



Hydrogen and Helium Isotopes in Materials Conference
February 6-7, 2007

“Unit Cell Expansion in ErT₂ Films”

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Overview

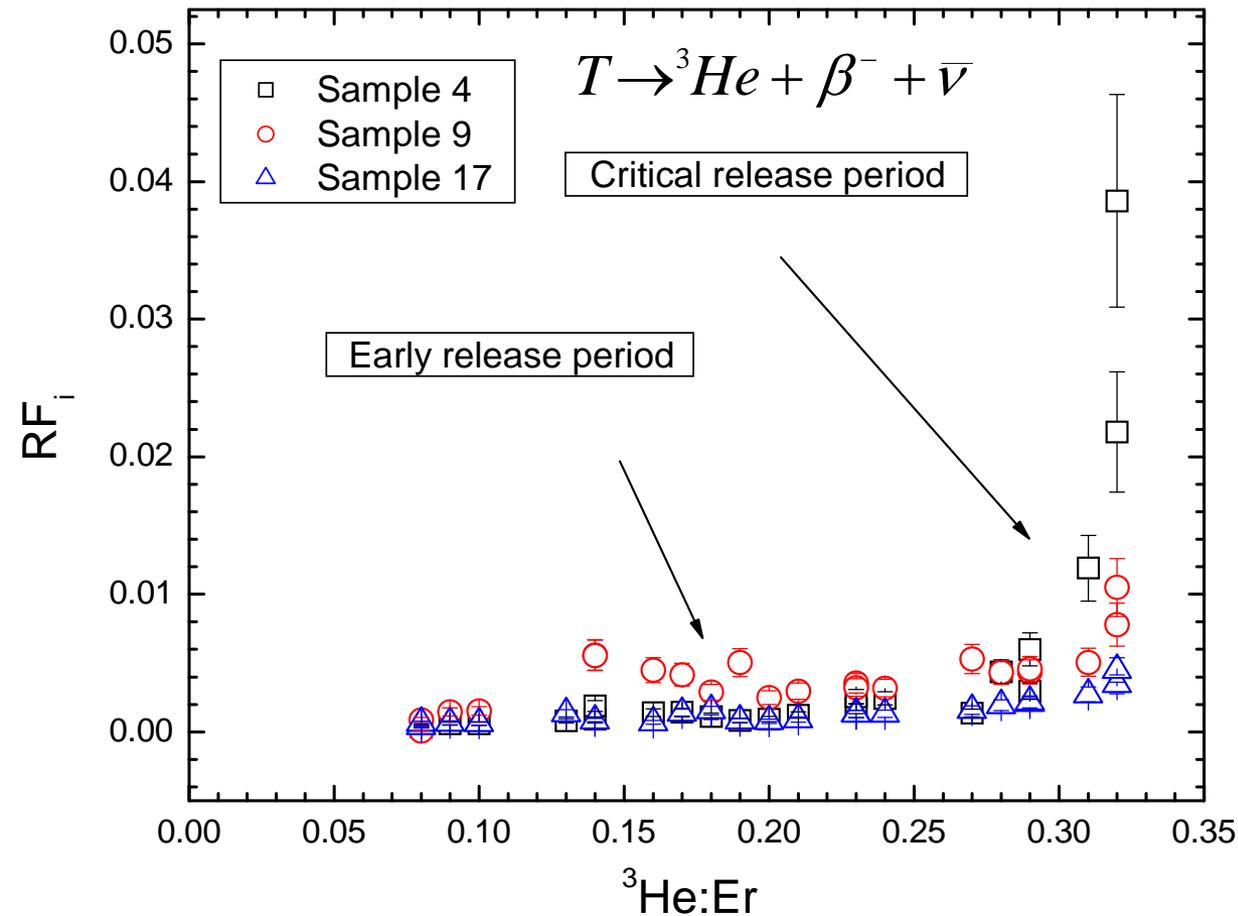
- **Introduction**
- **Experimental**
- **Results**
 - **Expansion data with time**
 - **Texture analysis and microstructure**
 - **Macro-strain**
 - **Skewed peaks**
- **Emerging model**
- **Summary**

Research objectives

- **Research goal:** to obtain a scientific and technical basis for understanding tritium decay in Er-tritide.
 - ^3He Bubble formation and growth
 - Influence of Microstructure on ^3He bubble retention
 - Texture
 - Macrostrain
 - Structural analysis of ErT_2 phase
 - Lattice parameter values

Focus of this presentation

Monitoring of ^3He release fraction shows an Early Release and Critical Release period

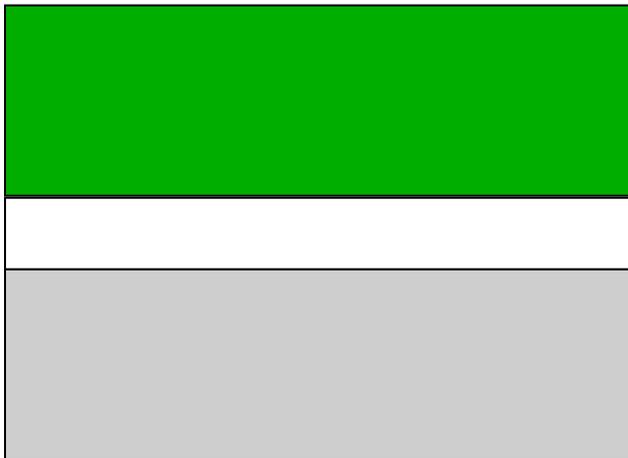


Typical ^3He release characteristics indicate most ^3He generated remains in lattice.

Question:
How will the presence of ^3He alter the ErT_2 structure?

Experimental

- E-beam PVD 5000Å Er/1000Å Mo/Si
- Tritide layer formed by exposure T_2 gas.
- Characterized via IBA, TEM and XRD.

