Crystal growth at the crossroad of high pressure physics and chemical thermodynamics

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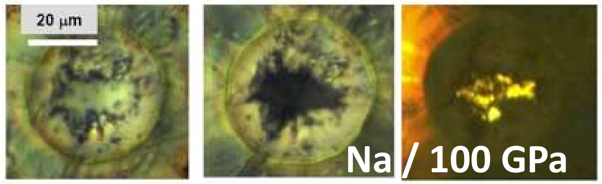
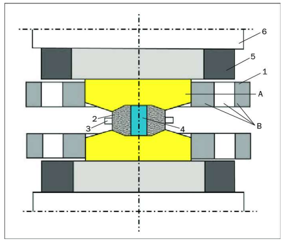
2 High pressure

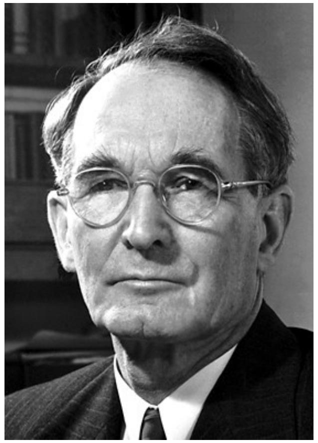
New physics at high pressure (HP)

- Pressure = **F / S**; natural range from crust (GPa) to core (TPa)
  - Access new structures, metastable phases, dense packing
  - Tune bonding, electronic structure, and properties

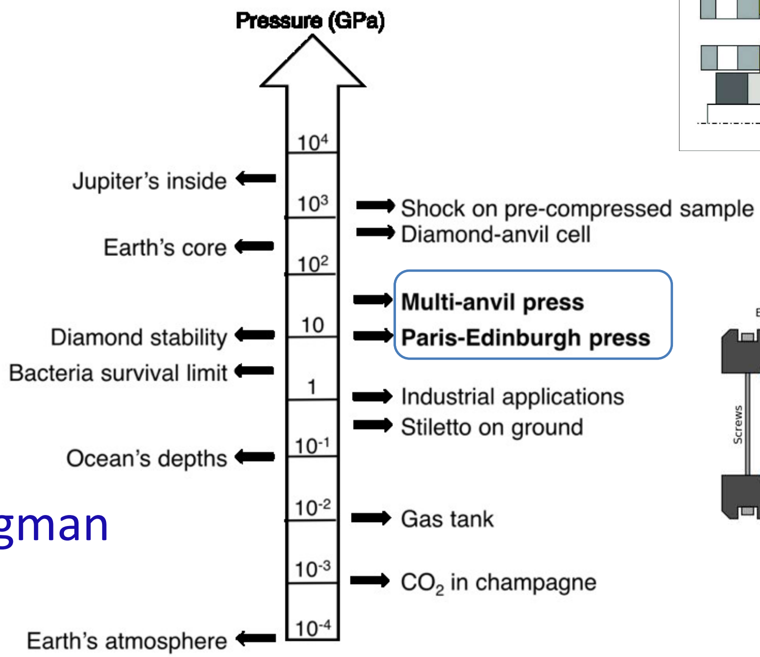
Ma et al., Nature (2009)

