Exploring Al_2O_3 Crystal Structures at TPa Pressures Using Ramp Compression

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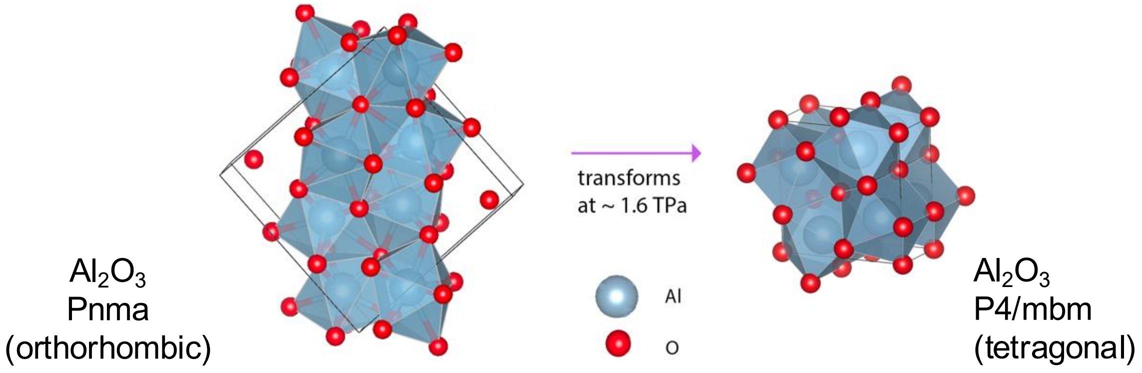
Compressing the stablest low-symmetry oxide at NIF: Why?

We don’t know how nature packs atoms beyond 1 TPa

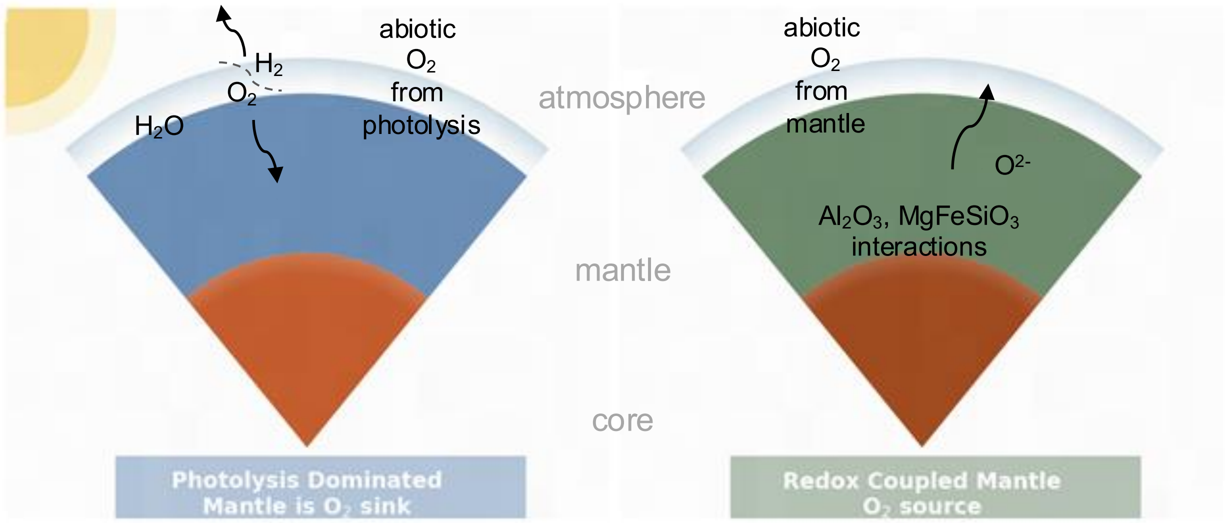
- NIF results will reveal whether low-symmetry oxides like Al_2O_3 transform into more close-packed or open structures, as observed in recent NIF studies of metals [1].



Al_2O_3 is predicted to transform from an orthorhombic to a tetragonal structure at 1.6 TPa [2]

Al_2O_3 can regulate planetary redox below 1 TPa

- NIF results on structural stability of Al_2O_3 will constrain redox models of rocky planets, improving interpretation of atmospheric observations of exoplanets [3–5].



