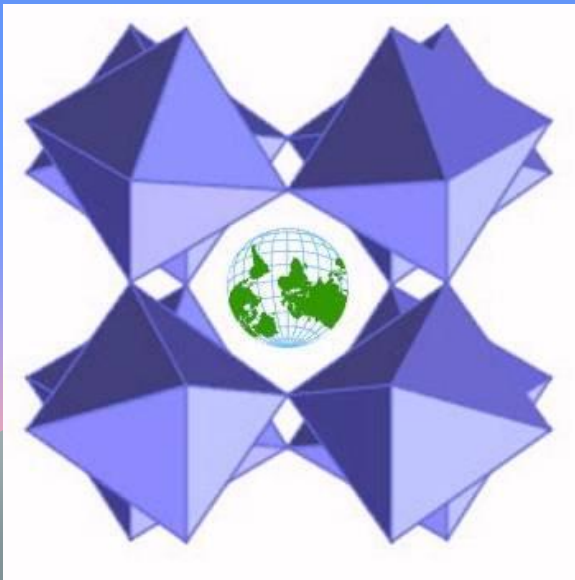


**Are there carbon bearing  
accessory minerals we have not  
thought of in the lower mantle and  
core?**

**Alexandra Navrotsky**

**UC Davis**



# High P and T

- **High T favors solid solutions**
- **High P may favor new structures**
- **All known parts of the Earth contain “accessory minerals”, why not the lower mantle and core for carbon bearing phases?**
- **Carbides have been found in poorly understood environments**

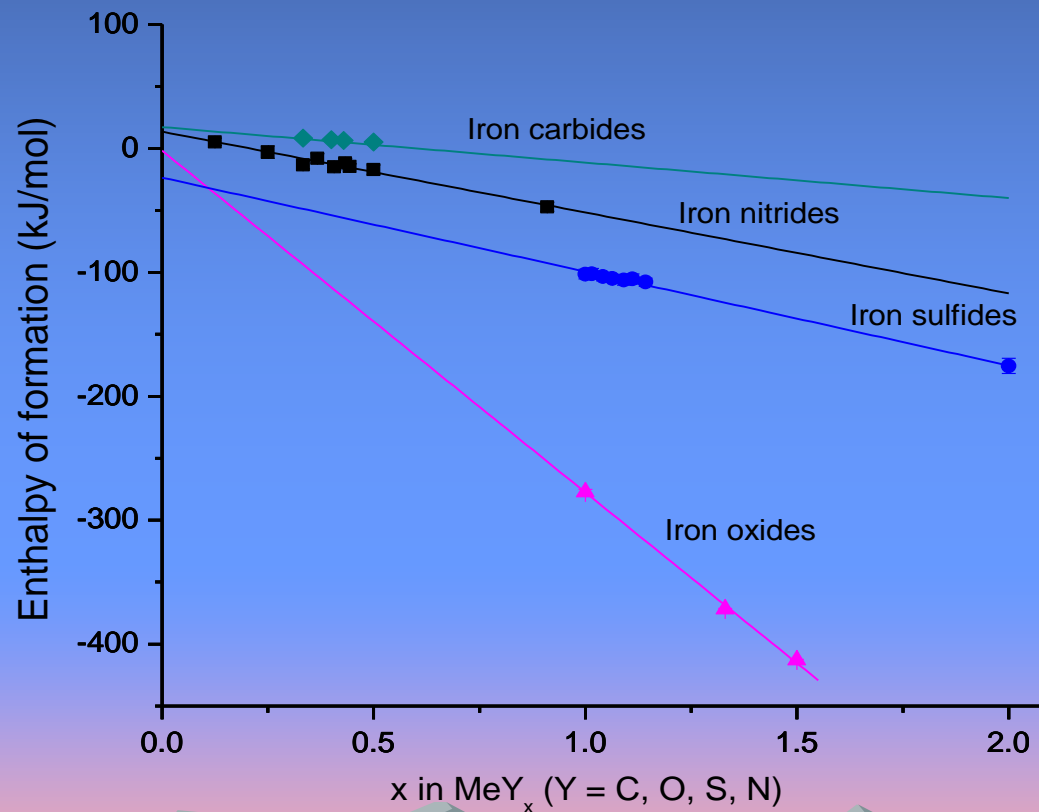


# Lessons from Materials Science

- **New phases - intermetallics, carbides, nitrides, sulfides, mixed anion materials**
- **A wider range of compositions for melts and amorphous materials**
- **Minor and grain boundary phases**



# Enthalpies of formation of iron oxides, sulfides, nitrides, carbides



# Carbide Formation Reactions, Relative Stability

- **A scale for reference: Iron Carbide + Metal Oxide = Iron Oxide + Metal Carbide**
- **Write reaction not involving any gas/fluid phases, then P,T dependence will be relatively modest and identify likely carbides to consider**
- **Carbothermic reduction by diamond of oxides to produce carbides + a fluid (CO<sub>2</sub>?) may need to be considered.**
- **Especially consider Si, W, Ta, Mo,Zr, Hf other transition metal carbides**
- **Ternary phases?**