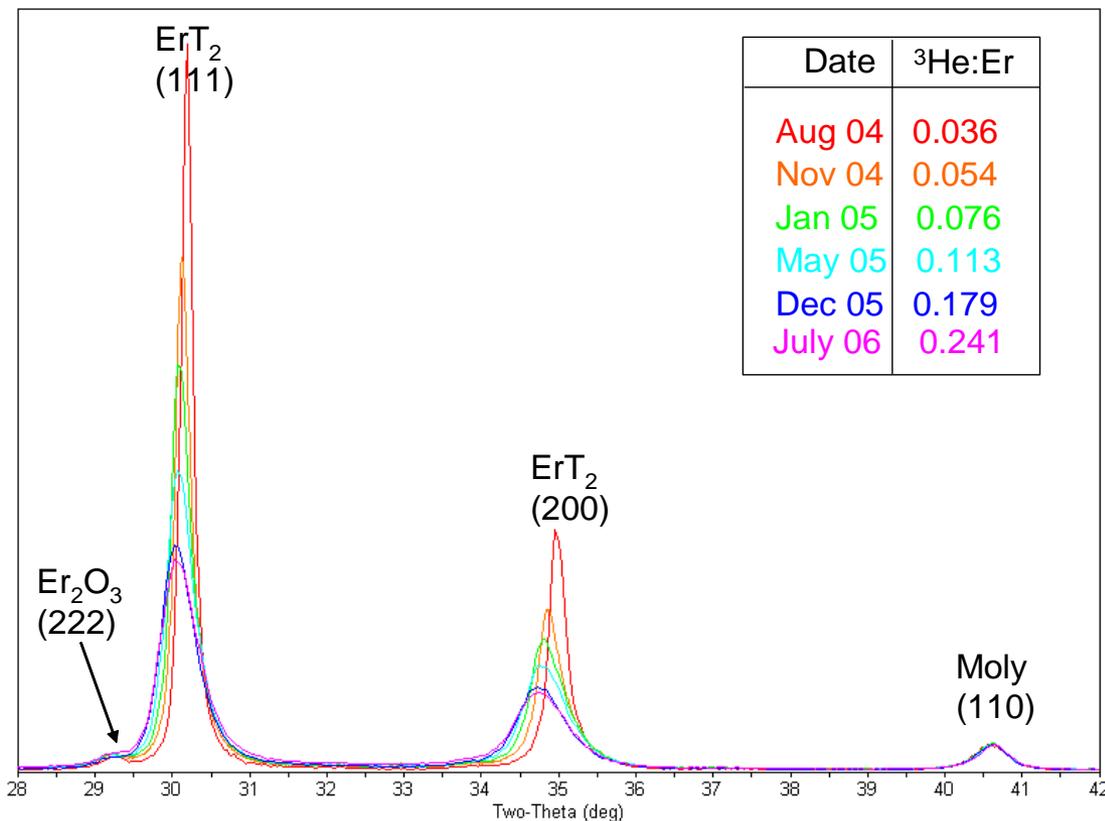


ErT_2 thin film

Molybdenum buffer layer

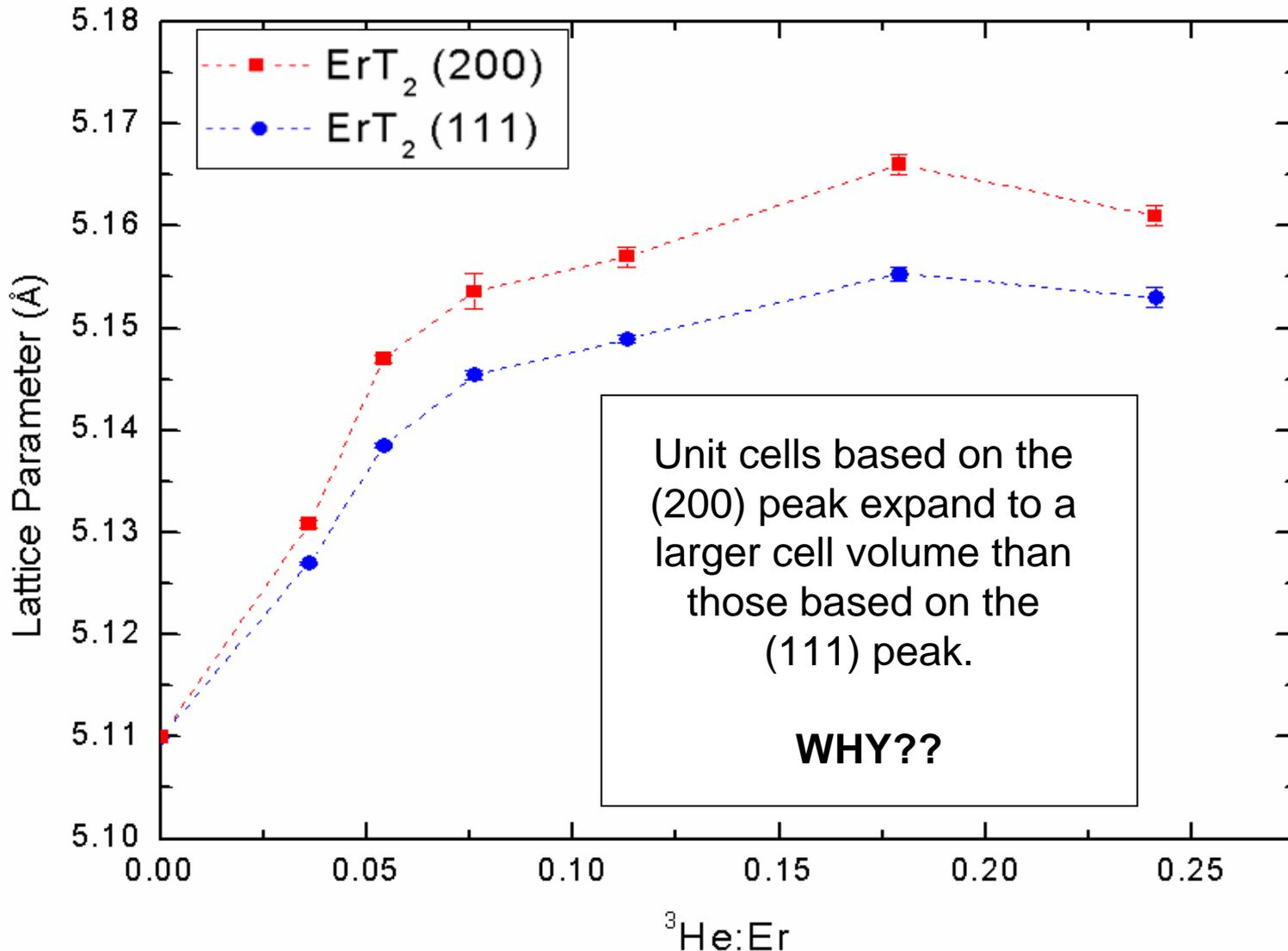
Si (111) substrate

Monitoring ErT_2 films with time shows unit cell expansion for standard $(\theta-2\theta)$ XRD scans