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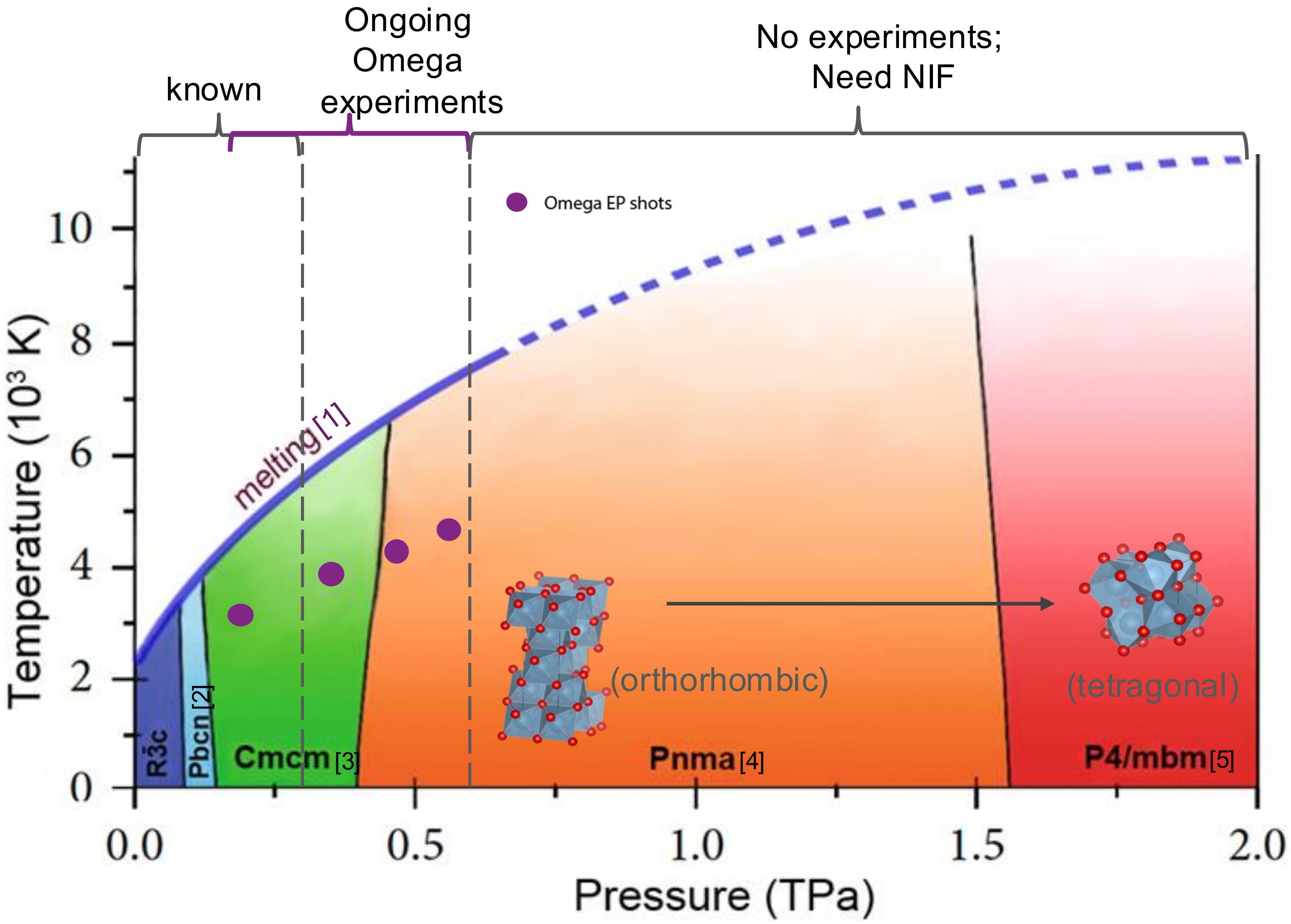
[1] Gorman et al., Nature 2022 [2] Huang et al., Research 2022 [3] Wordsworth et al., ApJ 2018 [4] Suer et al., in preparation [5] Hardegree-Ulmann et al, ApJ 2025

How do low-symmetry oxides transform at the TPa frontier?



ABO_3 Oxide Stability at Extreme Pressures

- Al_2O_3: Pnma predicted to be stable over a 1 TPa range then undergo symmetry increase to P4/mbm near 1.6 TPa [4, 5]
- $MgSiO_3$: Could dissociate between 0.6 and 1 TPa GPa [6]
- Fe_2O_3: An orthorhombic structure observed up to 0.4 TPa before amorphization [7]
- The NIF can provide structural information on these materials under TPa conditions [8]