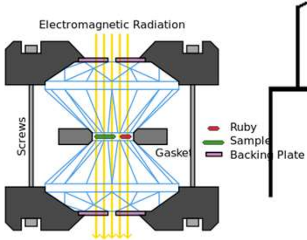


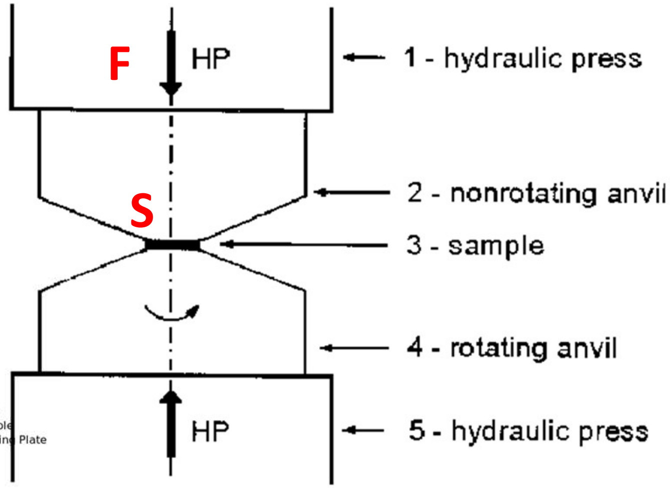




Percy Williams Bridgman
Nobel price in 1946







Elements and compounds under pressure & shear

3 High pressure & high temperature

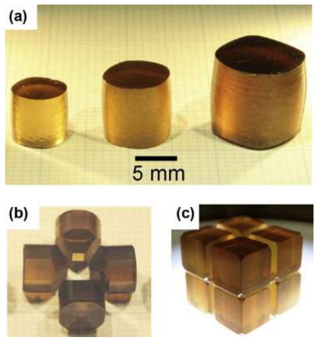
New chemistry at high pressure (HP)

- Artificial diamond and cubic boron nitride (cBN)
  - Steady 1800 K & 5 Gpa conditions, **C / Metal**