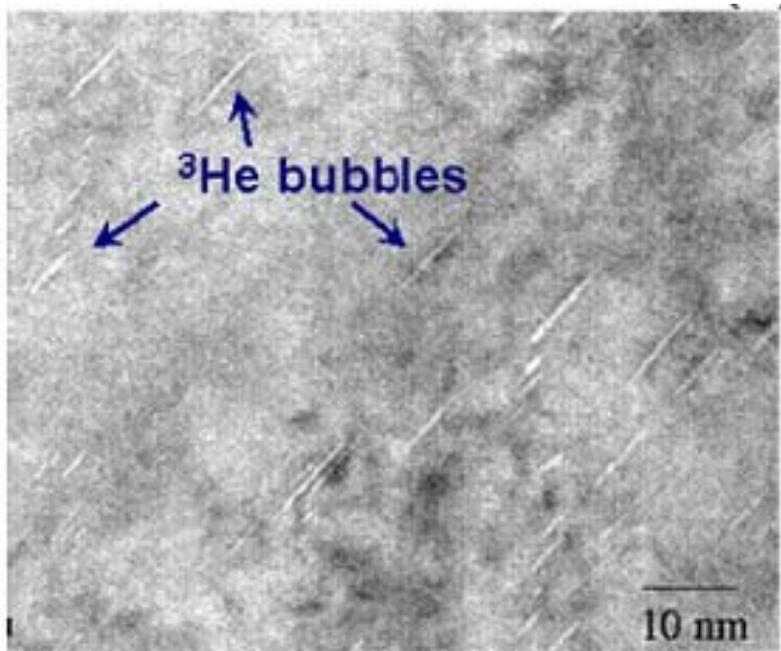


- ErT_2 peaks
 - broaden
 - shift to larger d-spacing
 - show skew
- Moly peaks
 - don't change

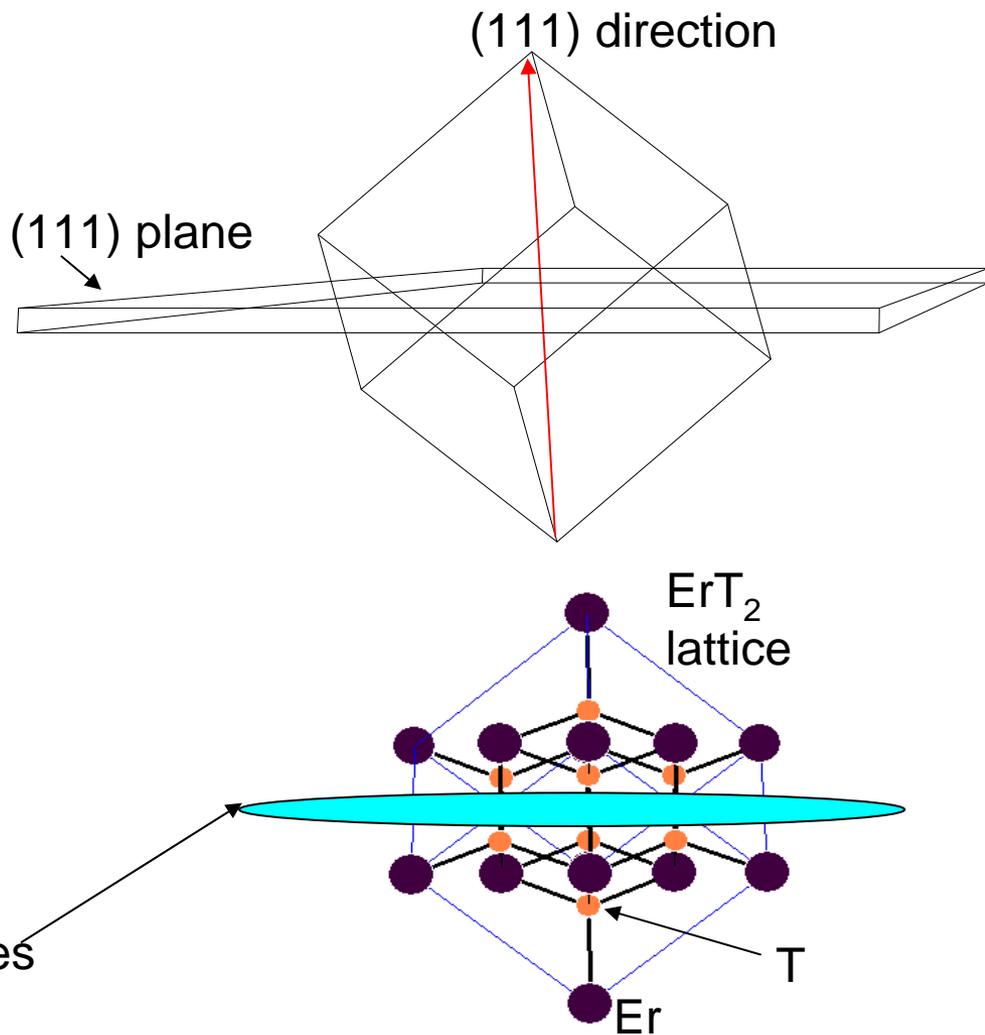
The unit cell lattice parameter for ErT_2 displays an *hkl dependence* of expansion with time