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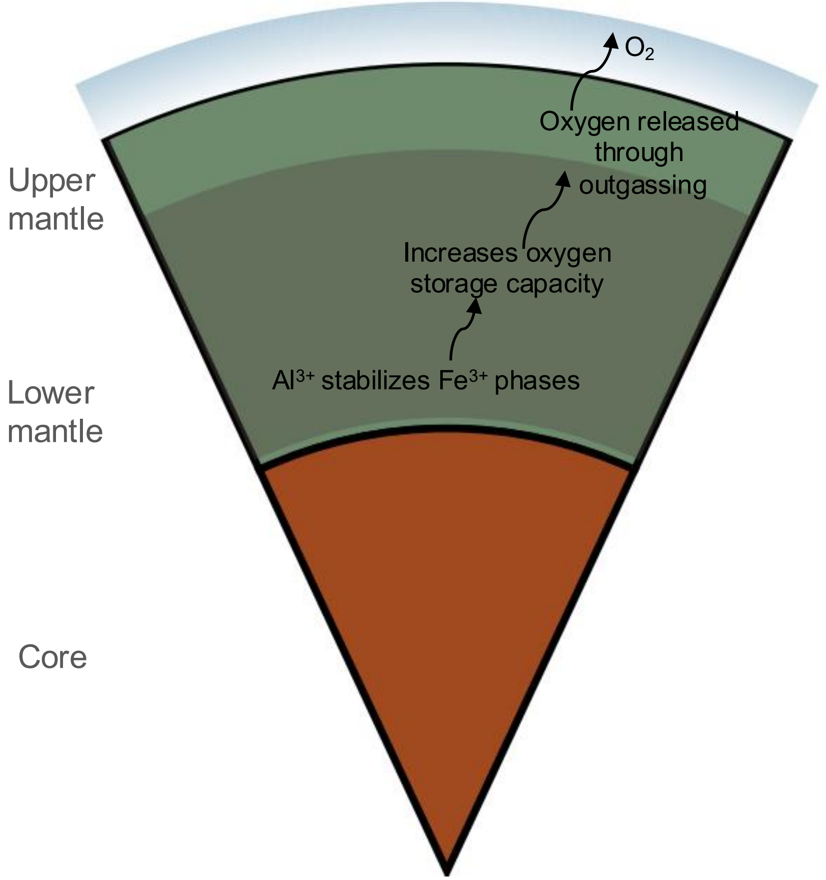
[1] Ostrik and Nikolaev, Journal of Phys conf., 2021 [2] Funamori and Jeanloz, Science 1997 [3] Ono and Oganov, PNAS 2005 [4] Umemoto and Wentzcovitch., PNAS 2008, [5] Huang et al., Research 2022
[6] Umemoto and Wentzcovitch, EPSL 2011 [7] Ocampo et al., in review [8] Gorman et al., Nature Physics 2022

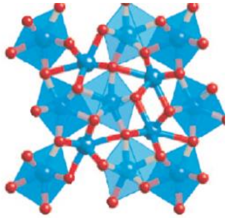
Structural transitions in Al_2O_3 may determine whether the deep-mantle oxygen cycle is active in super-Earths

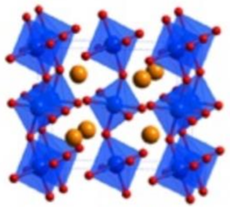


2 $Fe^{2+} \rightarrow Fe^{3+} + Fe^0$ transfers oxygen from metal to silicates. Al^{3+} stabilizes Fe^{3+} in $(Mg,Fe)SiO_3$, making this process efficient at driving mantle and surface oxidation—without adding oxygen from outside.

- Al_2O_3 is structurally similar to $(Mg,Fe)SiO_3$ (bridgmanite), the dominant mineral in Earth and super-Earth mantles.
- Al^{3+} drives $Fe^{2+} \rightarrow Fe^{3+}$ conversion in bridgmanite, sequestering more oxygen—key to long-term mantle and surface oxidation [1-4].
- This mechanism may operate in super-Earths if Al_2O_3 and related phases remain stable in similar orthorhombic structures such as Pnma and Cmcm.

Al_2O_3 Pnma [5]





$MgSiO_3$ PPv Cmcm [6]

- NIF TARDIS platform can resolve these structures under ramp to planetary mantle conditions

