Dynamic Compression of Iron Carbide at Planetary Core Conditions

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SSAA Annual Meeting - Feb. 15, 2023

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Our Team

Joint experimental & theory project

Experiments:

Sally Tracy, & **Postdoctoral Fellow** (Carnegie)

Simulations:

Ivan Oleynik, Kien Nguyen Cong (USF)

National Lab Collaborators:

Ray Smith, Federica Coppari, Jon Eggert, Marius Millot, Chris McGuire, & Samantha Clarke (LLNL)

Support from User Facility Staff at DCS and LLE

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University of South Florida

Lawrence Livermore National Laboratory

The Dynamic Compression Sector at the Advanced Photon Source

Laboratory for Laser Energetics, University of Rochester

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Planetary Cores

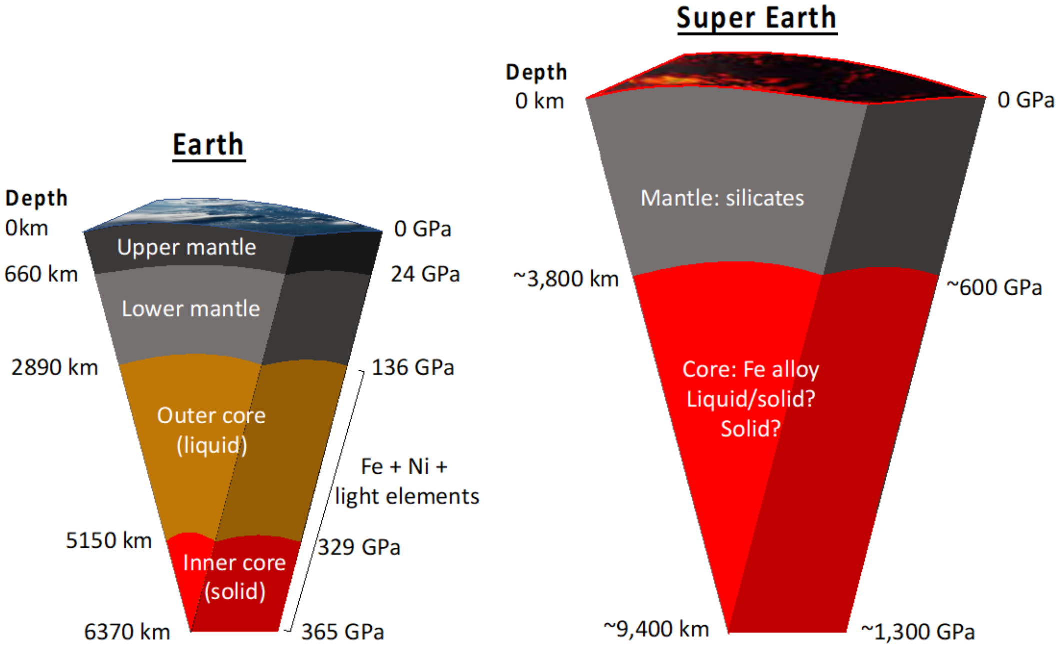
Structure & properties of core materials at the P-T conditions of Earth’s core and the core’s of larger super-Earth exoplanets

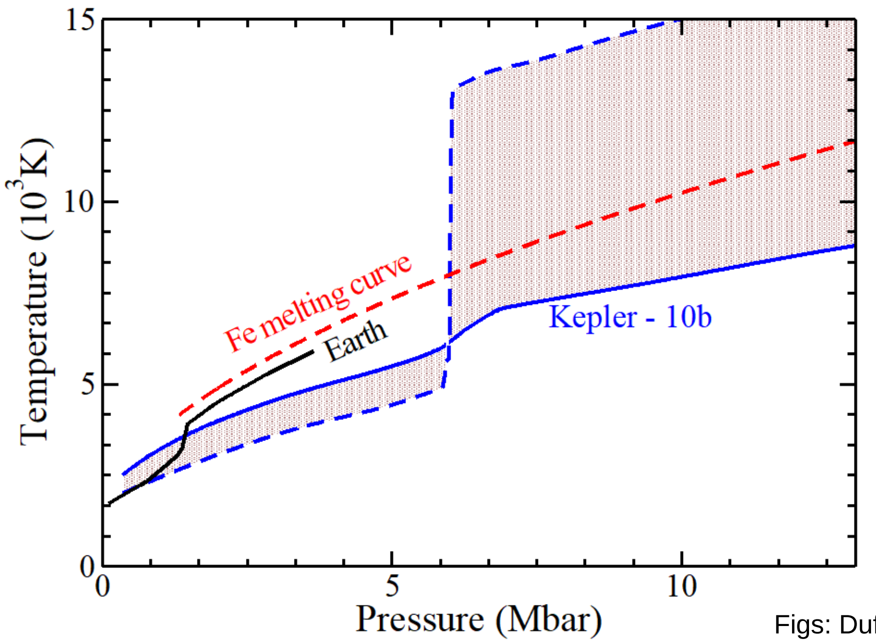
Earth’s Core:
Liquid outer core & crystalline inner core
Fe-Ni alloy with 10% lighter elements (C, Si, O…)

Super-Earths:
Abundant population of Earth-like planets with up to 10-Earth masses and internal Ps up to 4 TPa

Super-Earth are also expected to incorporate light elements

Focus of this project is on **carbon** an important candidate light element for Earth’s core as well as C-rich super-Earths





Figs: Duffy & Smith 2019

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Effects of Light Elements

Light elements effect melting temperature
Relative slopes of the liquidus and the planetary adiabat will determine if a planet has a coexisting liquid outer and solid inner core

Liquid outer core allows for a dynamo to form, generating a magnetic field which plays a role in habitability

Complex structures in the Earth's solid inner core

- Thin outermost layer
- West & East hemispheres with different elastic properties
- Distinct innermost inner core

Source of heterogeneities may be related to light-element-rich alloy phases.

Changes in crystallization over time that effect concentration of light elements in the precipitating solids.

