Research in Materials UC Davis May 2015

- Departments of Chemical Engineering and Materials Science, Chemistry, and Physics
- Emphasis on basic science
  - Inorganic materials for energy
  - Porous materials and catalysis
  - Soft and hybrid materials
  - Interactions with biology, medicine, vetmed, agriculture, food, wine, coffee

Focus Points and Collaborations

- NEAT- Nanomaterials in the Environment, Agriculture, and Technology
- Peter A. Rock Thermochemistry Laboratory
- Brazil collaborations through Profs. Ricardo Castro and Alex Navrotsky
- Faculty growth and renewal: 2020 and Chemistry Discovery District Project-

Experimental Materials Faculty

Chemical Engineering and Materials Science

Klaus van Benthem, Ricardo R.H. Castro, Sangtae Kim, Denise Krol, Subhash Mahajan, Alexandra Navrotsky, Subhash Risbud, Sabyasachi Sen, Yayoi Takamura

Chemistry

Ting Guo, Susan Kauzlarich, Kirillo Kovnir, Frank Osterloh

Physics

Nicholas Curro, Kai Liu, Dong Yu

NEAT

Play video

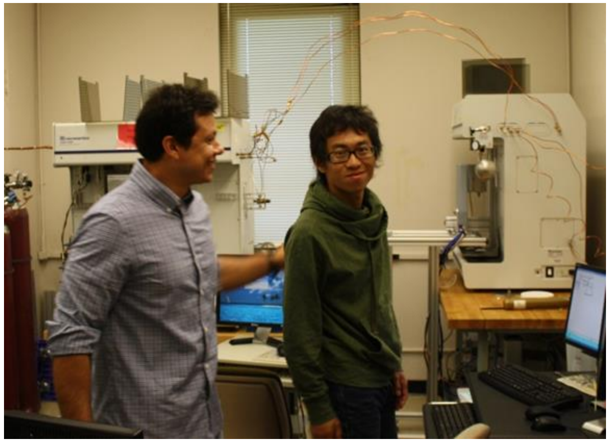
Peter A. Rock Thermochemistry Laboratory

Calvet –type instruments for drop, reaction and scanning calorimetry:

Four custom built calorimeters for solution and reaction calorimetry at 700° to 800° C
One Setaram AlexSys calorimeter for solution and reaction calorimetry ~600-1000 °C
Three Setaram C-80 and one Setaram BT2.15 calorimeter –150° to 300° C
Three Setaram Sensys (DSC 111) calorimeters used with gas dosing systems for measurements of enthalpies gas-solid interactions. Can also be used as DSC at -100 to 700° C. Two CSC 4400 isothermal calorimeters –40°-100° C

Systems for Differential Thermal Analysis (DTA) Thermogravimetry (TG) Differential Scanning Calorimetry (DSC) Thermomechanical analysis (TMA):

Netzsch 409 and 449 TG/DSC 25 -1650° C. Netzsch 404 DSC (-100° to 700° C) Netzsch 404 DSC (25°- 1500° C installed in the glovebox).
Setaram Labsys TG/DSC 25-1600 °C.
Setaram 9600 MHTC system for DSC, drop calorimetry and TG to 1500° C.
Two Setaram Setsys 1800 and one Setaram Setsys 2400 TG/DTA/TMA systems.



In-house synthesis and characterization:

Four Ar- and N_2-filled glove boxes, more than 10 furnaces, four to 1700 °C.
Synrad 100 W and 400 W CO_2 laser systems used with aerodynamic levitators and evaporation chamber for synthesis, pyrometers to 4000 °C to use with laser systems and Setaram Setsys 2400 thermal analyzer.
Bruker FTIR with DTGS and MCT detectors with gas cell and MKS Quad MS
Three Micromeritics ASAP 2020 and one Micromeritics Gemini gas sorption systems for analysis of surface area and dosing gas into calorimeters.
Bruker D8 Advance and Inel XRG 3000 X-ray diffractometers.