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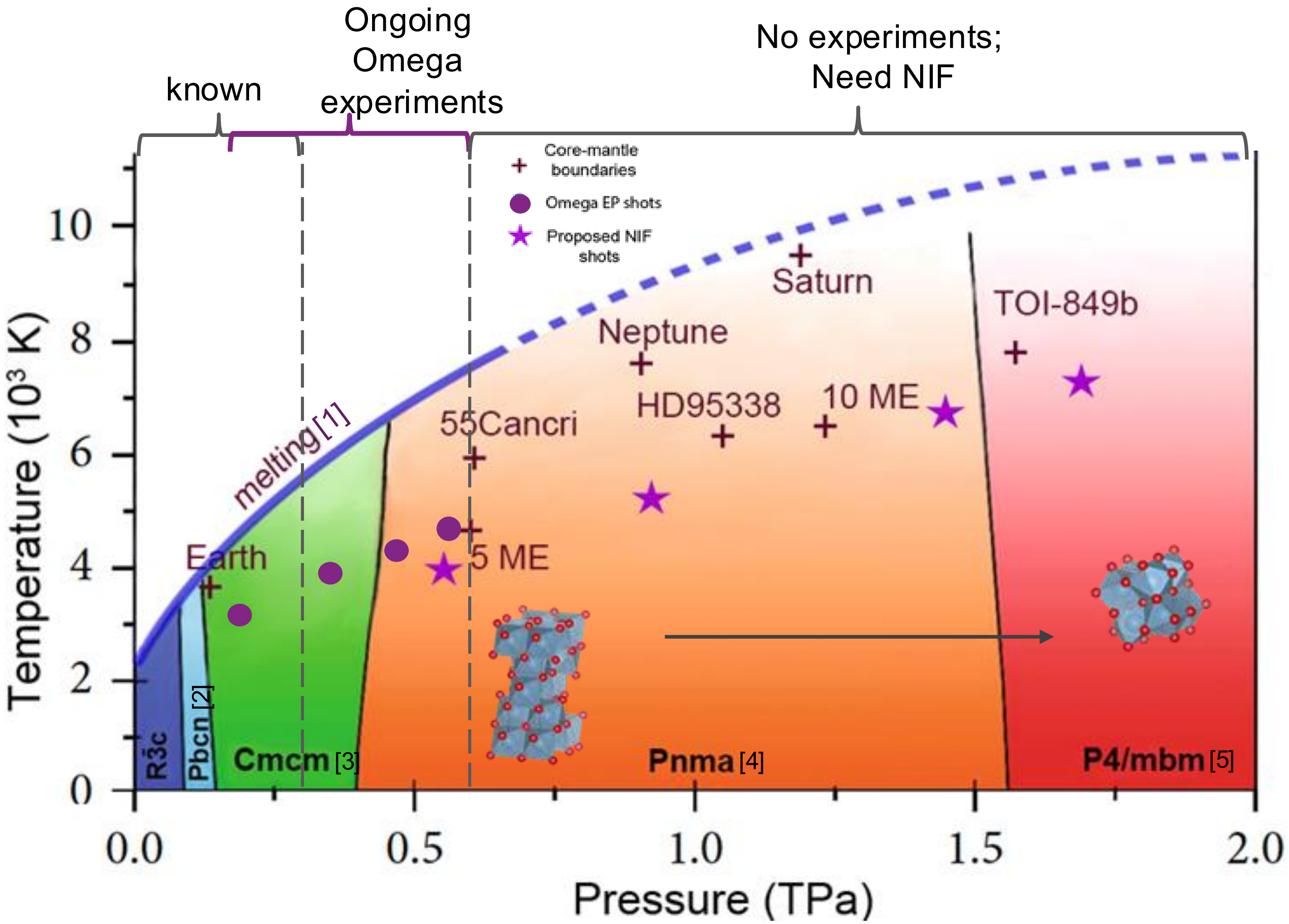
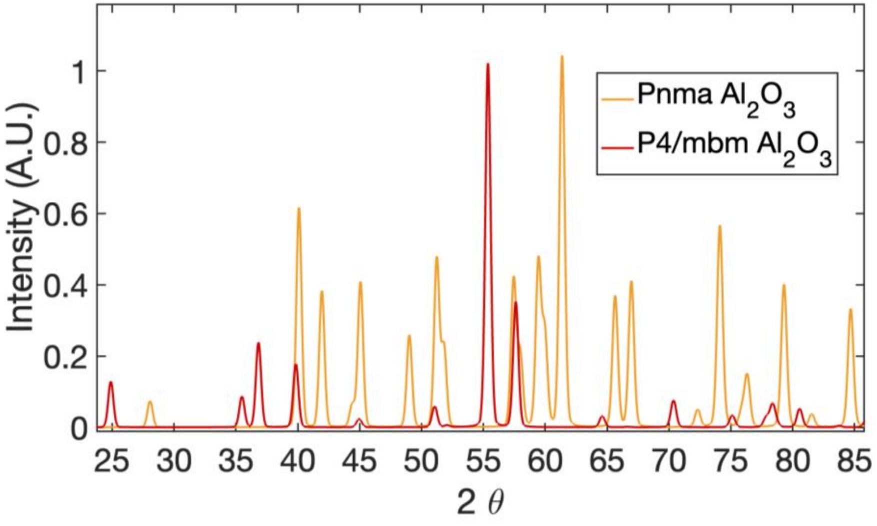
[1] Hirshmann, EPSL 2023 [2] Frost et al., Nature, 2004 [3] Oneill and Aubach, Scientific Reports 2022 [4] Andrault et al., GPL 2018 [5] Umemoto and Wentzcovitch., PNAS 2008 [6] Murakami et al., Nature 2005

Most of the Al_2O_3 phase diagram can only be accessed by the NIF



We plan to measure predicted structures (Pnma, P4/Mbm) of Al_2O_3 from 0.6 to 1.7 TPa, with the NIF



Candidate Al_2O_3 structures at 1.7 TPa with Ge x-ray source, 2° peak width [4, 5]