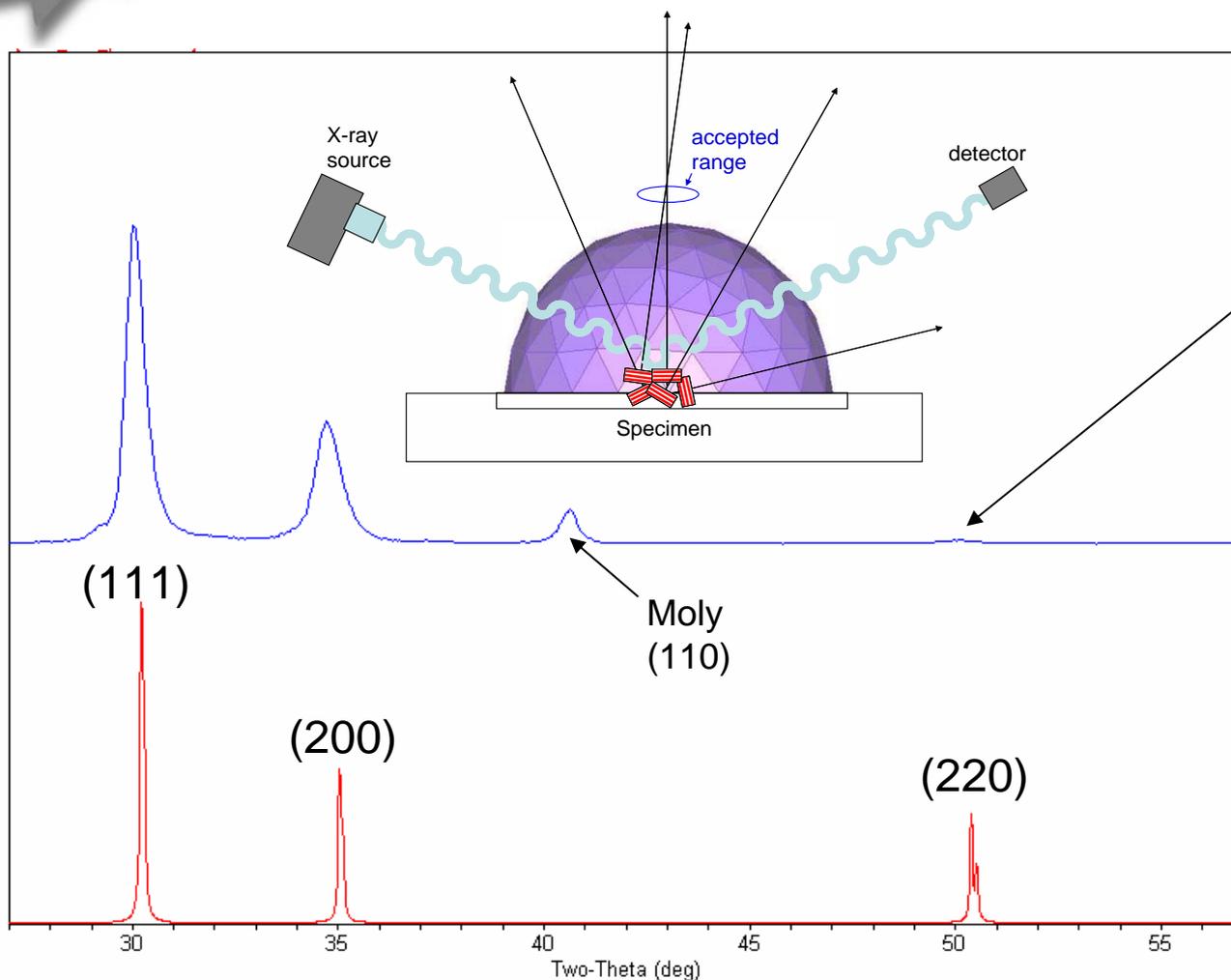
TEM analysis has demonstrated that ^3He bubbles form along the (111) planes in the fluorite structure



^3He bubbles are long thin plates that propagate along the (111) planes in the Fluorite-type ErT_2 lattice



Standard θ - 2θ XRD analysis only measures diffraction planes that are in the plane of the film

