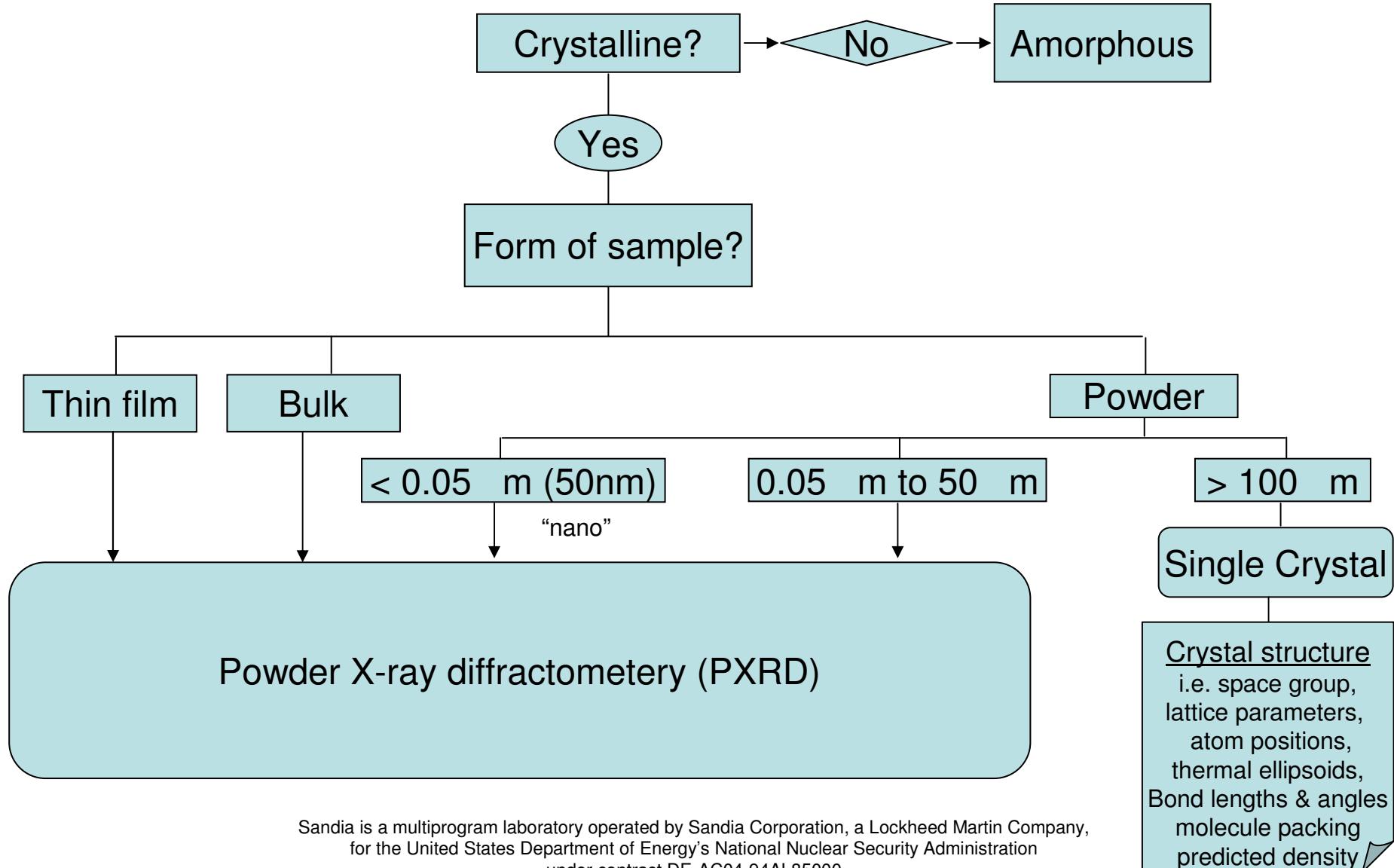
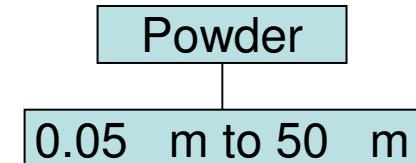


# XRD flow chart

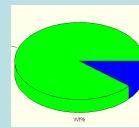


# Standard XRD



## Powder X-ray diffractometry (PXRD)

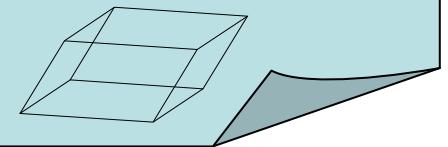
Phase identification: *What is this stuff?*



Phase fraction quantification via RIR: *How much is there?*

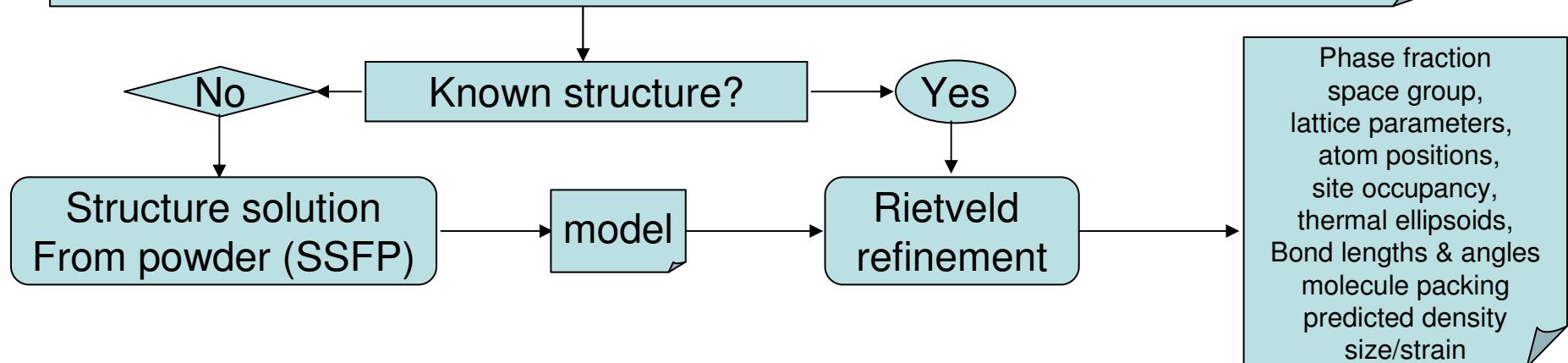


Out-of-plane preferred orientation: *Is sample non-random?*



Crystallite size / micro-strain: *What can I learn about the particles?*

Lattice parameter indexation / cell refinement: *What is the cell?*



**Nano-crystalline**

Powder

$< 0.05 \text{ m (50nm)}$

Mo tube:  $= 0.7107 \text{ \AA}$

Powder X-ray Diffractometry (PXRD)

Atomic pair distribution function (aPDF)

Phase identification?

Out-of-plane preferred orientation:

crystallite size / micro-strain:

Known structure?

aPDF  
refinement

space group,  
lattice parameters,  
atom positions,  
site occupancy,  
thermal ellipsoids,  
Bond lengths & angles  
molecule packing  
predicted density  
size/strain