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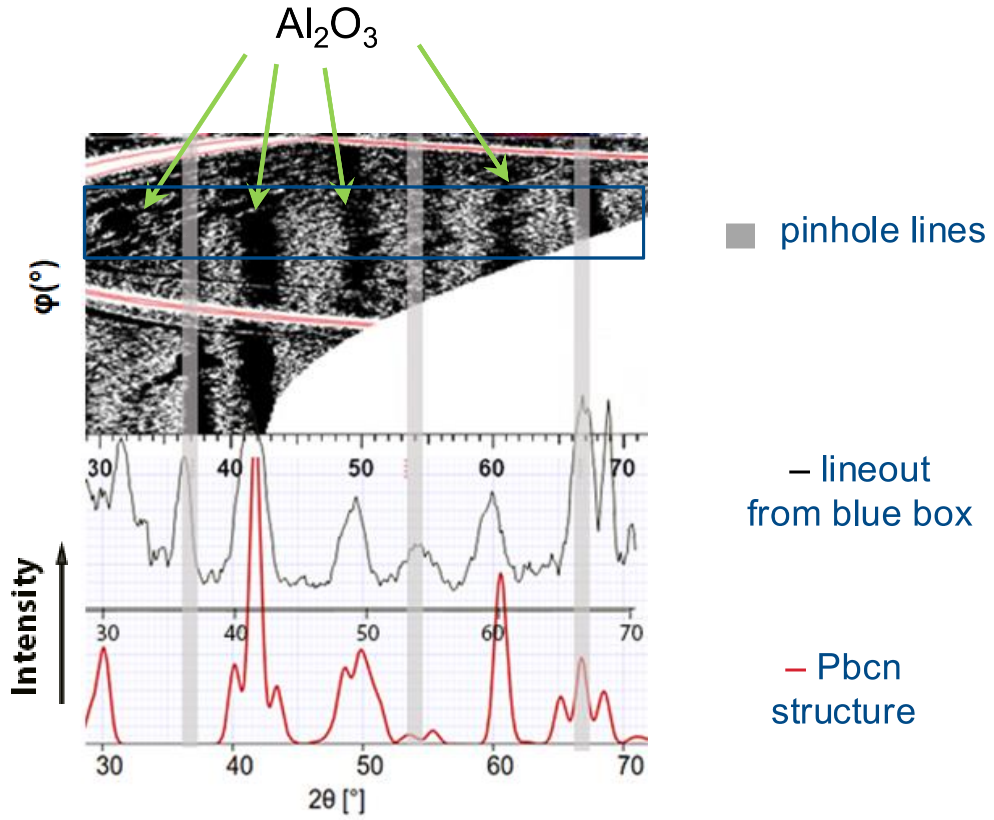
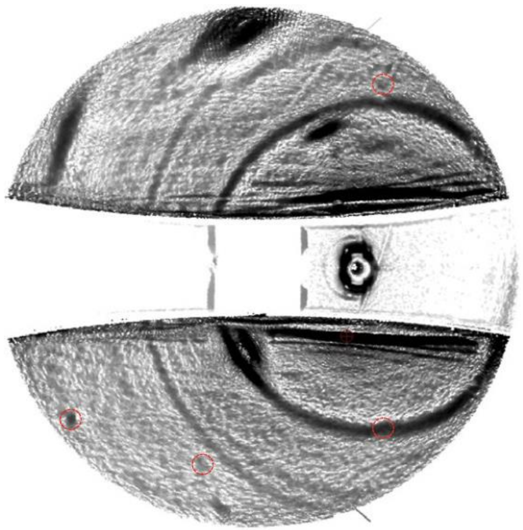
[1] Ostrik and Nikolaev, Journal of Phys conf 2021 [2] Funamori and Jeanloz, Science 1997 [3] Ono and Oganov, PNAS 2005 [4] Umemoto and Wentzcovitch., PNAS 2008, [5] Huang et al., Research 2022

Recent OMEGA-EP Results Motivate NIF experiments to Resolve Crystal Structure of Al_2O_3 at TPa Pressures

- Powder diffraction was collected from polycrystalline Al_2O_3 ramp compressed to ~400 GPa with a 20 ns pulse on Omega EP



- NIF enables long stable ramp drives (~40 ns) to reach 1.7 TPa while keeping temperatures below 10000 K.
- TARDIS provides high x-ray, SNR [1], broad 2-θ coverage, to enable high quality diffraction and resolution of structurally complex phases of Al_2O_3



Powder diffraction on Mg under ramp compression to ~1 TPa from a recent NIF study [2]. We expect similar signal to noise to this work due to similarity in atomic numbers with Al.

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[1] Rygg et al., Review in Scientific Instrumentation, 2020
[2] Gorman et al., Nature Physics 2022

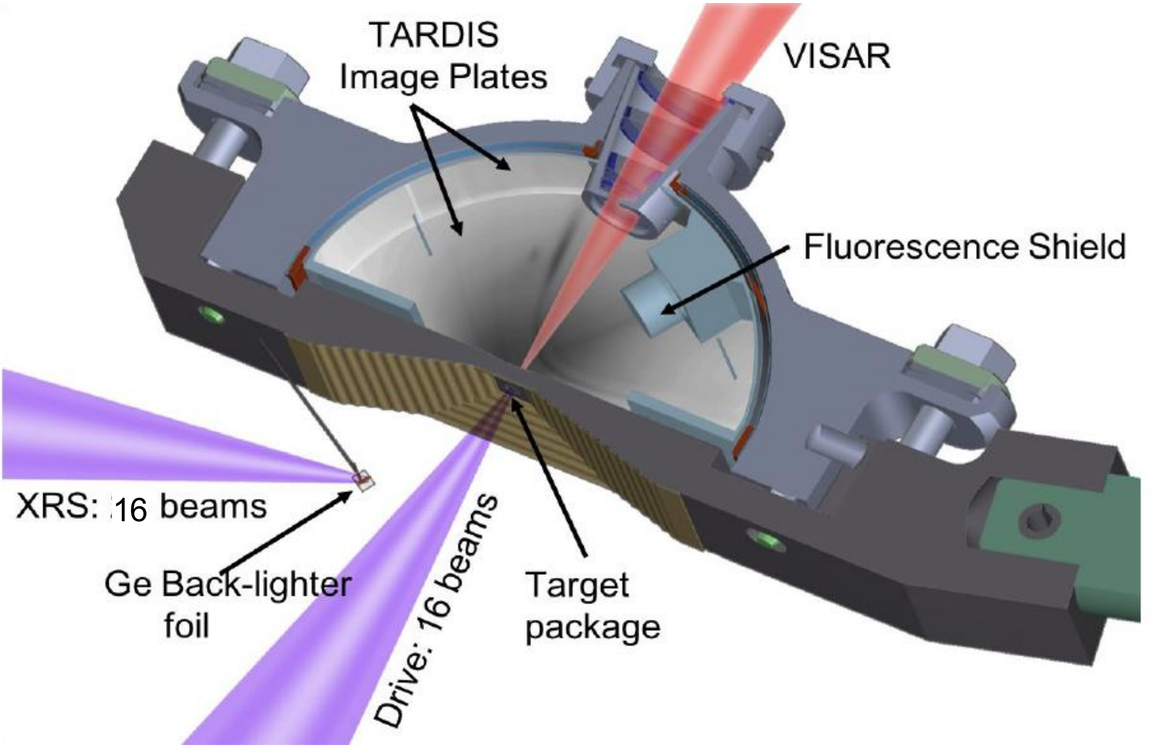
Experimental Approach/Requirements: We will use the TARDIS platform in a standard configuration