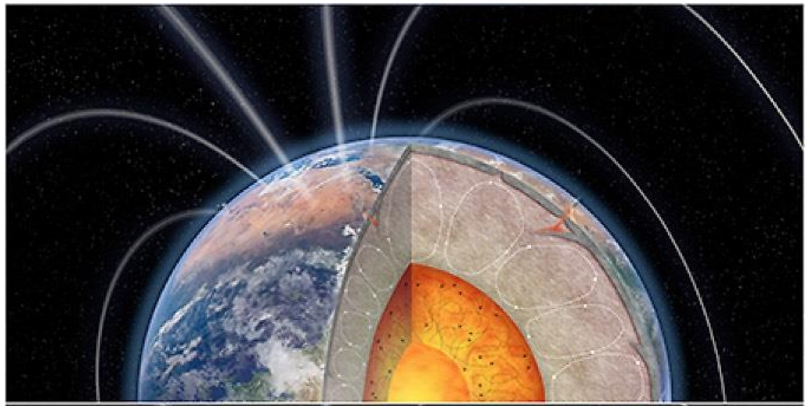


Fig: UC Santa Cruz

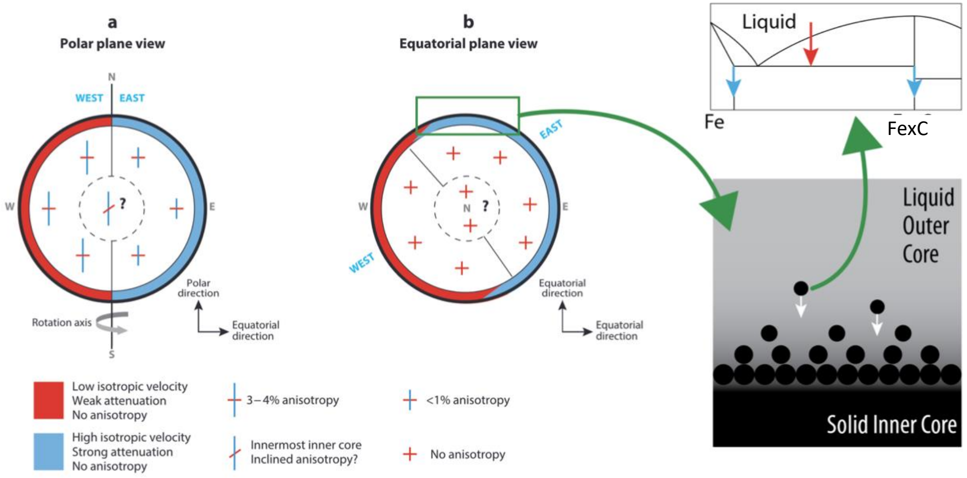


Fig: Deuss et al.

Iron Carbide Phase Diagram

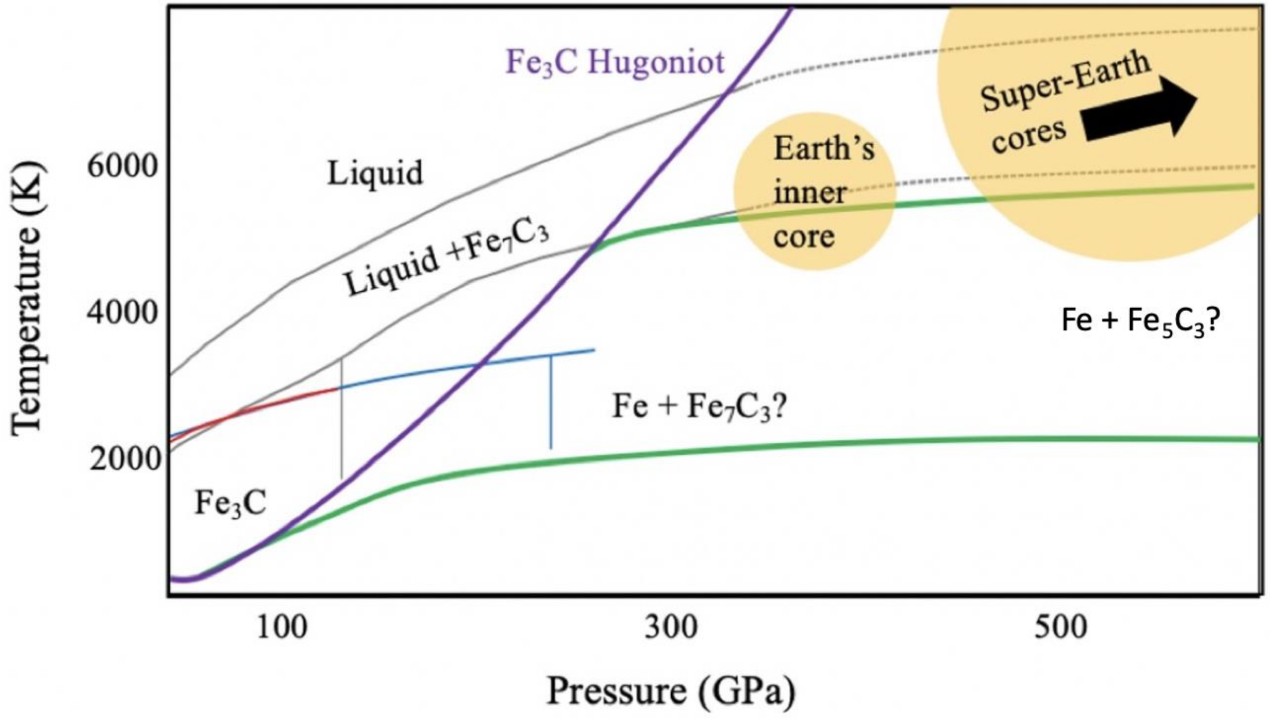
Understanding of C incorporation into the core is limited by poor constraints on the high-P Fe-C phase diagram

Carbon has limited solubility in HCP-Fe

Solid cores likely include Fe-carbide phases

Models based on long extrapolations predict Fe_3C was 1st phase to crystallize during solidification of the Earth's core

Recent results suggest Fe_7C_3 may instead be the favored phase such that Fe_3C melts incongruently



No experimental data at P-T conditions of inner core or cores of larger super-Earths

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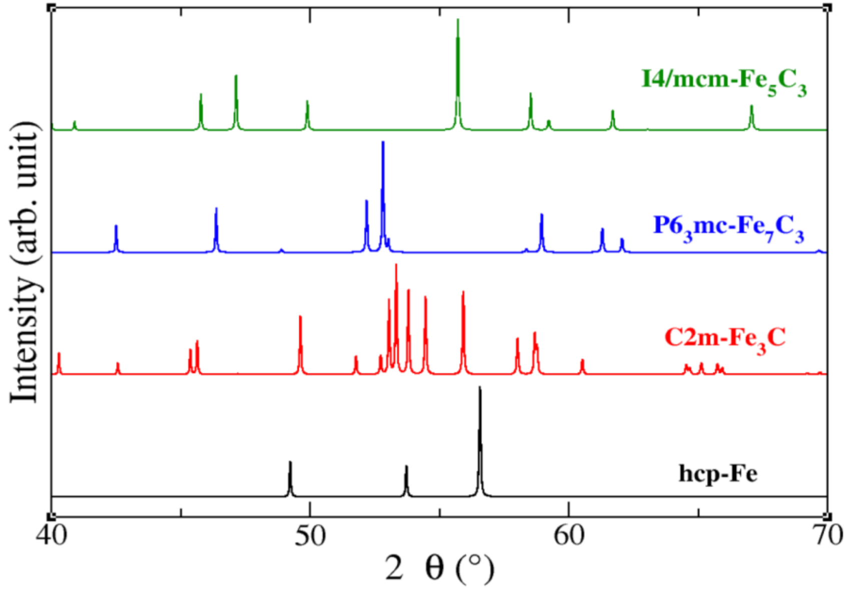
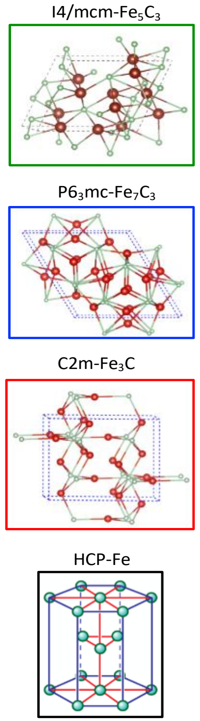
Structure Search Calculations

