X-ray Diffraction of Ramp Compressed Silicon

![Graph showing Si-LiF Interface Temperature (K) vs. Si bulk pressure (GPa)]

- **hcp** (this work)
- **fcc** (this work)
- **dhcp (?)**
- **hcp**
- **Cmce**
- **Melt Curve (PBEGGA)**
- **Isentrope (PBEGGA)**
- **Isentrope (PBEGGA)** (include plastic work heating)

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We observe hexagonal close-packed (hcp) structure from 33 to 99 GPa and face centered cubic (fcc) structure from 150 to 390 GPa in ramp compressed silicon.

- Angle dispersive x-ray diffraction allows us to observe crystal structure of ramp compressed silicon up to 390 GPa.
- Optical pyrometry is used to infer temperature of silicon. A statistical model is developed to estimate temperature below the traditional optical pyrometry detection limit.
- The predicted double-hexagonal close-packed (dhcp) phase was not observed, and the hcp phase persists to higher pressure than anticipated by theory.
- We observe deviation from the theoretical isentropic compression path.
Collaborators


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Theory predicts* a new dhcp phase above 400 K, and between 30 and 70 GPa. The fcc phase is predicted to be stable until 2.8 TPa.

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Silicon sample is ramp compressed to desired pressure using OMEGA EP laser, and x-ray is used to generate diffraction image at peak compression.

* VISAR: Velocity interferometer system for any reflector
Pressure is inferred from Si-LiF interface velocity measured by VISAR*

\[ \text{Pressure (GPa)} = \frac{\text{Sample Drive Intensity (TW/cm}^2\text{)}}{\text{Si-LiF Interface Velocity (km/s)}} \]

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characteristics method

1-ns x-ray
Two distinct types of x-ray diffraction patterns are observed.
At lower pressures between 33 and 94 GPa, we observe hcp structure, as opposed to dhcp predicted by theory.

Shot 32081 @ 52 ± 4 GPa
At lower pressures between 33 and 94 GPa, we observe hcp structure (as opposed to dhcp predicted by theory).

The pattern matches well with hcp structure.

The absence of (103) peak of dhcp suggests dhcp is not the right structure.

The absence of (101) peak of simple hexagon (sh) also rules out this structure.
At pressures above 152 GPa, fcc is observed, and persists to the highest pressure we reached, 390 GPa.
The temperature of ramp compressed silicon is measured using SOP*

- For streaks shorter than 50 ns, the SOP signal from self-emission of sources below 5000 K is not easily distinguishable from the noise.
- A statistical model is developed to untangle self-emission signal and background noise, therefore determining the temperature of the silicon emitter.

* SOP: Streaked Optical Pyrometer
We observe deviation from theoretical isentropic compression path.
Plastic work heating due to strength of silicon partially accounts for the deviation from ideal isentropic path.

\[ \text{Plastic work heating due to strength of silicon partially accounts for the deviation from ideal isentropic path} \]

\[ \text{Melt Curve (PBECCGA)} \]

\[ \text{Isentrope (PBECCGA)} \]

\[ \text{(include plastic work heating)} \]

\[ \text{DAC data\textsuperscript{*}} \]


The predicted dhcp phase was not observed. We instead observe hcp phase persists to higher pressure than anticipated from theory, before transforming into fcc structure.

![Graph showing Si-LiF Interface Temperature (K) vs. Si bulk pressure (GPa)](image)

- hcp (this work)
- fcc (this work)

Melt Curve (PBE GGA)

Isentrope (PBE GGA)
(include plastic work heating)

Isentrope (PBE GGA)

Summary

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