Experimental Approach

- Ramp compress polycrystal Al_2O_3 targets with the NIF following protocol developed in recent NIF-TARDIS experiments [1–4].
- **Sample Drive**: 4-quads (16 beams, standard DPP); 40 ns ramp pulse shape; total laser energy ~50 kJ (~3 kJ/beam); total peak power of ~0.5 TW/beam
- **Backlighter Drive:** 6-quads (24 beams, no DPP); ~ 2ns pulse shape; total laser energy of ~150 kJ (~6.25 kJ/beam) and a total peak power of ~2 TW/beam.
- Use velocimetry and XRD diagnostics to probe sample state and structure.
- Compare XRD results to ongoing structure searches by the theory team.

Diagnostic Requirements

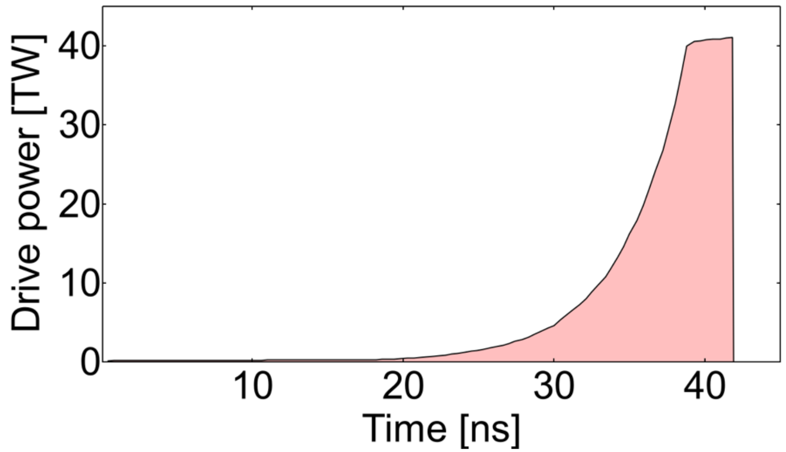
- Primary: TARDIS, VISAR
- Secondary: NXS/DISC or GXD/Supersnout
- No new diagnostics or modifications



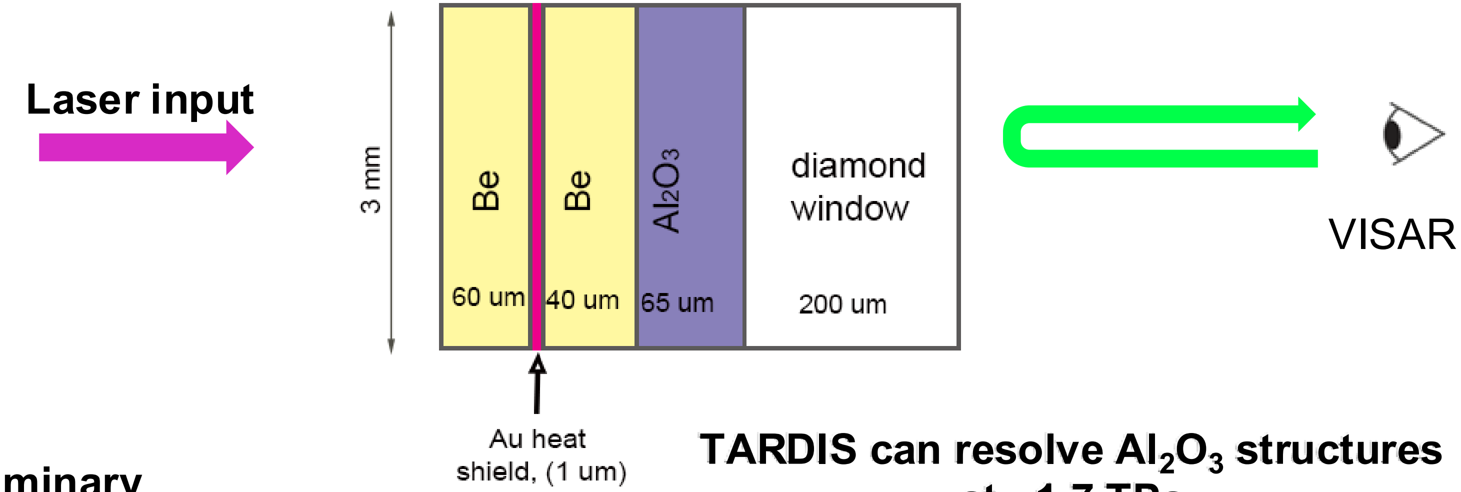
[1] Rygg et al., Rev.Sci.Inst 2020 [2] Gorman et al., Nature Physics 2022 [3] Lazicki et al., Nature 2020
[4] A. Krygier et al., Phys. Plasmas 2022