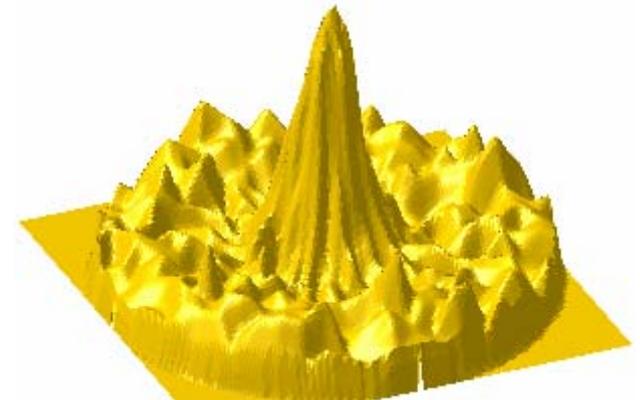
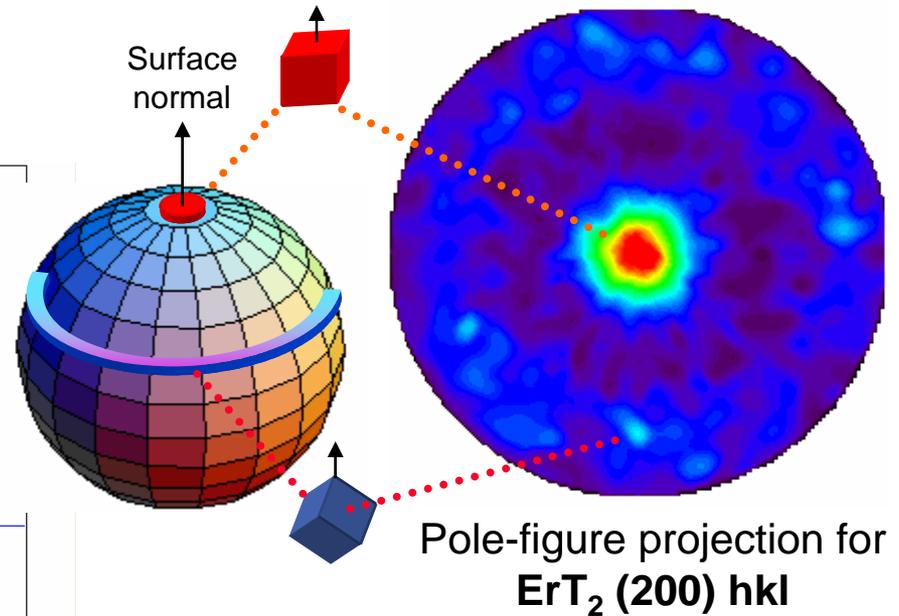
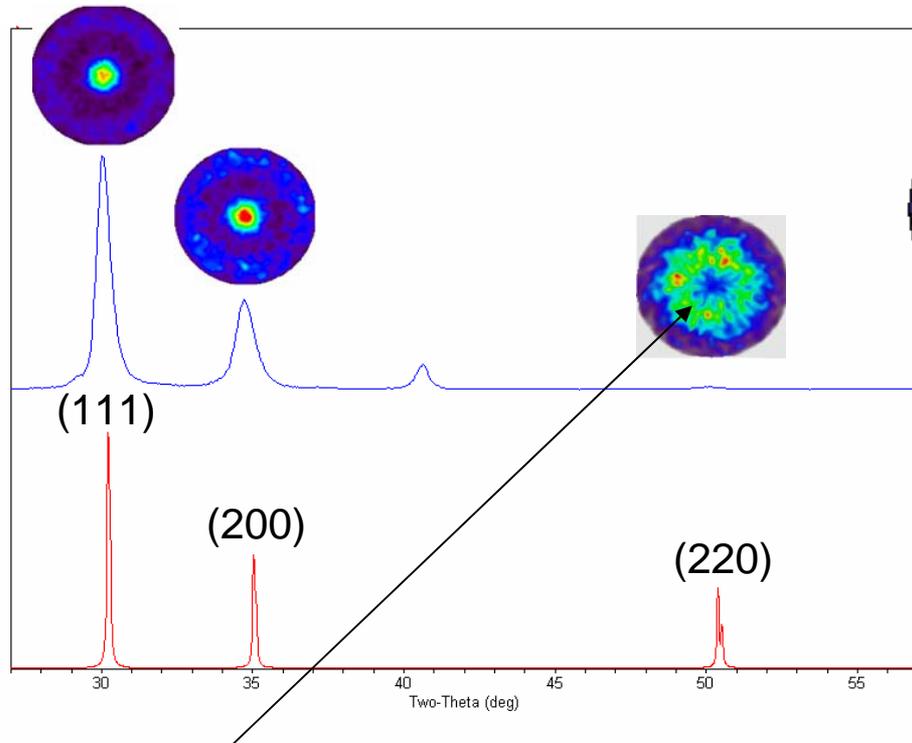


Peak intensity of ErT_2 (220) in observed pattern is suppressed: **Texture effect**