Alexandra Navrotsky research projects May 2015

- Critical materials institute- DOE energy innovation hub – rare earth thermodynamics
- Materials science of actinides – DOE energy frontier research center- fluorite oxides, clusters, hybrid materials
- Fluid interface reactions, structures and transport (FIRST) – DOE energy frontier research center – carbon materials and MAX and MXENE phases
- Ultra high temperature materials
- Thermochemistry of oxides with electrochemical and energy applications – perovskites, spinels, others
- Energetics of nanomaterials and materials under confinement
- Thermodynamics of minerals stable near the earth's surface
- Thermodynamics of slags

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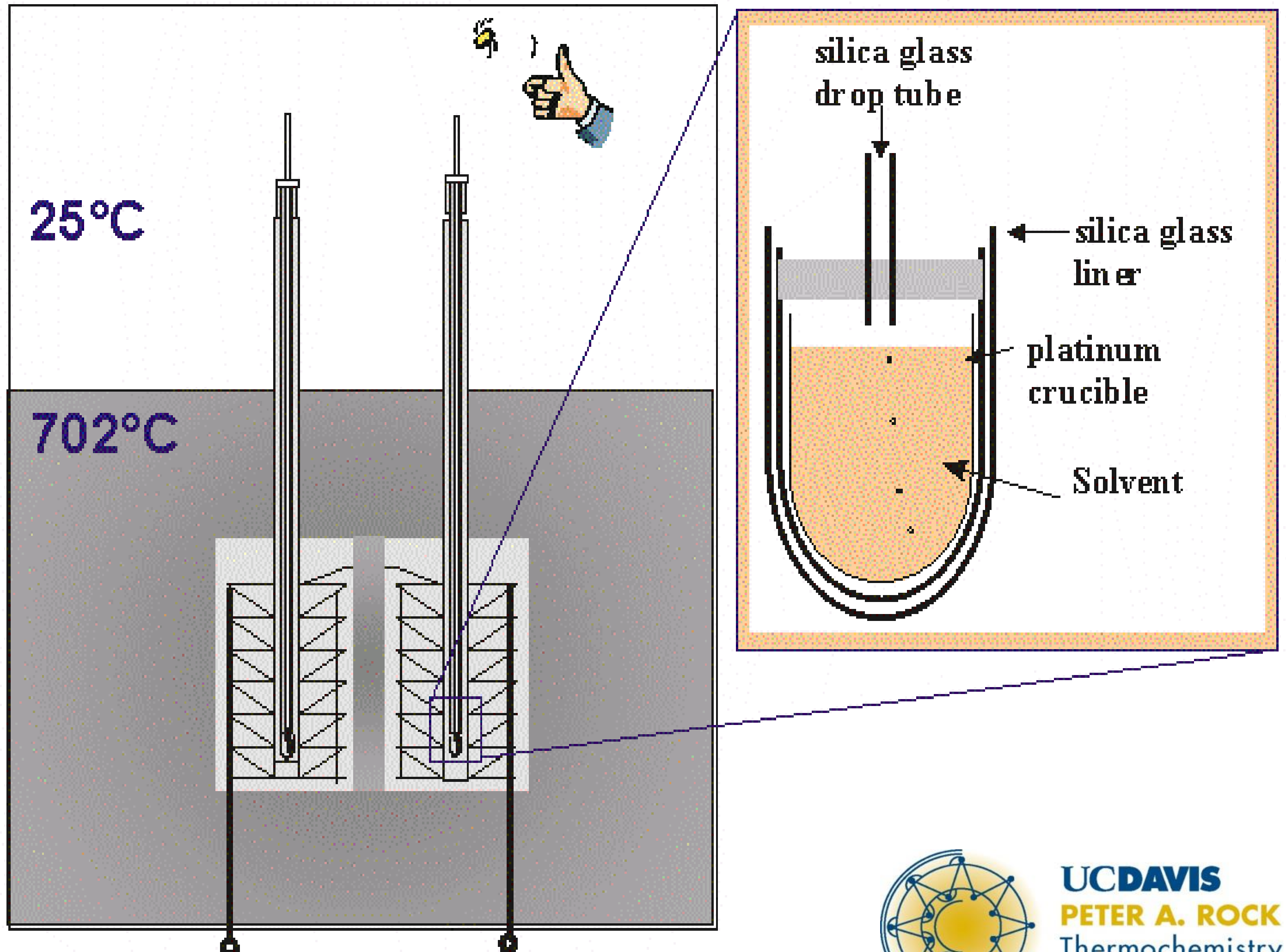
Laboratory