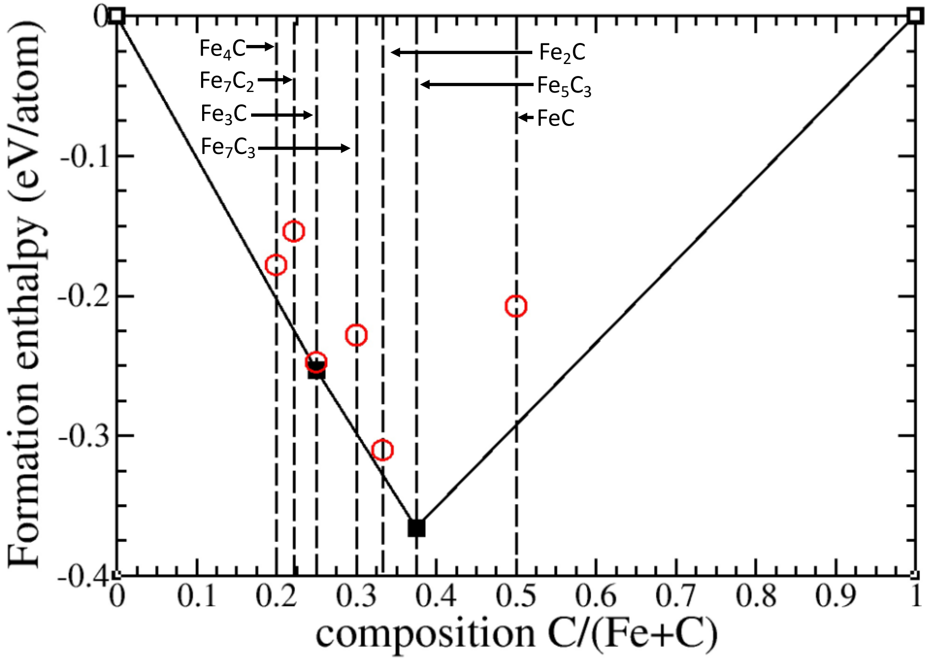
Theoretical calculations predict Fe_2C to be more stable than either Fe_3C or Fe_7C_3 at inner core conditions





Our recent structure search results indicate a new Fe_5C_3 structure is the lowest enthalpy phase at 500 GPa

Based on these results, we expect Fe_3C may will break down into HCP Fe + carbide phases of different stoichiometries



Kien Nguyen Cong (USF)

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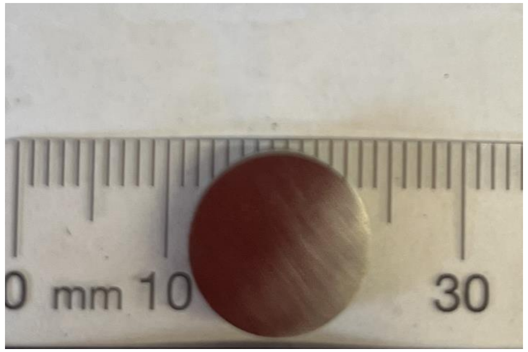
Fe_3C Synthesis at Carnegie

Start with Fe_3C allowing us to explore Fe-C phase stability with a well-constrained stoichiometry (6.7 wt% C)

98% dense polycrystalline Fe_3C sample synthesized by solid phase reaction between Fe and graphite powder at high-PT

Sintered at 4.8 GPa and 1100 °C for 15 min, using a large-volume cubic press



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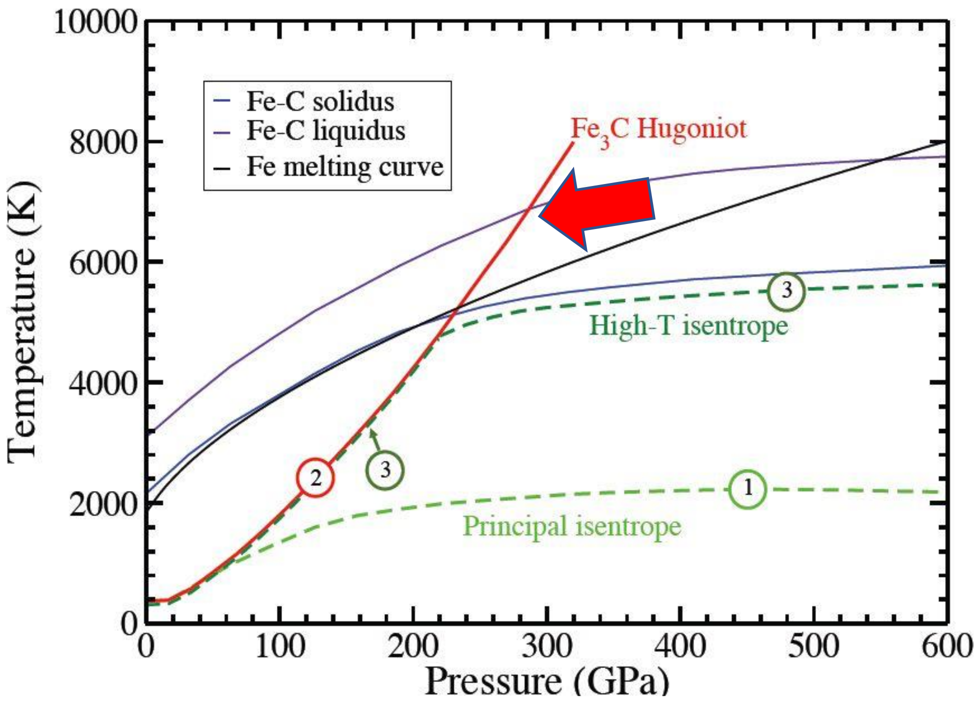
Structure of Fe_3C Under Shock Loading up to 250 GPa



X-ray Diffraction (XRD) along the Fe_3C Hugoniot

Questions

What is the crystal structure of Fe_3C under shock compression?

Can we constrain the Fe-C melt curve above 100 GPa?

Melting→ Loss of XRD peaks & appearance of diffuse scattering

Is melting is congruent or incongruent?

Implications

Explore stabilization of carbide phases in Earth's inner core

Assess carbon's effect on suppression of the liquidus at Earth-core conditions

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In Situ Diffraction Under Laser Shock Loading at DCS

Image: ANL

Laser (<80 J, 5-10 ns pulse length) is focused on a plastic ablation layer generating a plasma which expands backwards sending a shock wave into the sample

During the shock state, sample is probed with XRD data is recorded using a transmission geometry

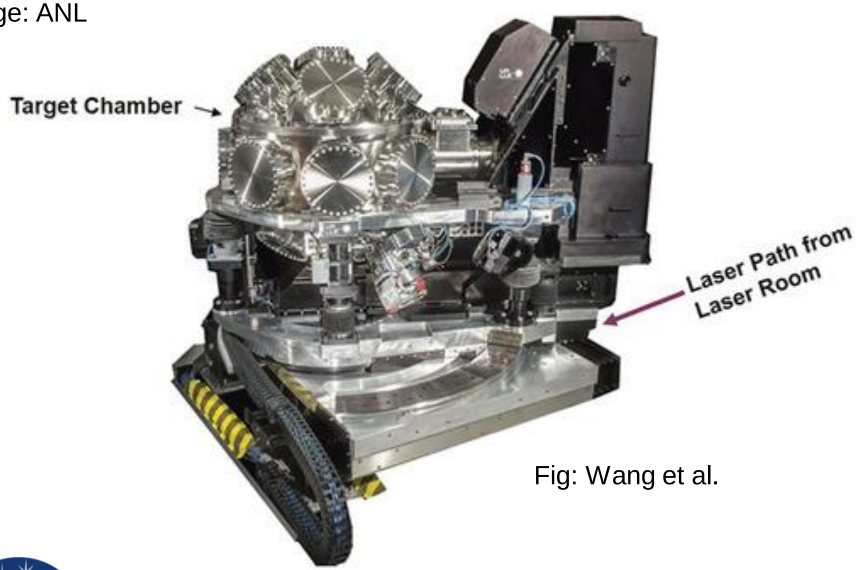


Fig: Wang et al.