Observed ErT_2 XRD (Dec '05)
 $^3\text{He}:\text{Er} = 0.179$

Simulated ErT_2 XRD pattern

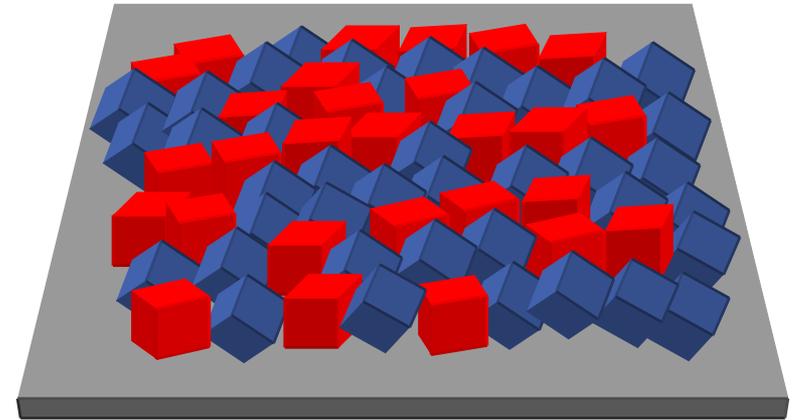
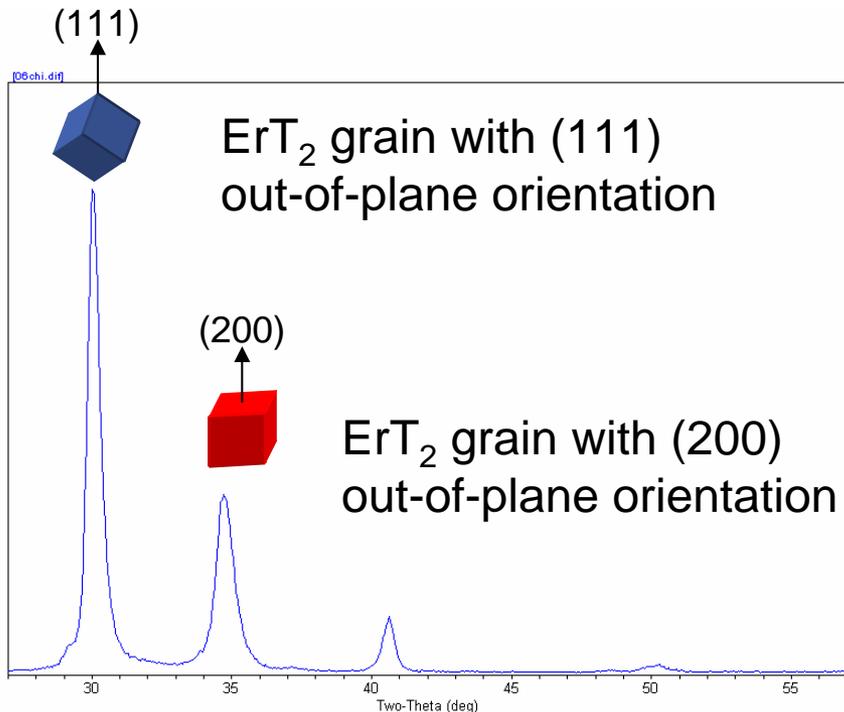
Pole-figure analysis confirms bi-modal (111)/(200) out-of-plane texture, in-plane fiber texture



Ring of intensity in the ErT_2 (220) Pole-figure is critical for accurate diagnosis of texture

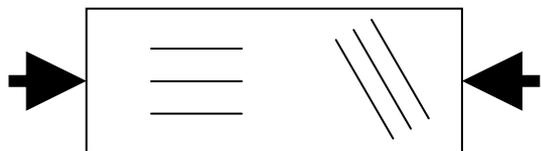
Texture analysis yields an important picture about the microstructure of the ErT_2 films

For simplicity, let us say that the grain morphology is the same shape as the unit cell symmetry (i.e. cubic).

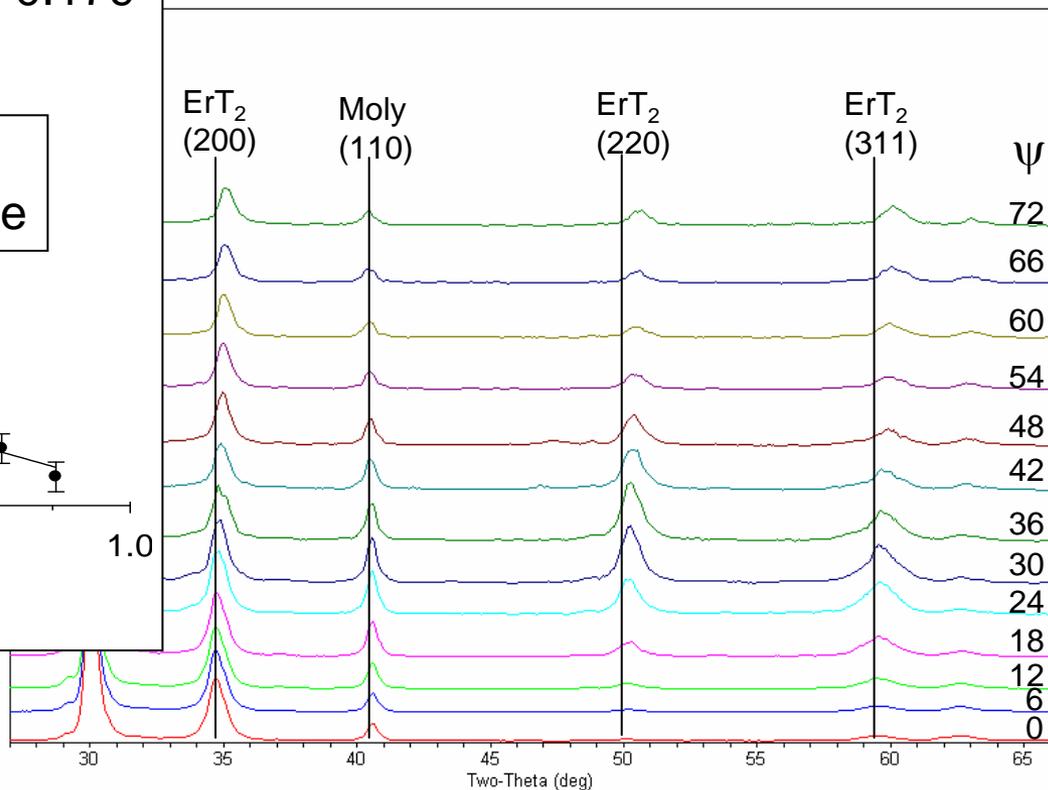
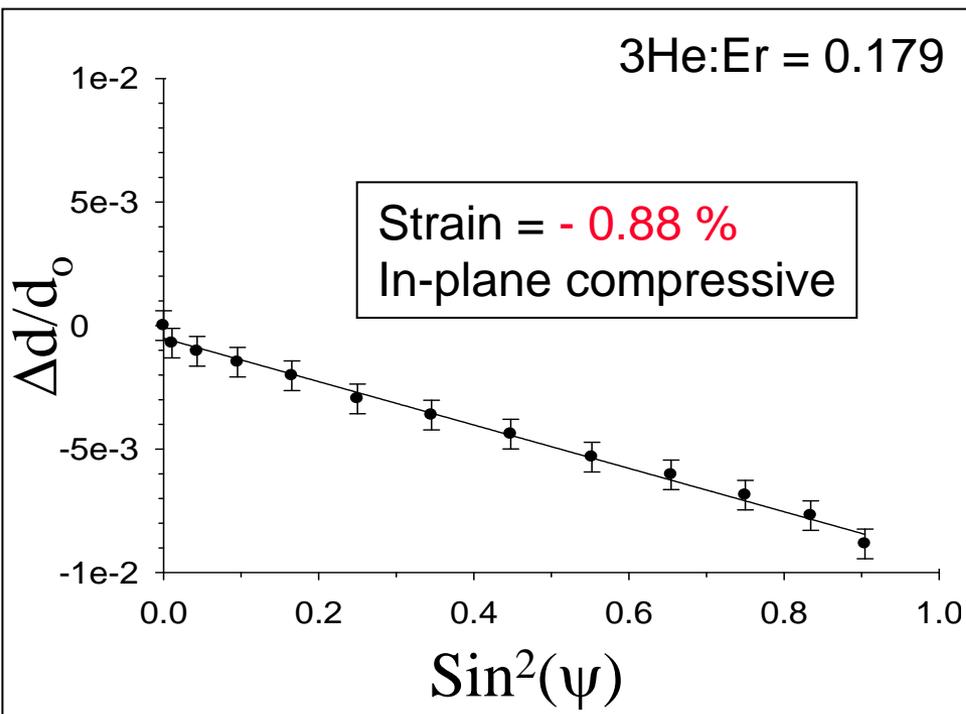