Tracy Hall, General Electric 1954

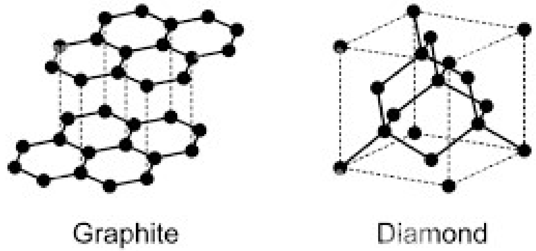
Bundy et al., *Nature (1955)*

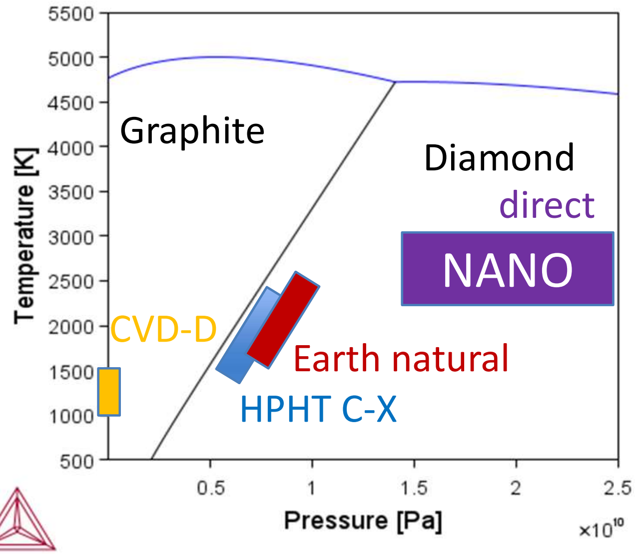
Nano diamond

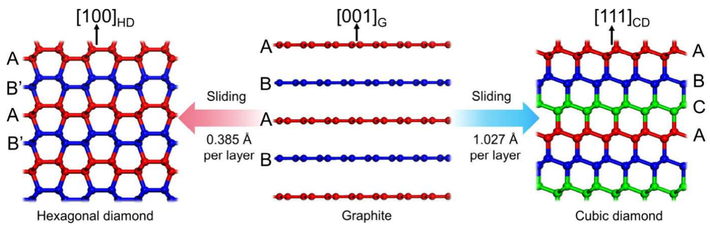


T. Irifune, Sumitomo 2003

Irifune et al., *Nature (2003)*







Materials design by explorative in situ HP crystallography

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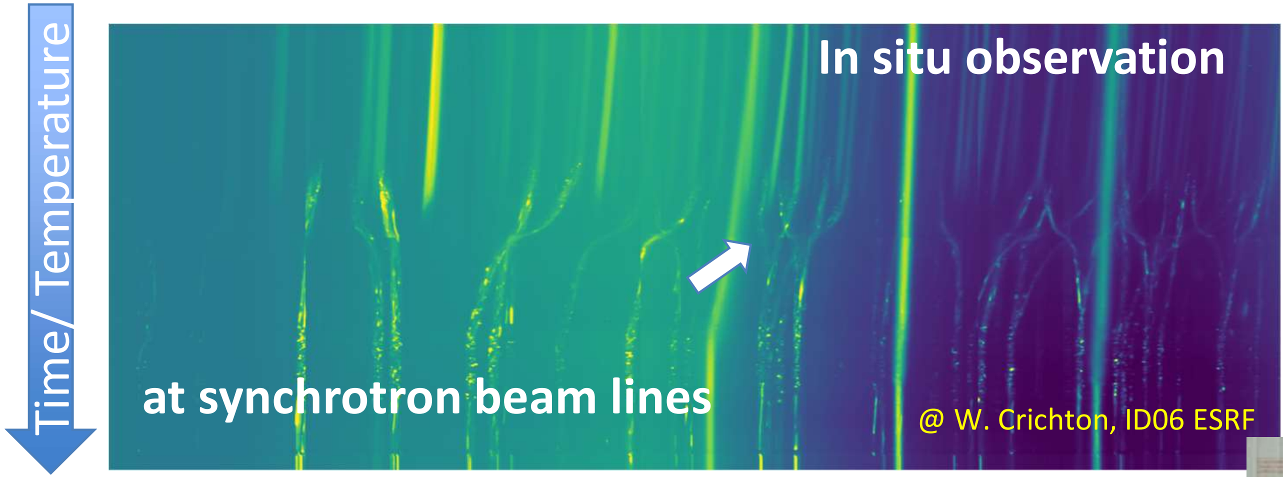
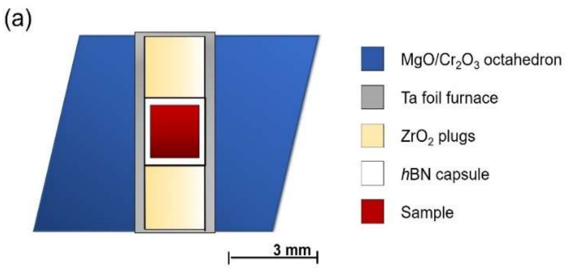
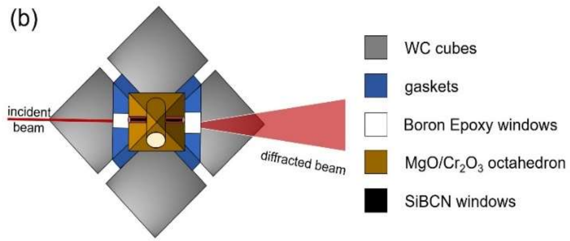
4 In situ HPHT crystallography at synchrotrons

- Synchrotron XRD: time-resolved, HP cell tomography, multi-sample experiments
- Advantages: Large sample volume (mm^3); Temperature homogeneity
  - Diffraction + imaging
- Typical data: chemical reactions, phase identification, kinetics, nucleation, transformations







ESRF

Paris-Edinburgh (PE)

Multianvil (MA)

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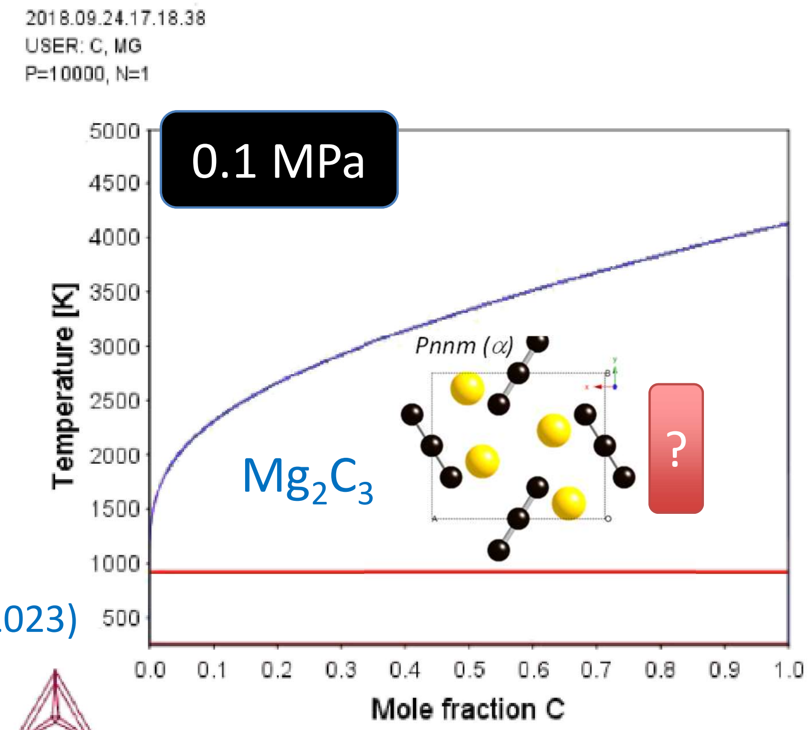
5 Phase diagram of Mg-C system