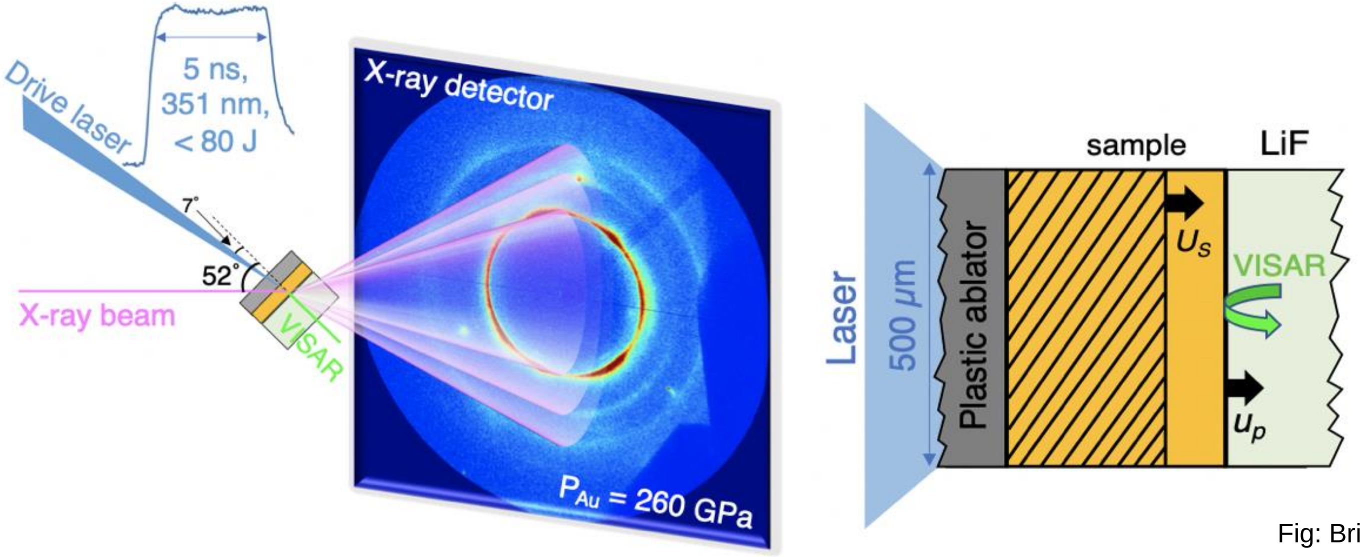
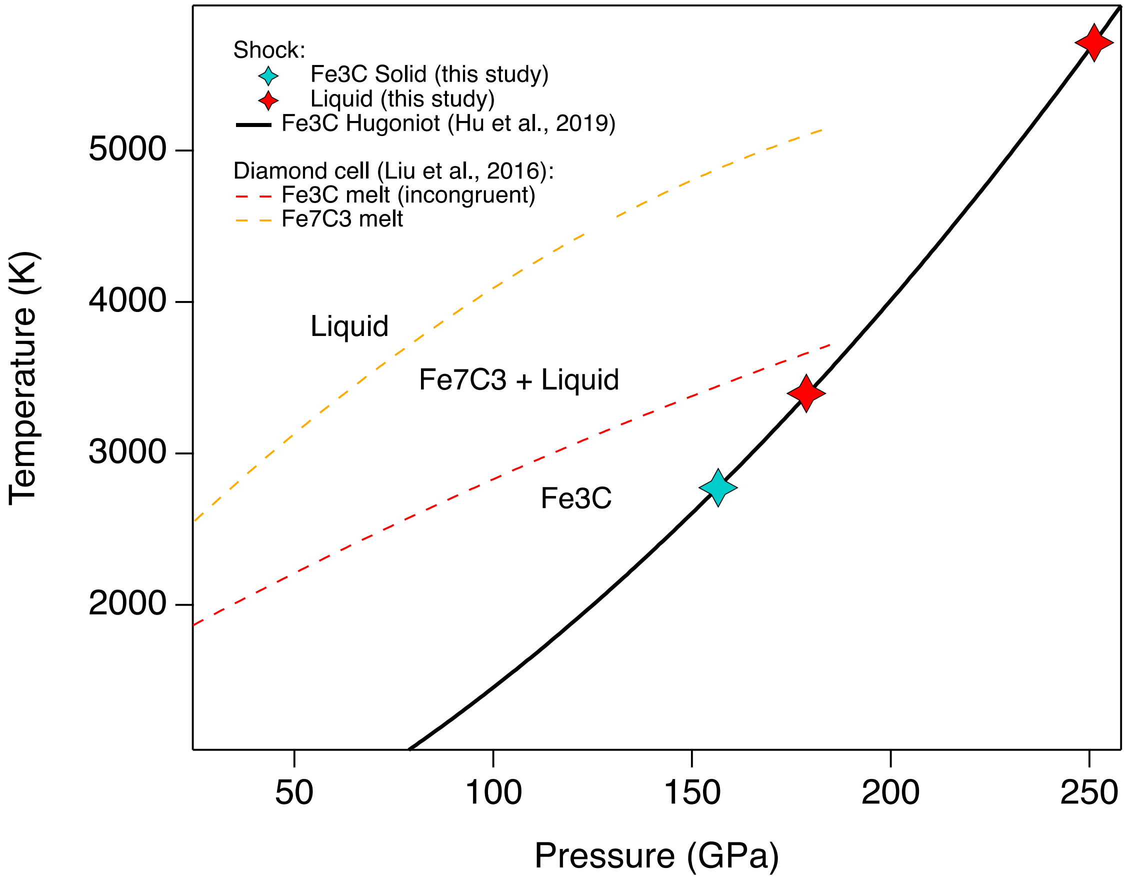
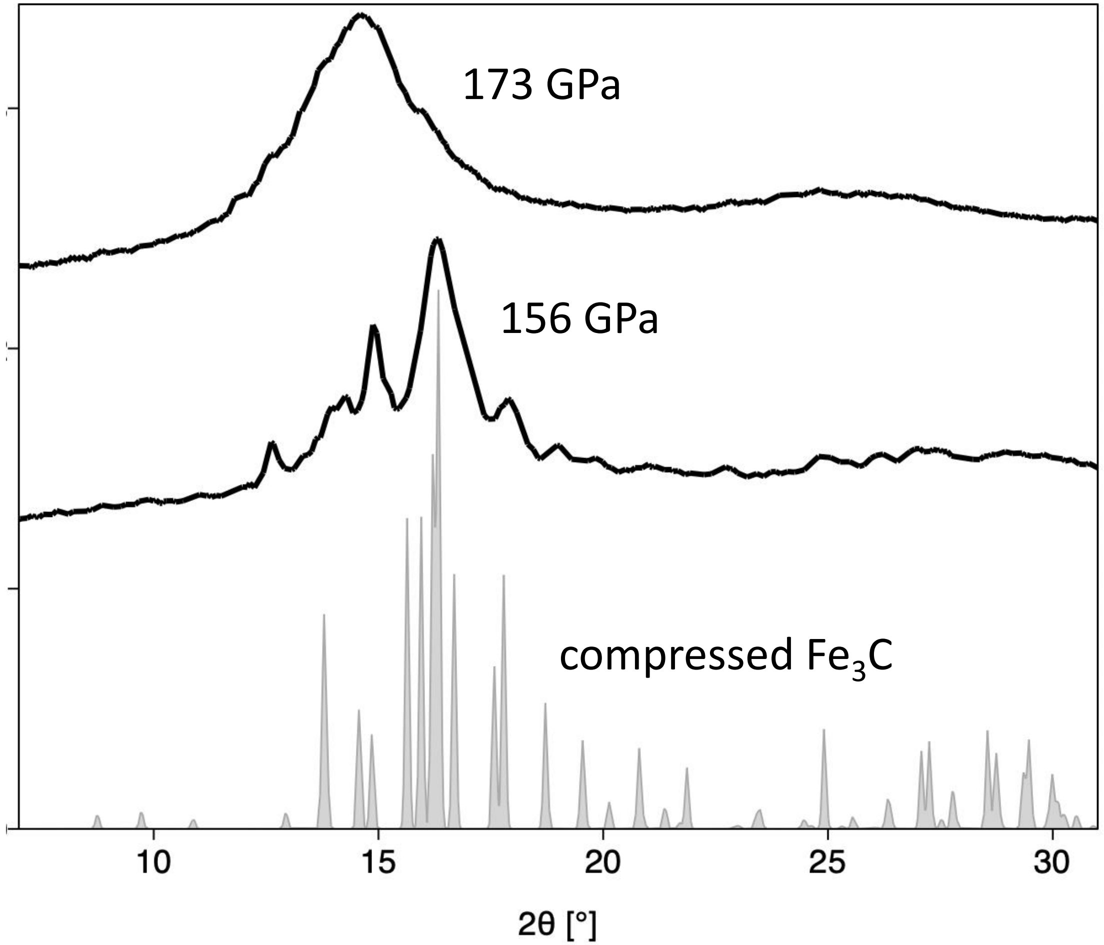