High temperature oxide melt drop-solution calorimetry



Differential Thermopiles

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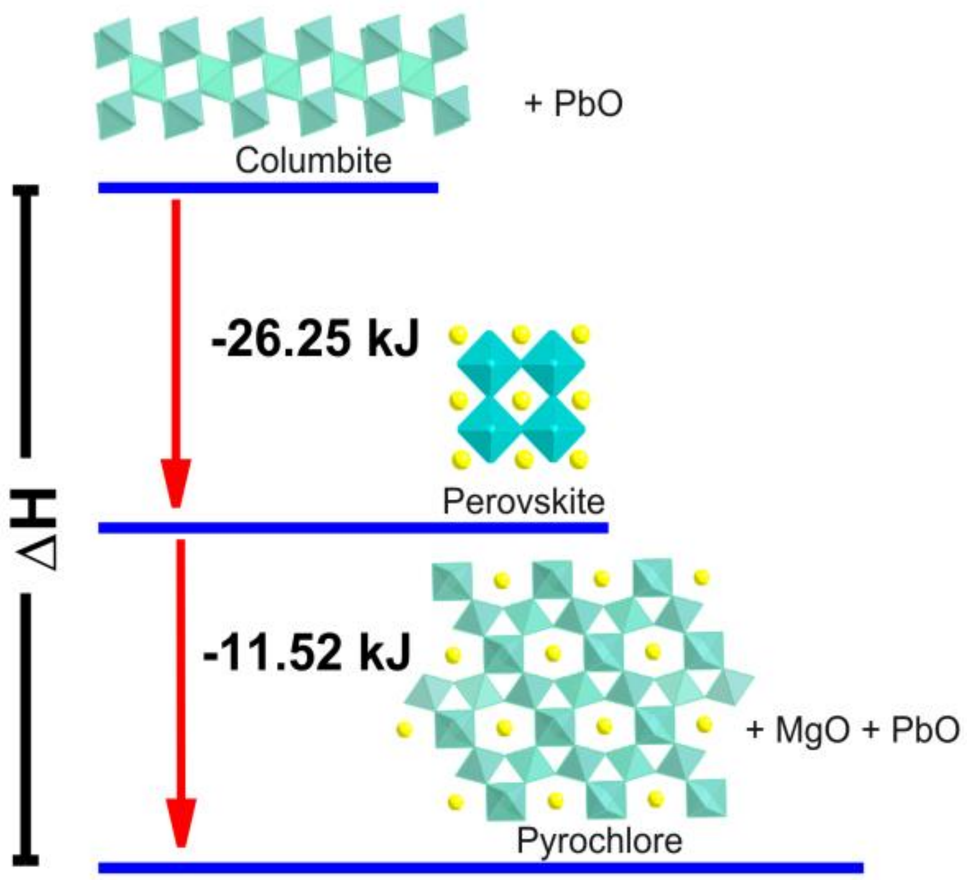
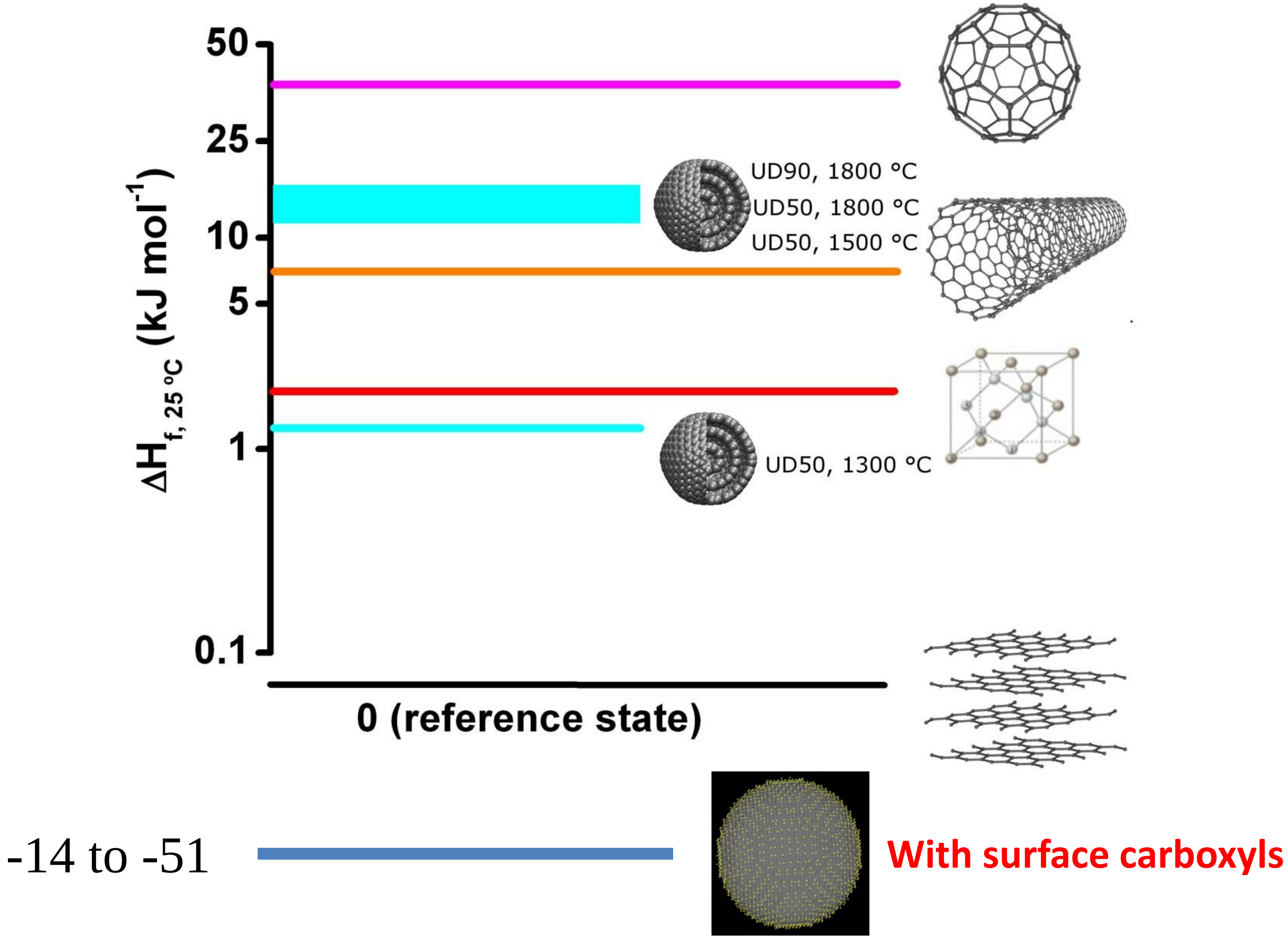
Thermodynamic Constraints on PMN (lead magnesium niobate) Synthesis