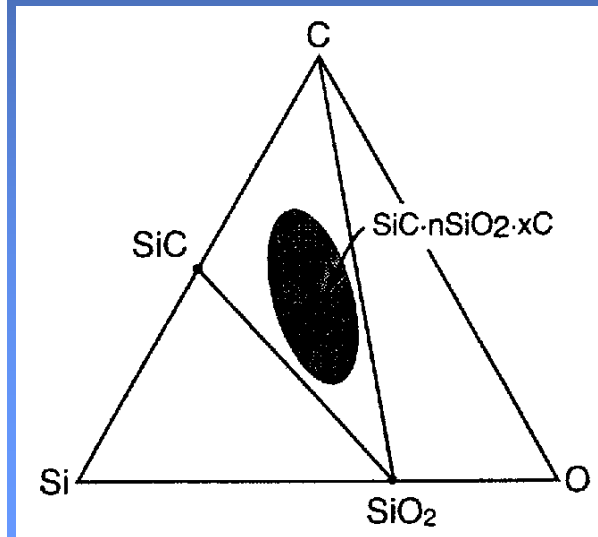
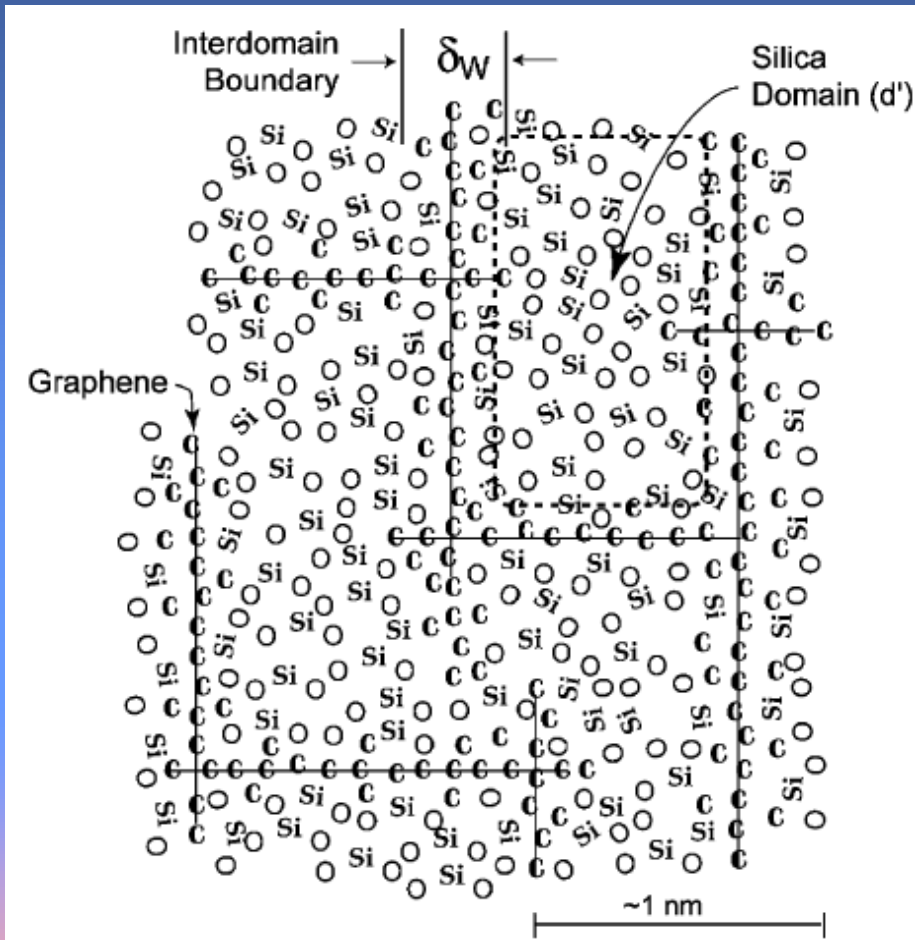


# Si-C-N-O Materials

- CO polymers, photochemical reactions
- Tetrahedral C in CO<sub>2</sub> and silicates
- Carbothermic reduction of silica, iron oxides, etc. Occurs above 1500 °C under ambient conditions, what happens at high P,T, low fO<sub>2</sub>.
- Amorphous Si-O-C-N stable ceramics



# Si-C-O X-ray amorphous but nanostructured materials



# Enthalpies of Formation from Crystalline SiO<sub>2</sub> + SiC + C

- Almost all  $\Delta H$  values are negative (-7 to -130 kJ per g atom), implying energetic stability of amorphous phase relative to crystalline end members. No simple compositional dependence.
- Entropy of amorphous phase is higher than that of crystalline, so  $DG$  is also negative.
- Explains why samples do not crystallize until they decompose due to carbothermic reduction of silica above 1500 °C



# Possible Path Forward

- Investigate binary and ternary carbides and oxycarbides at high P, including elements like Zr, Ti, Fe, W, Mo, Nb
- Use “analogue materials”, lower P analogues of high pressure phases
- Need insight from metallurgy
- Are amorphous phases out of the question?
- Other planets?
- Think outside the box

