

# TIME-RESOLVED X-RAY DIFFRACTION AT EXTREME CONDITIONS

ATOMIC

MICRO

BENCH

SYSTEMS

DEPLOYMENT

## IMPACT

Interrogating chemical and structural transformations of critical materials at a wide range of extreme pressures and temperatures.

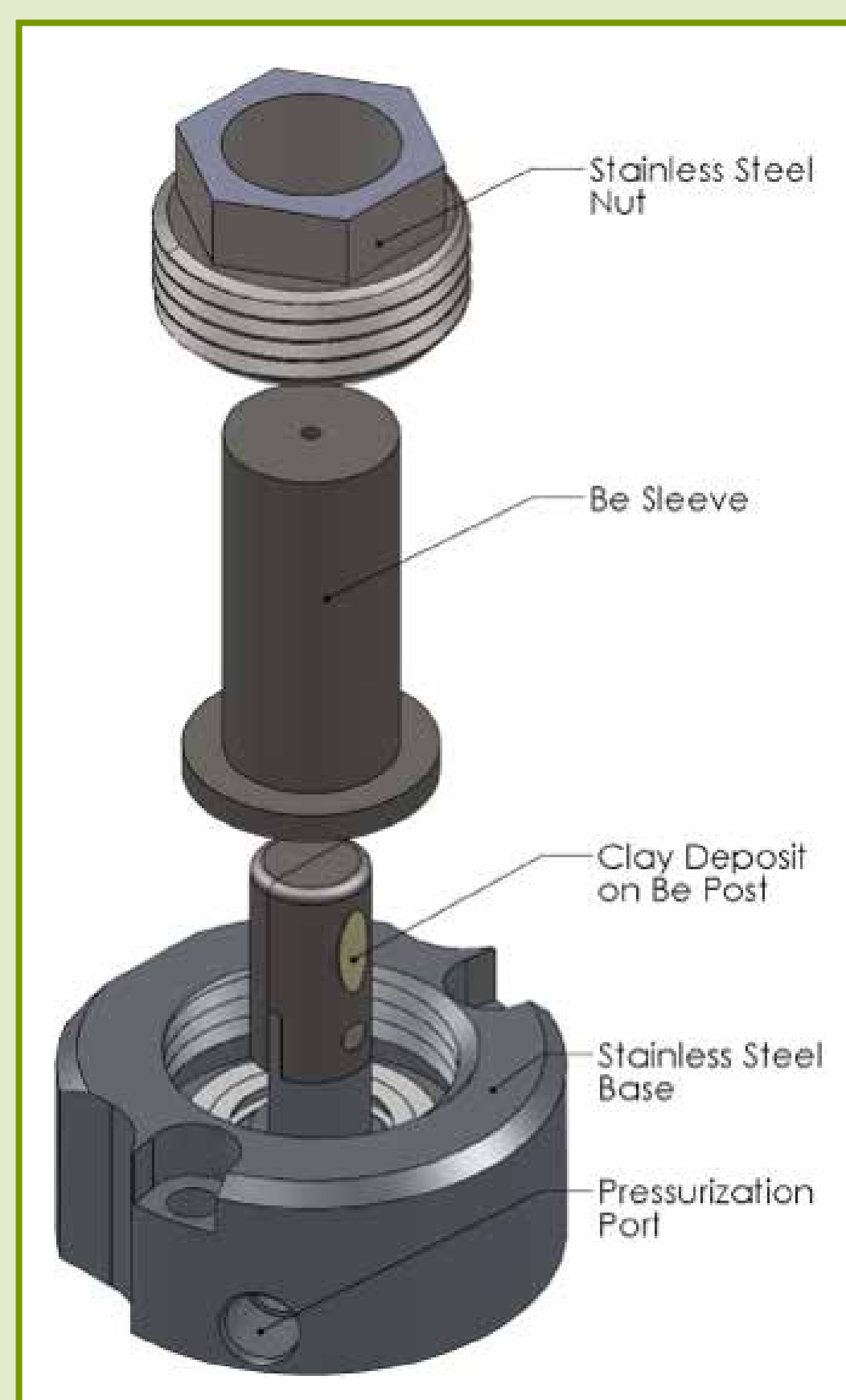
## APPLICATION

- Optimize hydrocarbon and geothermal resource recovery
- Synthesis and monitor performance of critical energy materials
- Isolate and characterize transient metastable materials
- Long-term predictions of subsurface CO<sub>2</sub> fate and transport
- Hydrothermal stability of architected capture materials