Fig: Briggs et al.

Preliminary DCS Results





Fe_3C melts at 160 GPa into a single liquid along the Hugoniot

Contrast expected incongruent melting (Fe_3C→ Fe_7C_3 + Lq.)

Future: Quantitative analysis of liquid structures between 160-250 GPa

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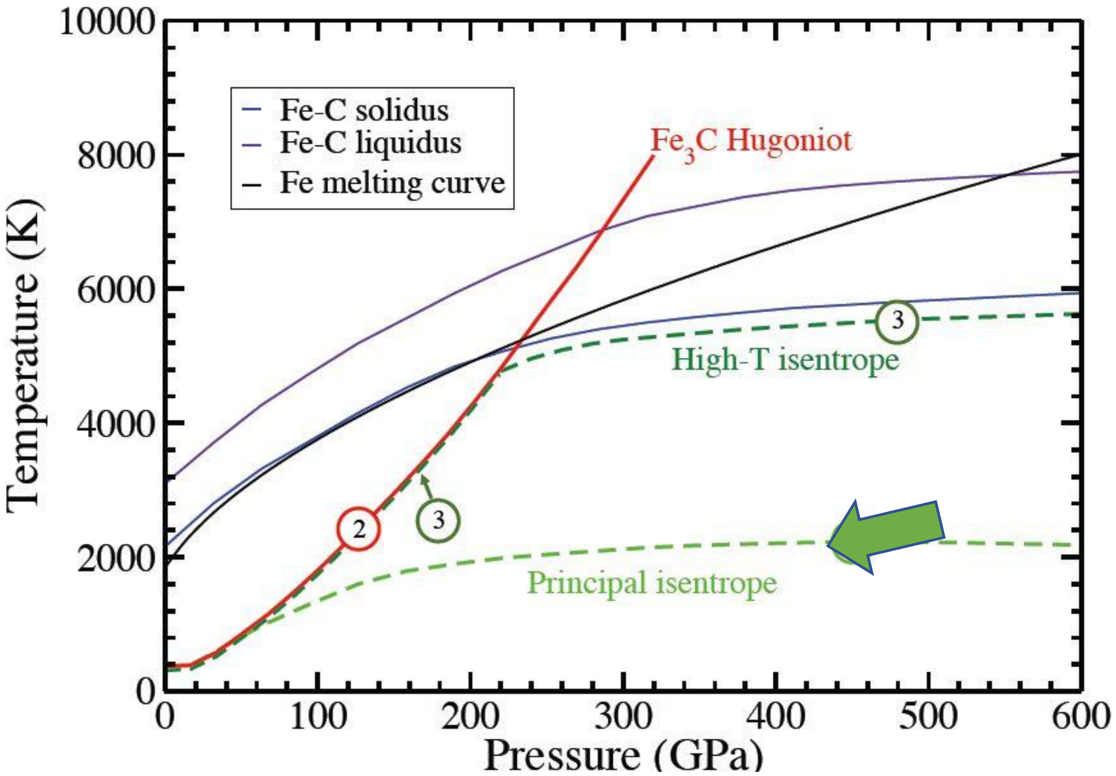
Structure of Fe_3C Under Ramp Loading up to 600 GPa



Questions

What is structure and EOS of iron carbide at conditions of the super-Earth cores?

Does Fe_3C undergoes decomposition into HCP Fe and higher carbon content carbides (e.g., Fe_3C_5) at ultrahigh pressures?

Implications

Explore stabilization of carbide phases in cores of up to 2-Earth mass terrestrial exoplanets

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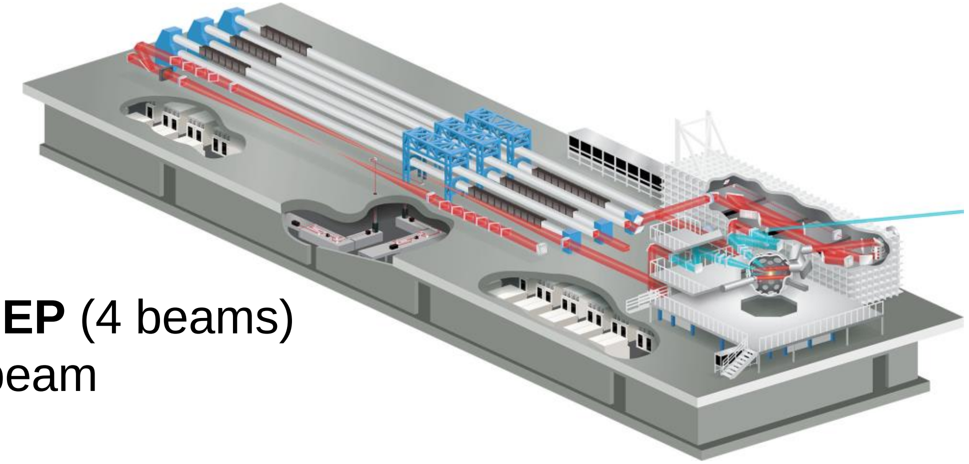
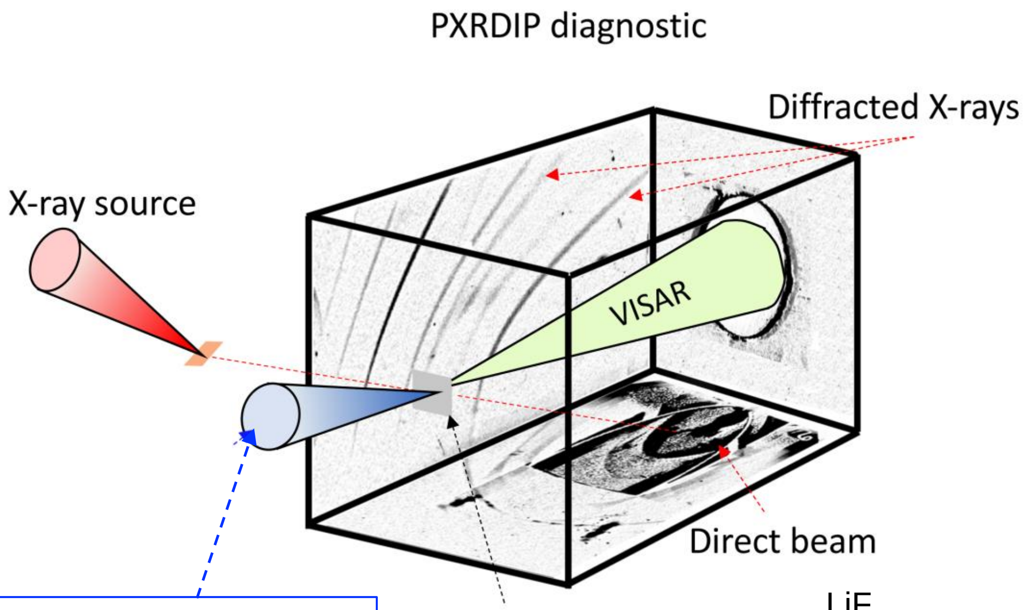
Plasma X-Ray Source at Omega EP Laser