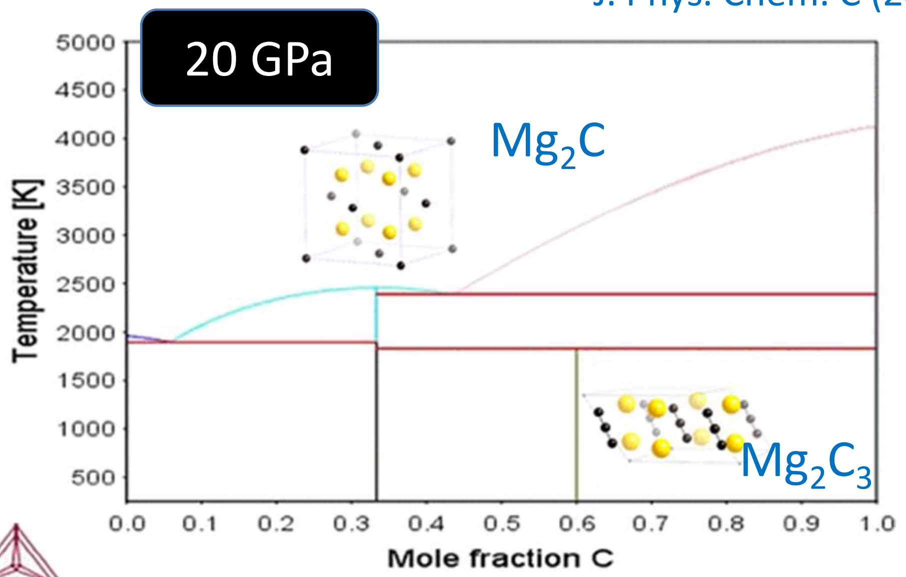
- Simple thermodynamics of Mg–C system at ambient pressure.
- **Pressure-induced chemistry**
- Rich ambient-pressure "metastable" chemistry
  - MgC_2 (*P4mnm*)
  - Mg_2C_3 (*Pmmn*)

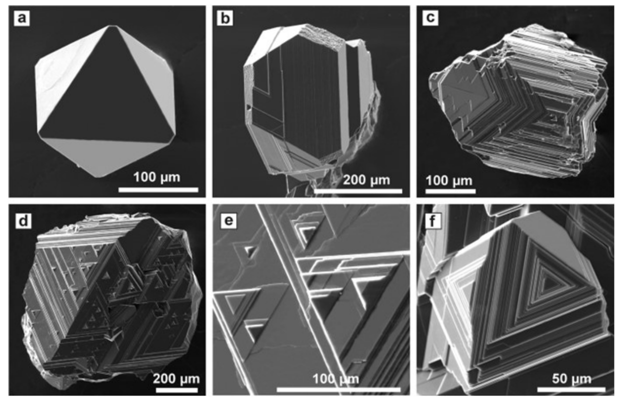
Soft chemistry

Patents on C to C_3H_4 transformation

Turkevich et al.,
J. Phys. Chem. C (2023)