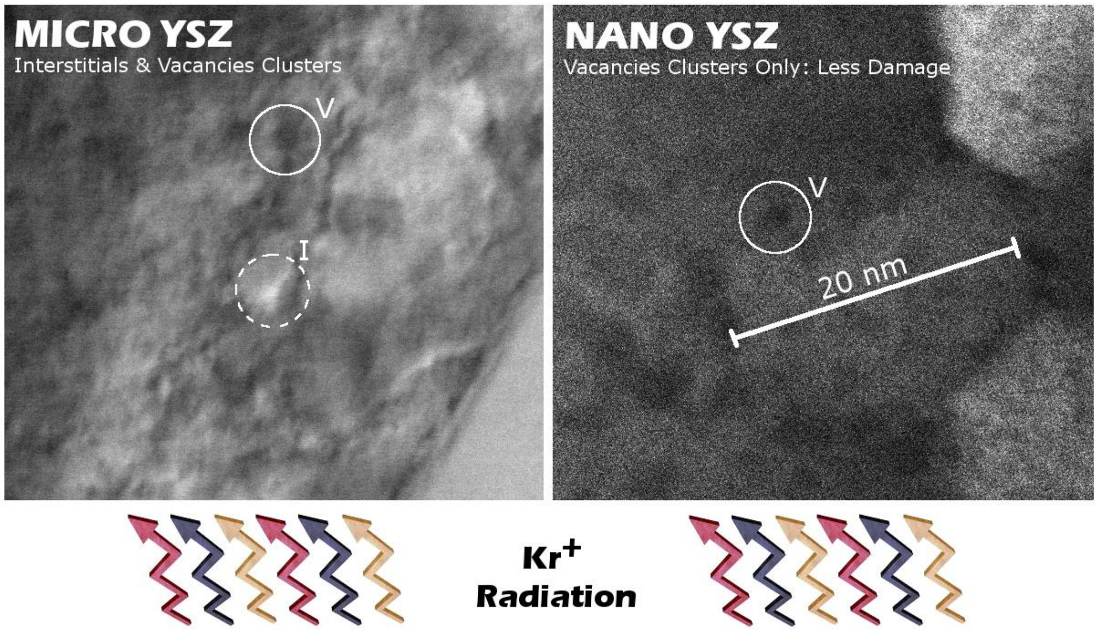


Work by Gustavo Costa

Enthalpies of formation at 25 °C (ΔH_f) of carbon forms relative to graphite

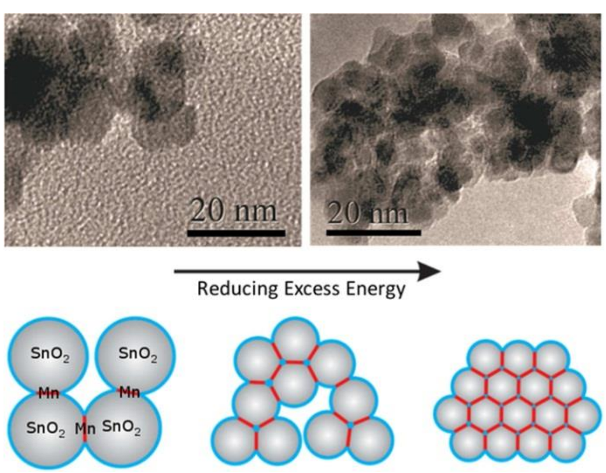


Radiation Tolerance of Nanocrystalline Materials Ricardo Castro



Nano YSZ shows less damage due to **defect-sink** nature of GBs. Performance is related to GB energies.

Sci. Rep. 5, 7746.
doi:10.1038/srep07746

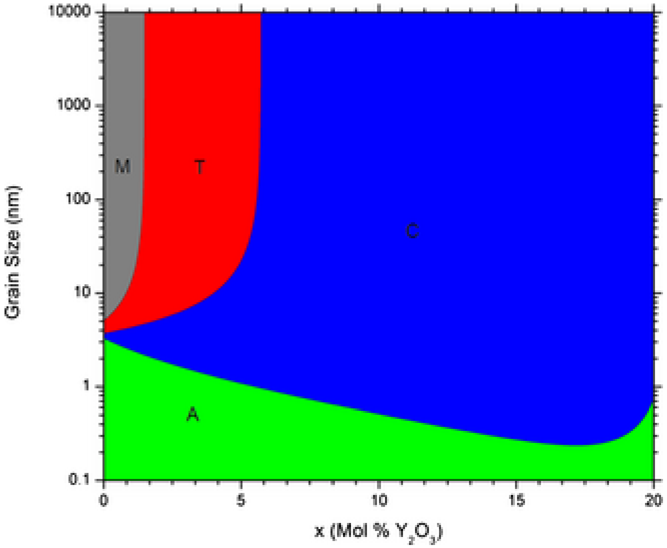


Improved Stability of Nanoparticles

Decreasing surface and grain boundary energy of oxides using dopants. Examples: CeO_2, SnO_2, $MgAl_2O_4$, YSZ.

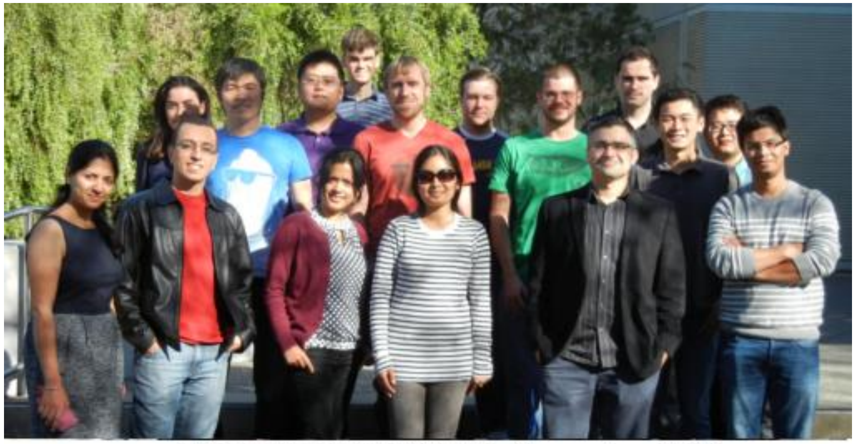
J. Phys. Chem. C, 119, pp. 6389, 2015
J. Phys. Chem. C, 118, pp. 30187, 2014
J. Phys. Chem. C, 118, pp. 10142, 2014

Phase Stabity of Nanocrystals



Predictive stability phase diagram of YSZ as a function of Y content considering bulk and surface energies measured by microcalorimetry.

J. Am. Ceram. Soc. 98, 1377, 2015 (COVER)



Castro Research Group - December 2014

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