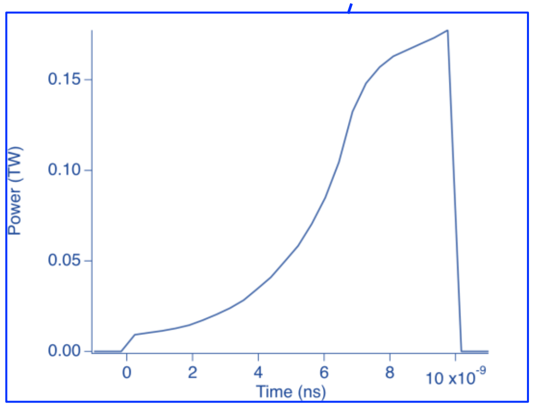


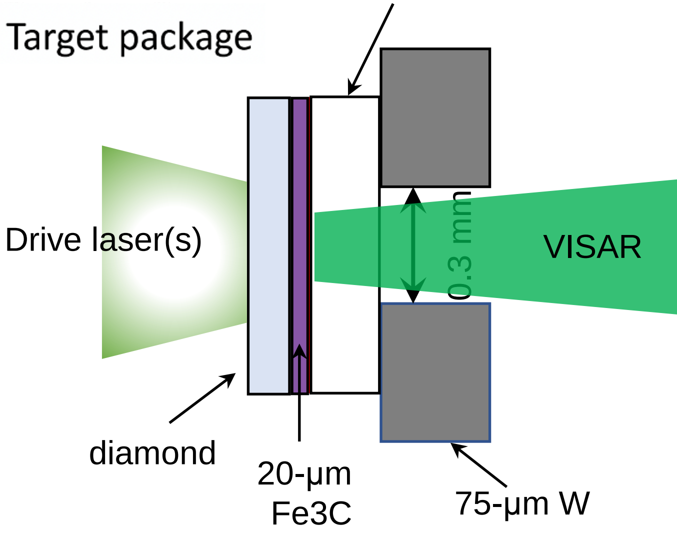
Omega-EP (4 beams)
6.5 kJ/beam

High-power multibeam laser facility where we can drive samples with a kJ pulse & tailored pulse shapes

Drive a thin Fe foil with a 2^{nd} high-intensity laser pulse which induces He_{α} emission of quasimonochromatic X-rays







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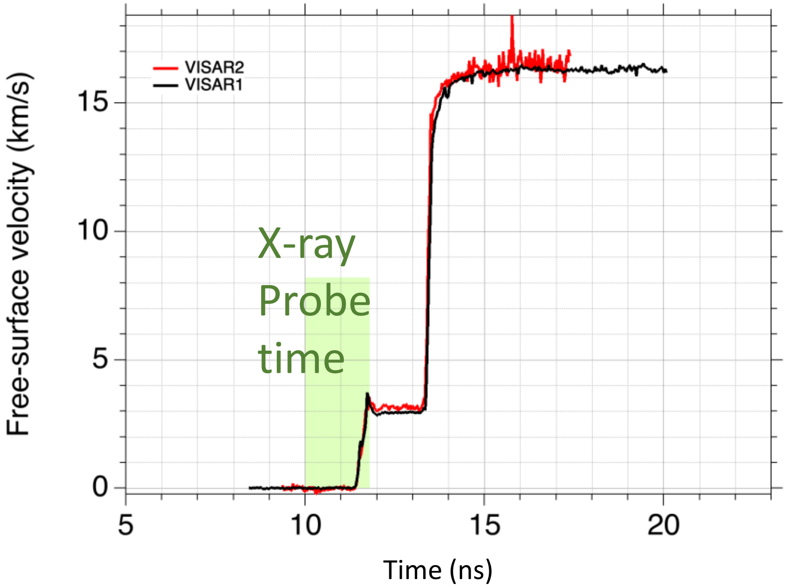
Laboratory for Laser Energetics
University of Rochester