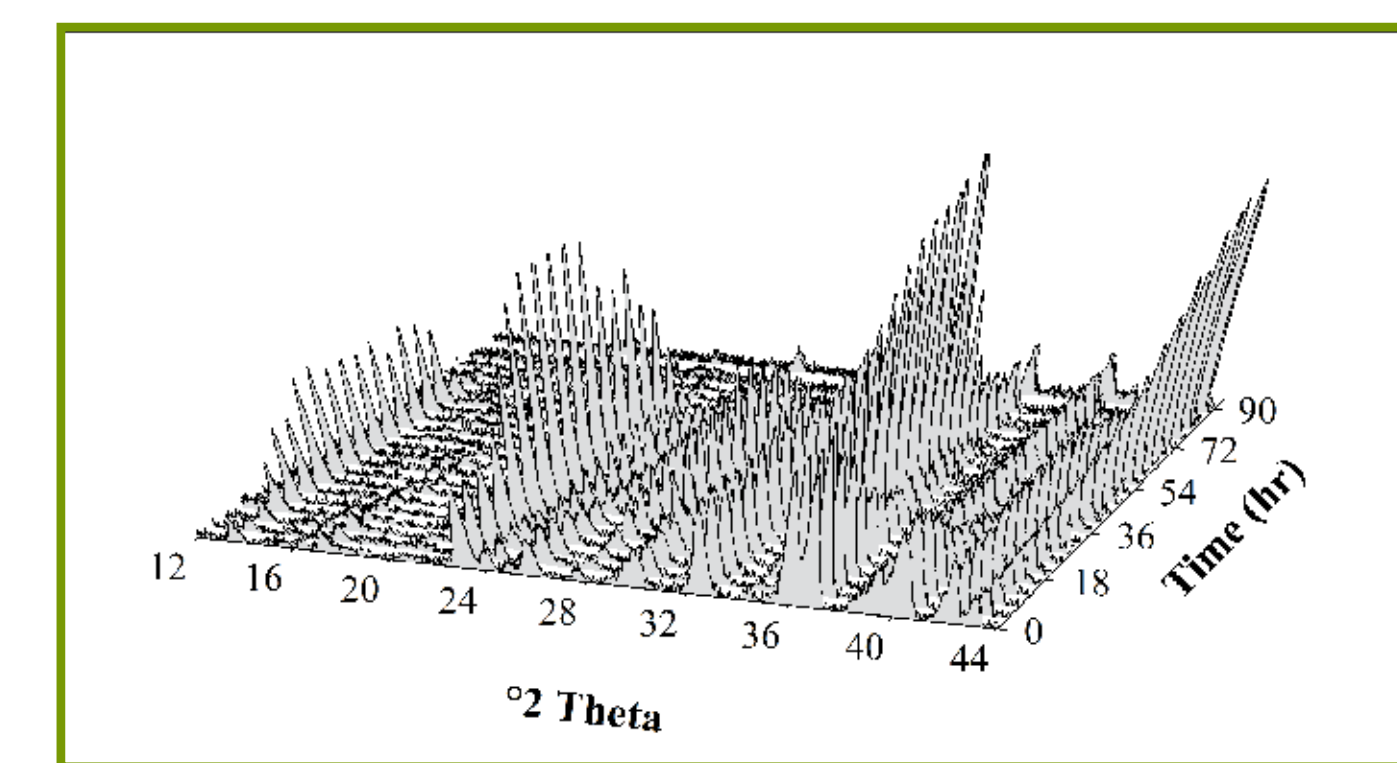
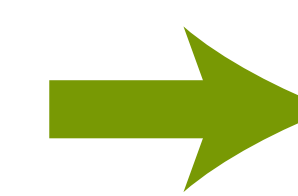
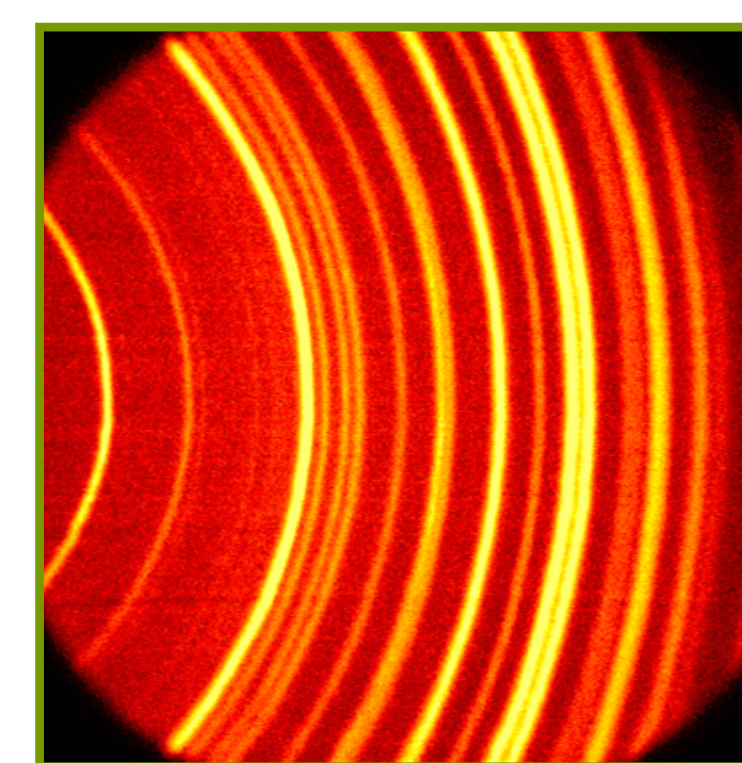
## PROBING SOLID-FLUID TRANSFORMATIONS AT EXTREME CONDITIONS