Schematic showing a *bi-modal* (111) and (200) out-of-plane preferred orientation for ErT_2 grains.

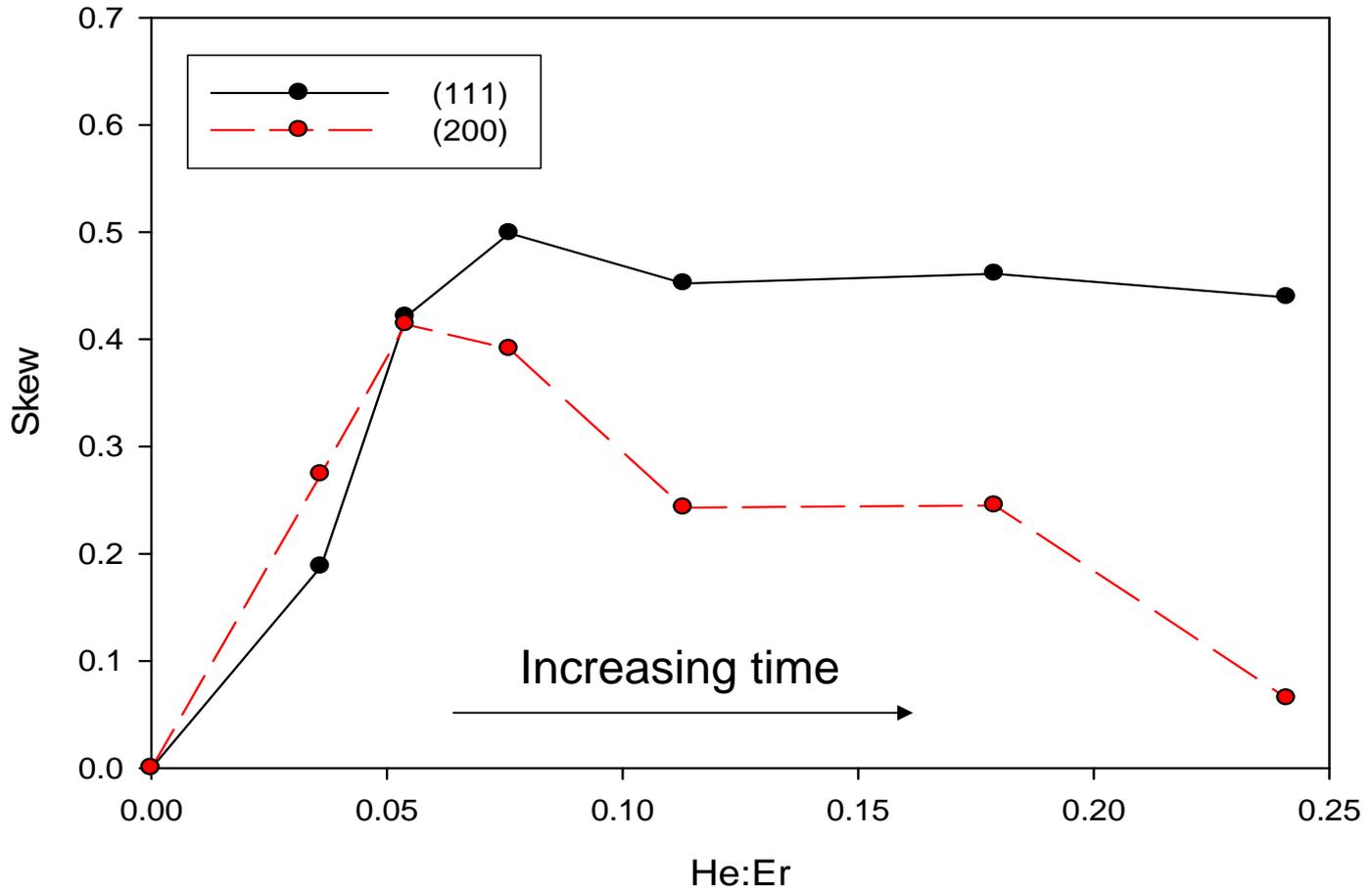
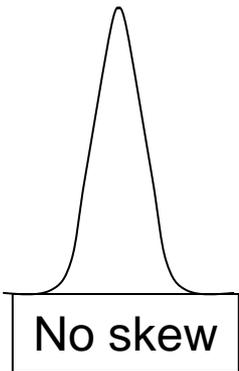
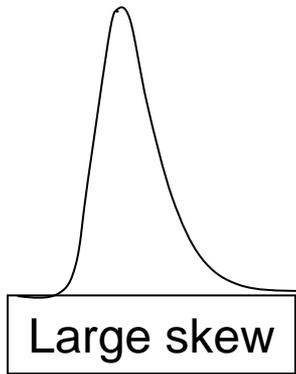
Sin²ψ analysis revealed significant in-plane strain in the Dec '05 film



