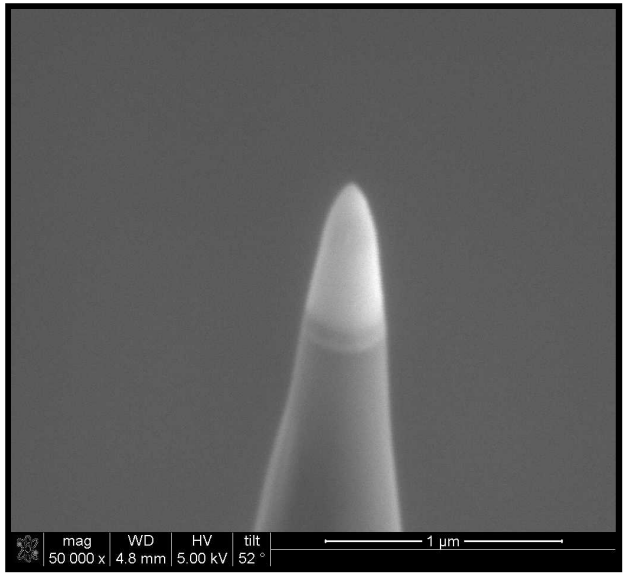
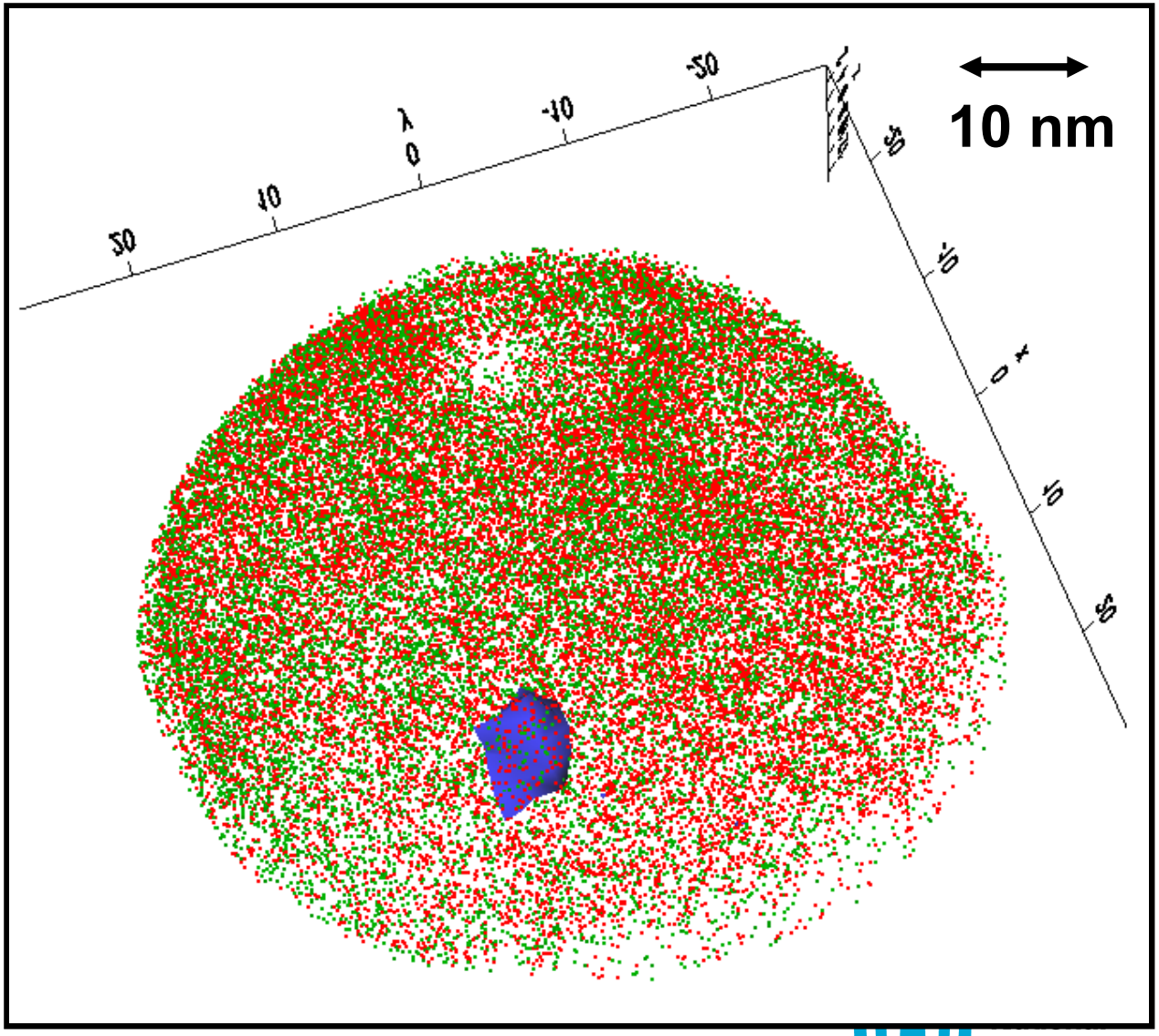
Preliminary atom probe results: small