We will measure the phase of Al_2O_3 ramp compressed between 0.5 and 1.7 TPa, where it is predicted to stabilize or transform to a more symmetric phase

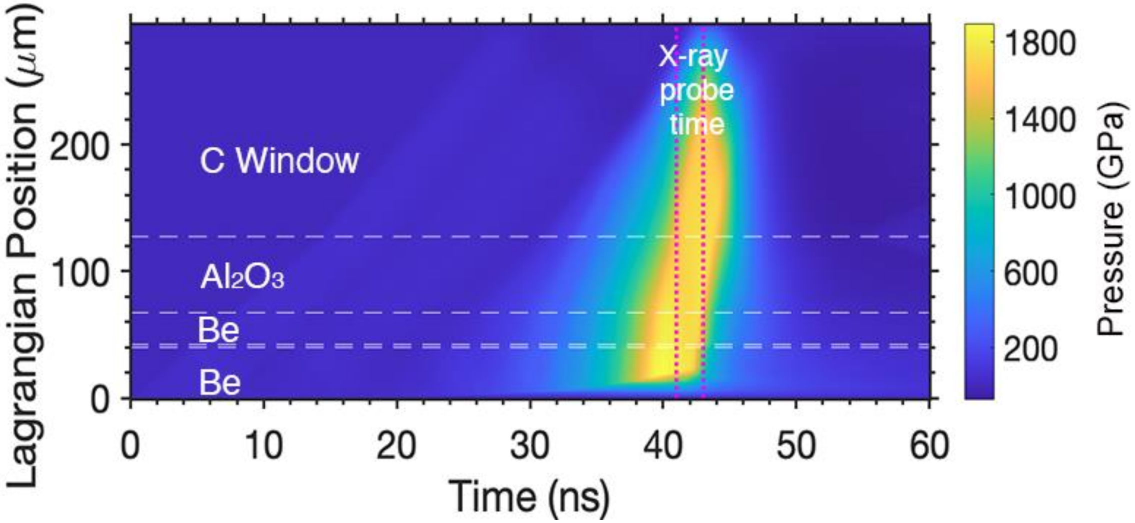
Ramp pulse shape



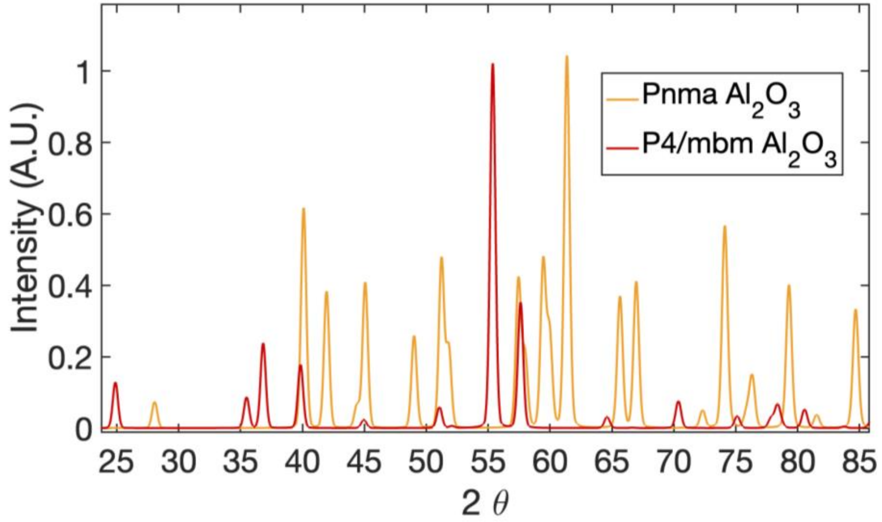
propose target geometry



Pressure evolution of target from preliminary simulation of the target for requested NIF shots