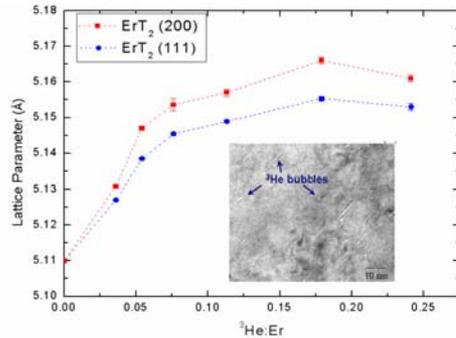
An in-plane compressive force develops because ErT₂ grains wish to expand but the film geometry limits this. Out-of-plane expansion is not likewise hindered.



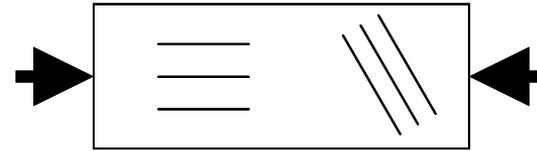
(111) oriented out-of-plane grains saturate at a high skew value, while the (200) out-of-plane grains re-normalize to a more symmetric peak profile.



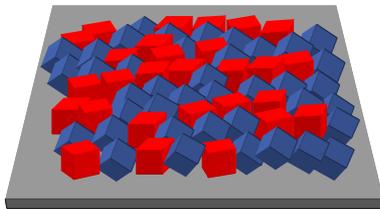
Summary of observations for our analysis: what does it tell us?



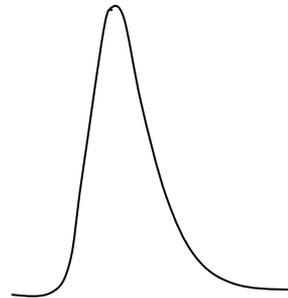
hkl-dependent
out-of-plane expansion



In-plane compression



Bi-modal texture



hkl-dependent
skew behavior

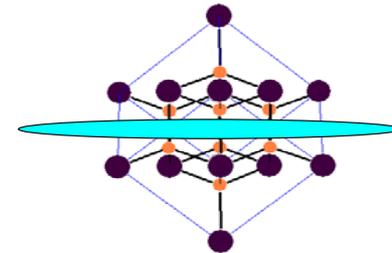
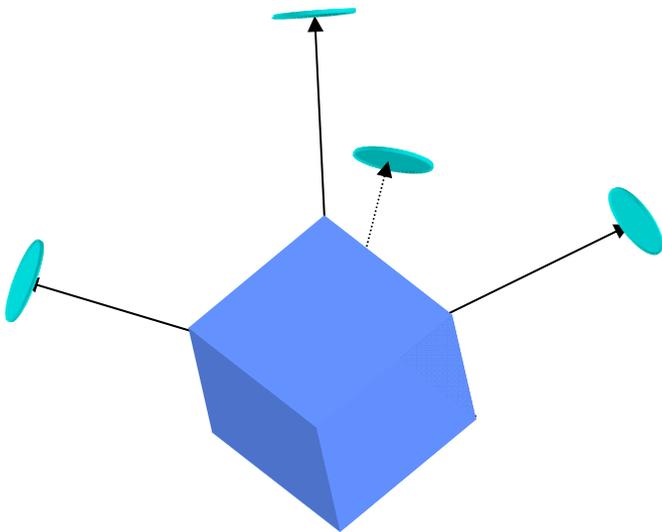


Plate-like ^3He bubbles
along ErT_2 (111) plane

Our developing theory

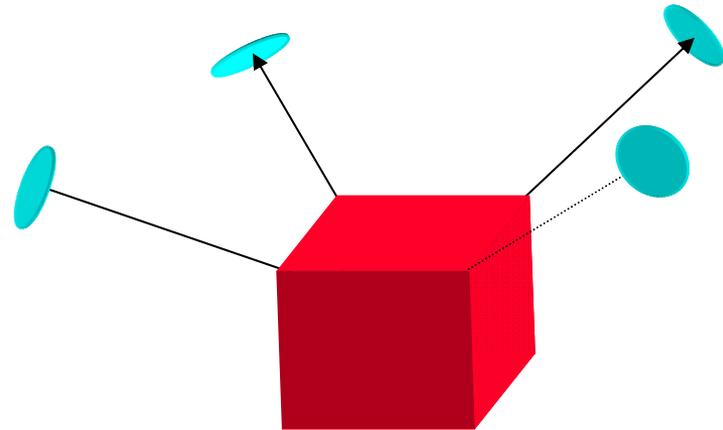
(111) out-of-plane grains

- One (111) direction out-of-plane
 - expands easily
- Three additional (111) directions just 20° from in-plane
 - hindered expansion



(200) out-of-plane grains

- All four (111) directions have **equivalent components** both in and out-of-plane
 - more uniform expansion
 - less internal opposition from other (111) directions





Summary

- Different expansion rates and magnitudes are observed in the (200) out-of-plane grains as compared to (111).
- Our ErT_2 films showed a bimodal (111)/(200) out-of-plane texture.
- In-plane compressive strain exists in ErT_2 films with significant Tritium decay.
- Peak skew with T decay is markedly different for (111) and (200) out-of-plane grains.
- Observations can be explained in terms of ^3He bubble expansion along (111) planes in the ErT_2 lattice.
- This effect might result in different ^3He release characteristics for the differing grain orientations.