oxides observed



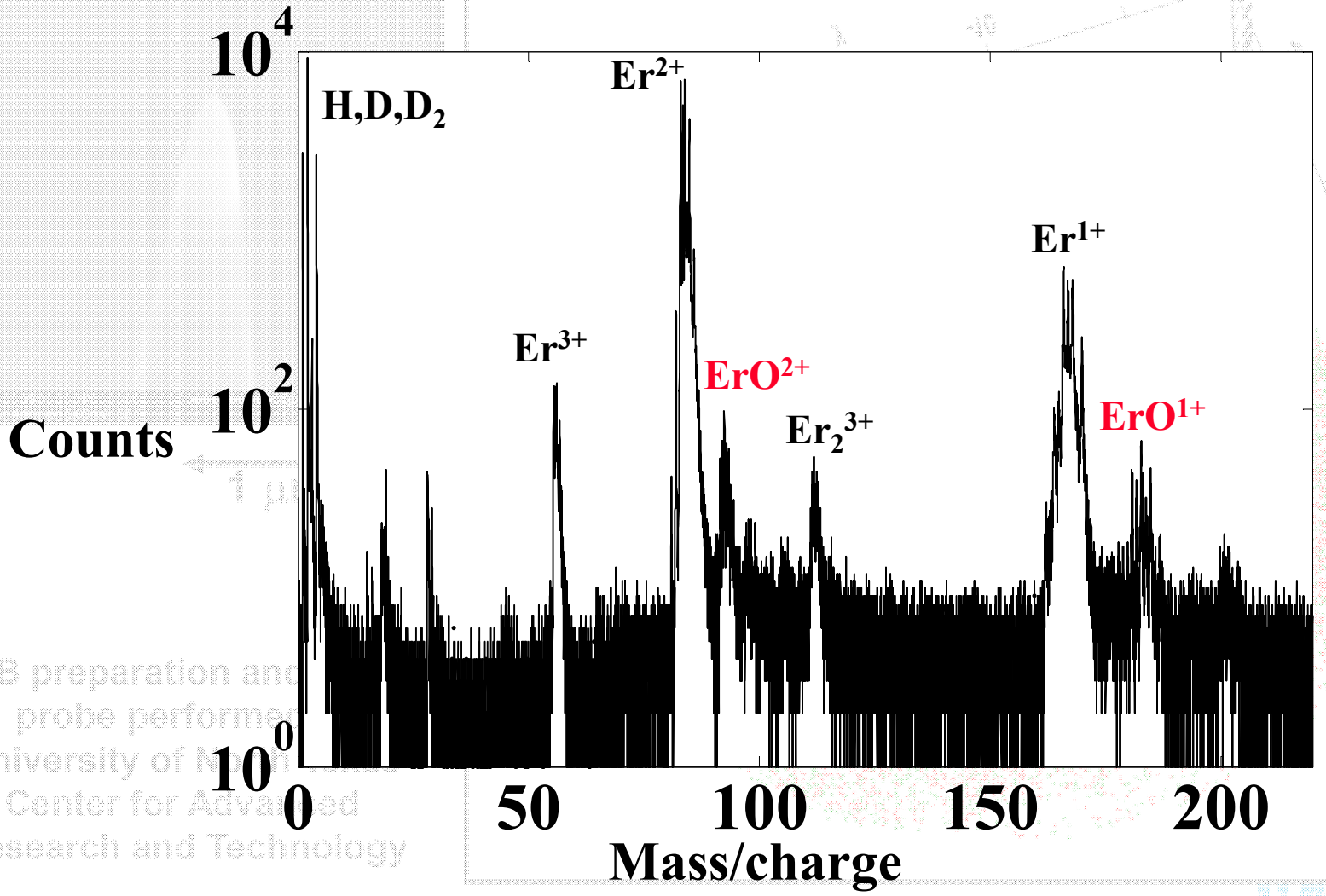
1 µm



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