Figs: D. Kim

Preliminary EP Results

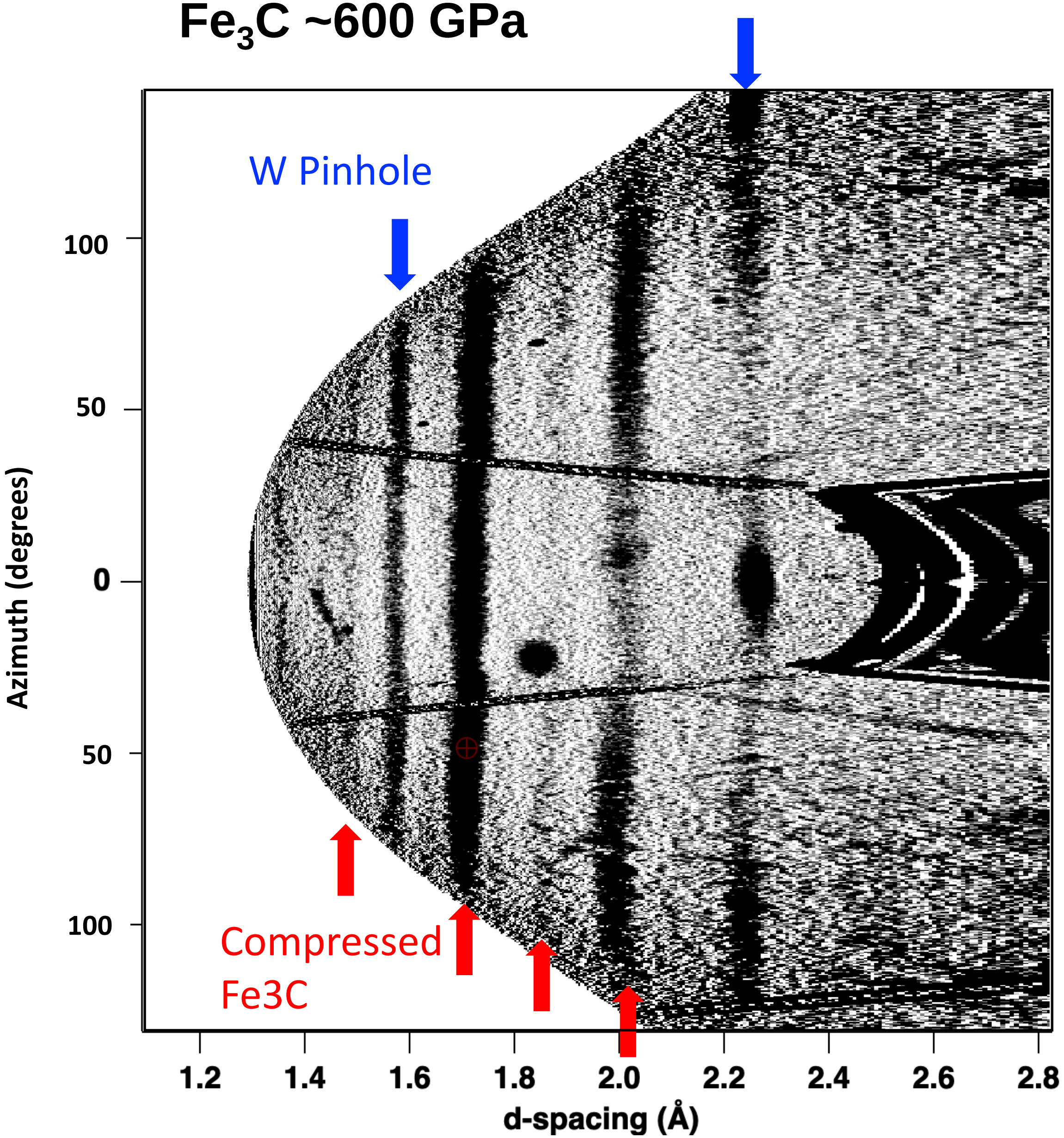


Collected 7 shots between 200-600 GPa

Orthorhombic Fe_3C phase observed up to highest pressure

No evidence for phase transition or breakdown into HCP-Fe + carbides

Fe_3C ~600 GPa



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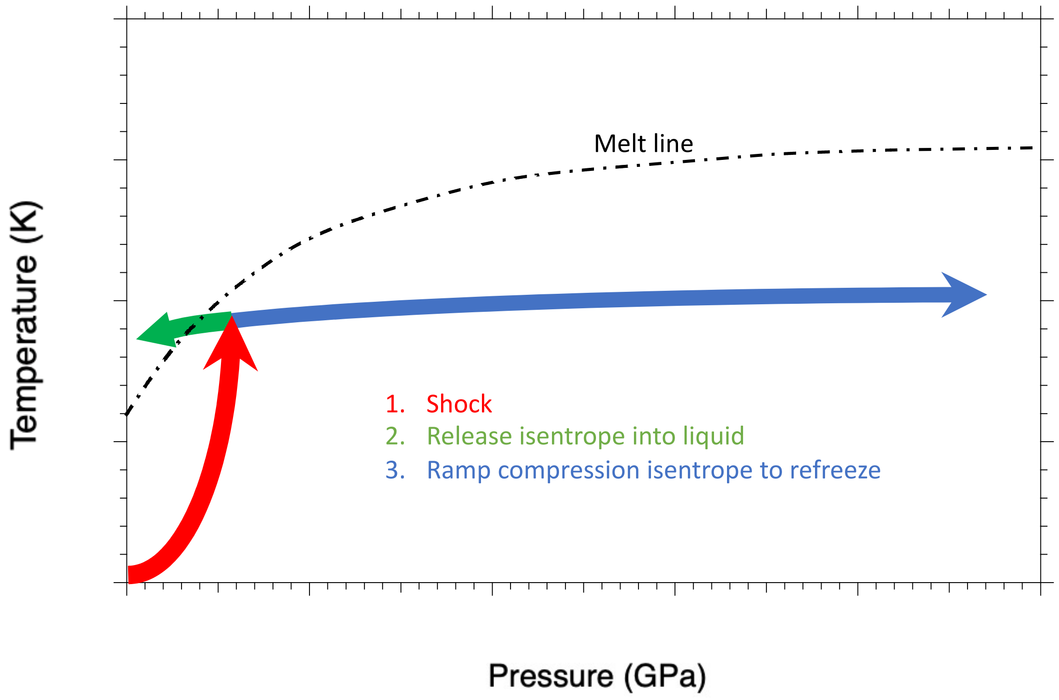
Up Next: Recrystallization at Omega EP

What role does kinetics have on our observations?

Fe_3C predicted to break down into HCP-Fe + carbide phases of different stoichiometries

Decomposition reactions are diffusion limited so may not be observed in ns dynamic compression experiments

Shock-Ramp – Melt-Refreeze
Recrystallization of the stable phase assemblage from the liquid



<u>Implications</u>
Direct measure of phase(s) crystallizing from the high-P melt at the pressures of Earth's inner-outer core boundary