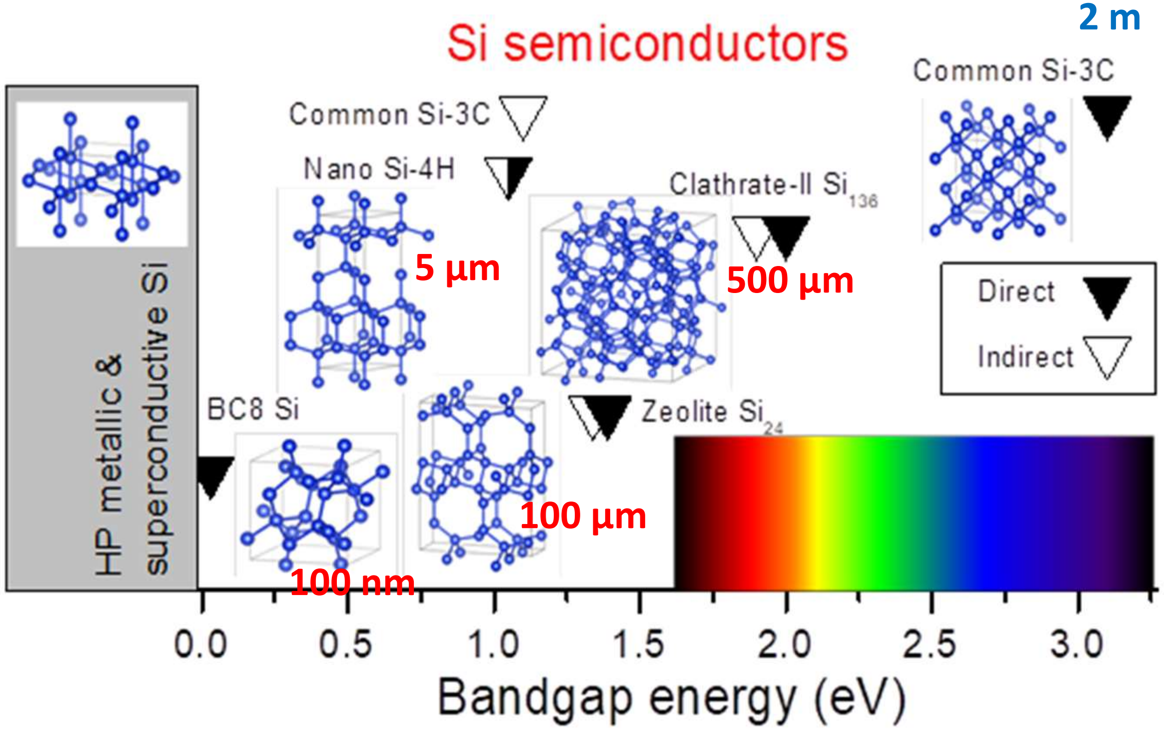


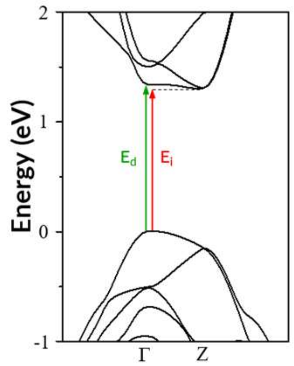
Polyanov et al., CrystIngCom (2015);
Diam. & Relat. Mater. (2016)

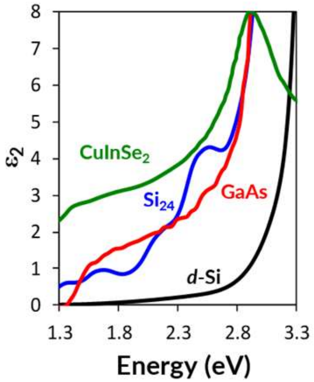
6 Single crystals in Na-Si system

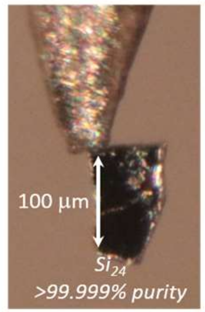
- Si_{136} (*cF136*), Si_{24} (*oC24*), Si-III (BC8 or *cI16*), Si-VI (4H or *hP8*).
- The search for ideal bandgap Si
- Physical measurements of systems undergoing chemical reactions

Guerette et al., J. Phys. Cond. Mater. (2020)
Cryst. Grow. Des. (2018)

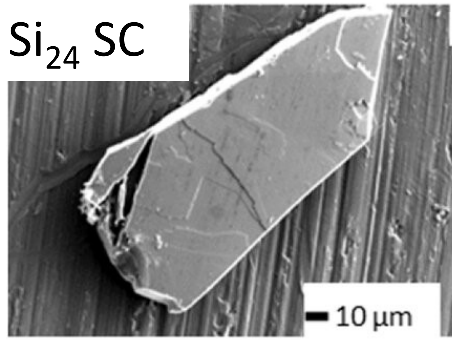








Clathrate Si - Si_{24} SC



Ideal silicon

Nano Lett. (2018); Phys. Rev. Lett. (2017); Inorg. Chem. (2016); Nat. Mater. (2015)