The in situ pressurized X-ray diffraction technique is a non-destructive analytical tool that reveals information about the crystal structure, chemical composition, and physical properties of materials. We have advanced this technique to allow probing of these properties under extreme conditions with a range of unique environmental chambers. This PNNL capability is typically restricted to synchrotron beamline user facilities, which have limited access and time-constrained investigations.

- Geochemical transformations of mineral under hydrothermal or supercritical conditions
- Structural changes to swelling clays induced by competitive gas intercalation
- Capturing solid phase transformations of energy materials
- Decomposition of catalysts and capture materials



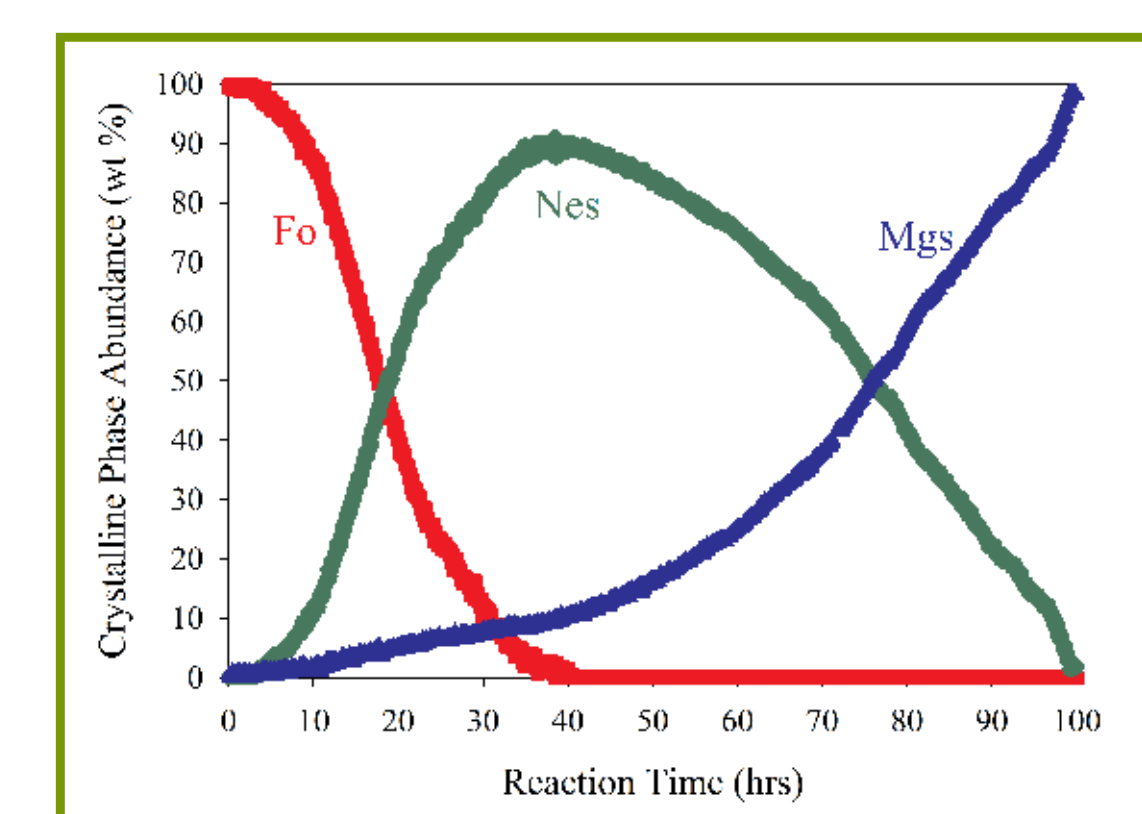
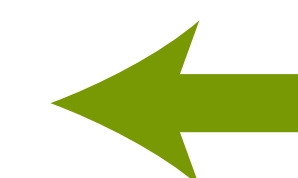
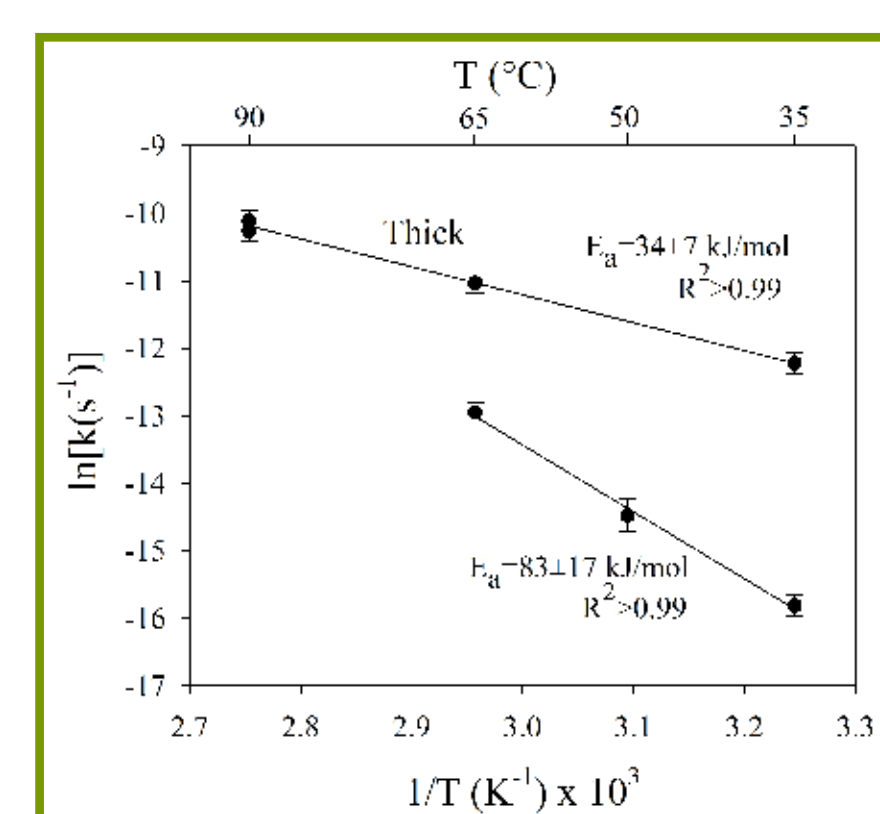
In situ diffraction patterns at elevated temperature and pressure



Time-resolved diffractograms indicate what phases are present during the reaction(s)



Extracted kinetic parameters (rates and activation energies) allow for the prediction of long-term fate of subsurface CO<sub>2</sub>



Time-resolved quantitative phase abundances reveal the importance of metastable intermediate phases