Understand kinetics of nanosecond dynamic experiments

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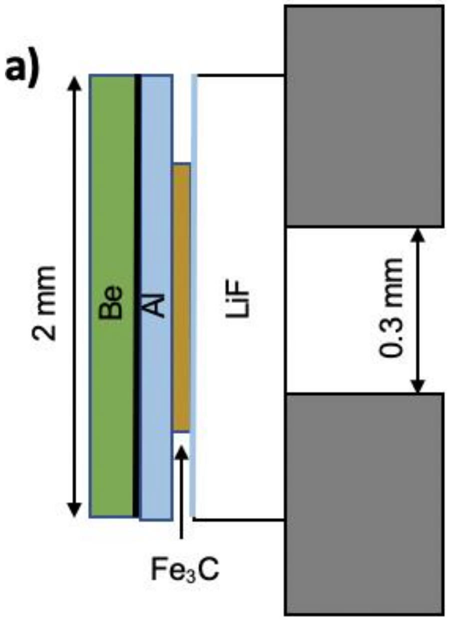
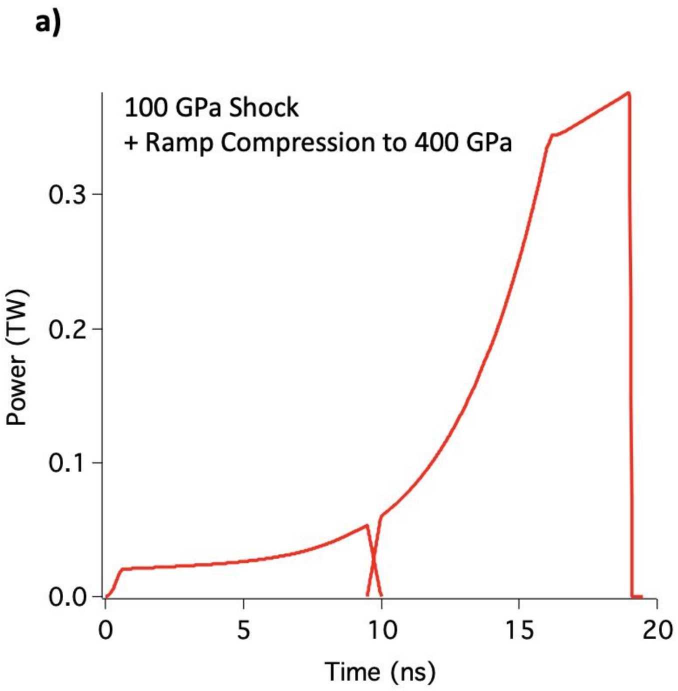
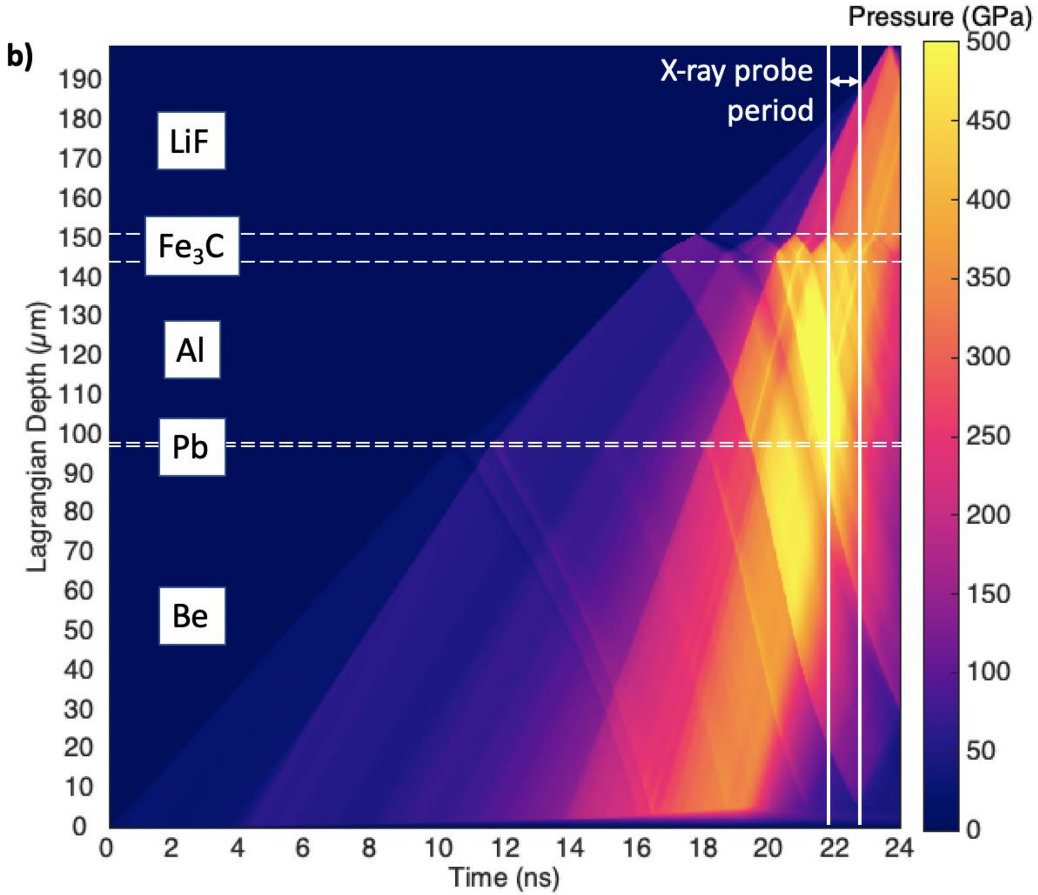
Shock-Ramp experiments







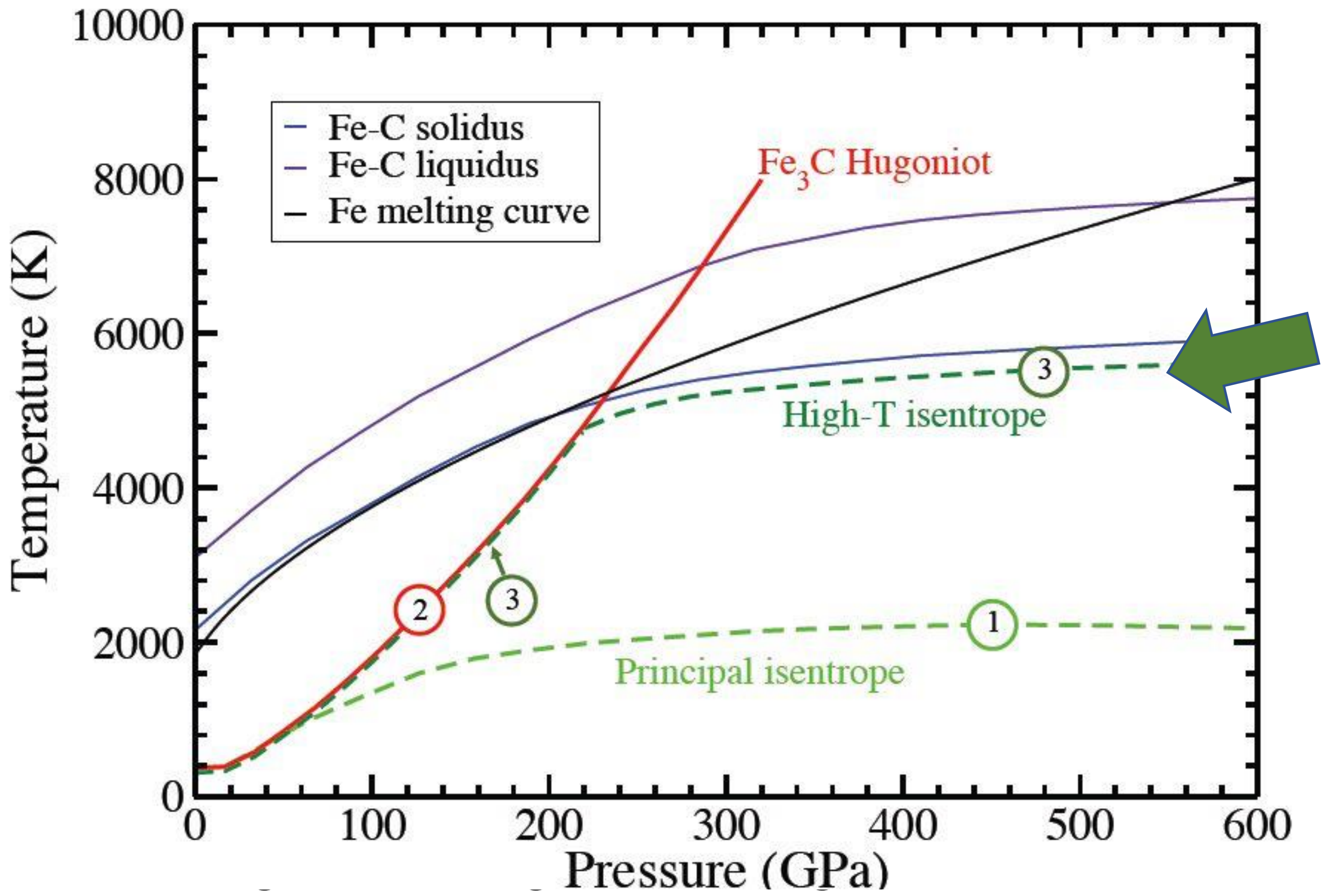
Conclusions

- Fe-C structure searches show evidence for stability of Fe_7C_3 and Fe_5C_3 at planetary core pressures.
- Fe_3C melts at 160 GPa into a single liquid along the Hugoniot
- Orthorhombic Fe_3C was observed under ramp compression up to 600 GPa, with no evidence for phase transition or breakdown into HCP iron and C-rich carbides

Future Directions

- Shock-ramp and melt-refreeze experiments at Omega EP
- Liquid structure analysis of DCS Data
- Molecular Dynamics calculations of temperatures along variable compression pathways

Shock-Ramp experiments 400 GPa



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