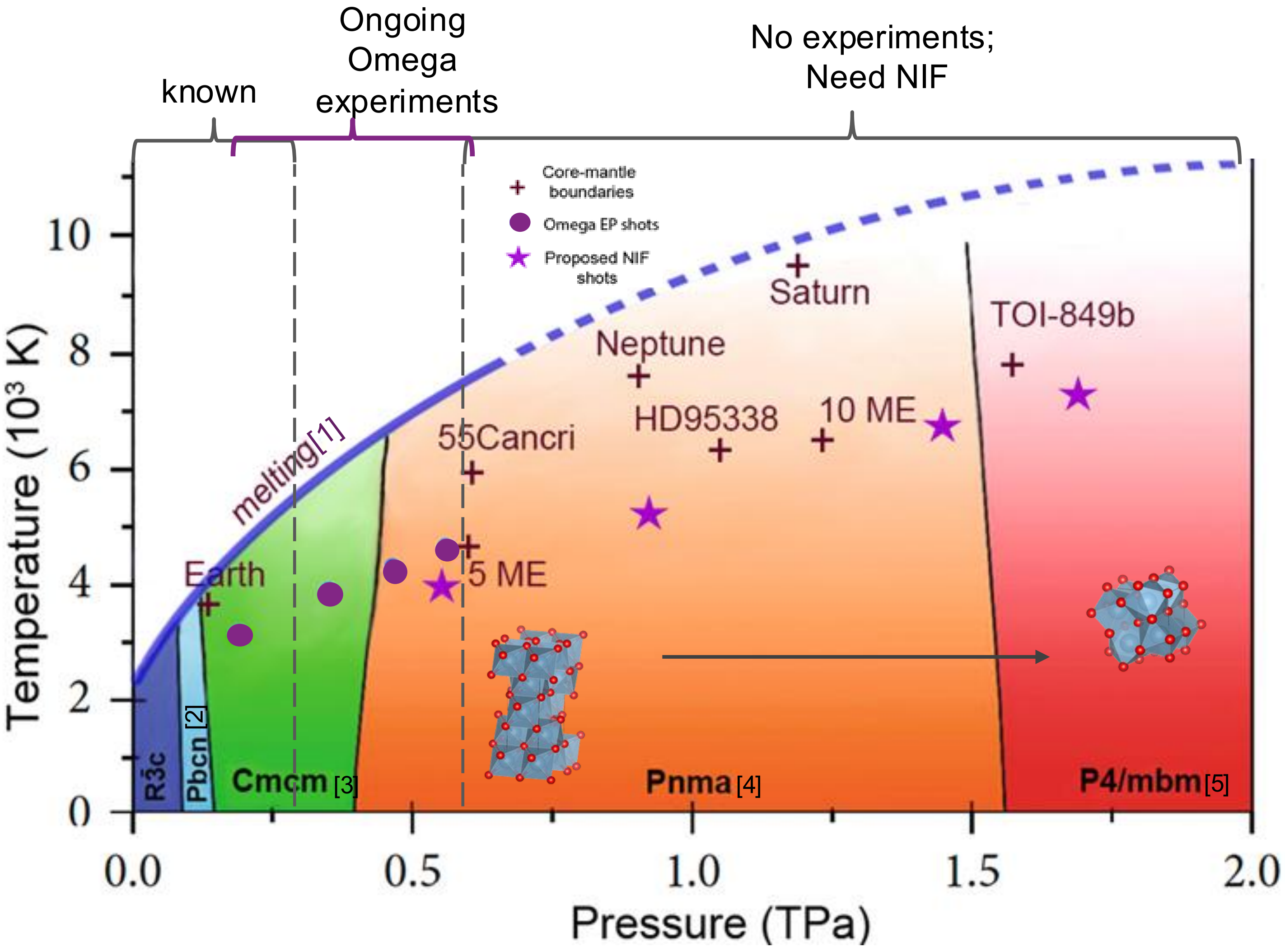
TARDIS can resolve Al_2O_3 structures at ~1.7 TPa



Candidate Al_2O_3 structures at 1.7 TPa with Ge x-ray source, 2° peak width [1, 2]

[1] Umemoto and Wentzcovitch, PNAS, 2008
[2] Huang et al., Research 2022

Four shots will probe the Al_2O_3 structures at key pressures to address our two main scientific objective



Proposed shot plan

Shot #	Objectives	Target P (TPa)
1 [FY26]	Establish background levels, signal to noise and test pulse shape	0.7
2 [FY26]	Disambiguate structures seen in EP data and confirm phase stability	0.5 to 1
3 [FY27]	Search for P4/mbm structure/Identify stable phase	1.7
4 [FY27]	Refine phase boundary between Pnma and P4/mbm in this pressure range	1 to 1.6

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[1] Ostrik and Nikolaev, Journal of Phys conf, 2021 [2] Funamori and Jeanloz, Science,1997 [3] Ono and Oganov, PNAS 2005 [4] Umemoto and Wentzcovitch., PNAS, 2008, [5] Huang et al., Research, 2022

Our team

- **LLE:** Planetary Materials, NIF, TARDIS,

Terry-Ann Suer, Danae Polsin, Gilbert Collins, Ryan Rygg, Michelle Marshall, Xuchen Gong, Alex Chin, Grigoriy Tabak

- **LLE; University of Buffalo; Cambridge University:** Density Functional Theory

Shuai Zhang, LLE, Stefano Racioppi, Eva Zurek

- **LLNL:** NIF, TARDIS, Planetary materials

Jon Eggert, Federica Coppari, Dayne Fratanduono, Amy Coleman (PoC)

- **MIT:** Exoplanet detection and characterization

Sara Seager

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