Observation of a New High-Pressure Solid Phase in Dynamically Compressed Aluminum

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We present the first in-situ high-pressure observation of bcc aluminum

- Aluminum and other prototypical sp-bonded materials are predicted to transform into complex, open, and incommensurate structures at multiterapascal pressures.
- High-power lasers ramp compressed Al and nanosecond in-situ x-ray diffraction (XRD) measured the crystal structure at pressures of 111 GPa to 547 GPa.
- The fcc–hcp and hcp–bcc phase transformations are observed at $216 \pm 9$ GPa and $321 \pm 12$ GPa, respectively.
- Texture evolution shows that even on nanosecond time scales, atoms can rearrange in the spaces between close-packed planes.

Summary

fcc: face-centered cubic
bcc: body-centered cubic
hcp: hexagonal close packed
Collaborators

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Outline

- OMEGA diffraction experiments
- NIF* experiment
  - dual backlighter
- Texture evolution

*NIF: National Ignition Facility
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The high-pressure EOS of many materials are referenced to the Al EOS*,**, 

Accurate knowledge of the Al equation of state (EOS) is required to avoid the introduction of systematic errors in high-energy-density (HED) measurements.

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‡VISAR: velocity interferometer system for any reflector
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Increasing structural complexity

Data are needed to provide benchmarks for density functional theory (DFT).


*X. Gong et al., POS.00007, this conference.

Aluminum is predicted* to undergo fcc–hcp and hcp–bcc solid–solid phase transitions as it is compressed at low temperatures

- Solid x-ray diffraction experiments are limited to 125 GPa along the principal Hugoniot because of shock melting
- Diamond-anvil cell (DAC) experiments measured the fcc–hcp transition at 217 GPa and 297 K

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**Y. Akahama et al., Phys. Rev. Lett. 96, 045505 (2006);
Ramp (shockless) compression is used to access high-pressure, low-temperature states

\[ P \text{ (GPa)} = 42 \left( \frac{I \text{ (TW/cm}^2\right)}{0.71} \]

*D. E. Fratantuono et al., J. Appl. Phys. 110, 073110 (2011).*
Pressure distributions in the Al samples are calculated using the measured Al–LiF interface velocities.
The x-ray backlighter was timed to probe the uniform pressure plateau in the Al pressure profile.

The sample is at a uniform, solid, high-pressure state at the time of the x-ray probe.
Monoenergetic x rays incident on an ideal powder sample will diffract in rings of uniform intensity at angles $2\theta$ with respect to the x-ray beam.

Compression of interatomic spacing ($d$ spacing) is determined by measuring diffraction angles ($2\theta$) and x-ray wavelength ($\lambda$).
Monoenergetic x rays incident on an ideal powder sample will diffract in rings of uniform intensity at angles $2\theta$ with respect to the x-ray beam.

Textured foils diffract into spots rather than continuous rings.
The powder x-ray diffraction image plate (PXRDIP)* diagnostic is used to record diffraction patterns on OMEGA EP

When pressure was increased from 111 GPa to 299 GPa, two diffraction lines were newly observed, consistent with hcp aluminum and distinct from fcc.
Above 321 GPa, a region of coexistence is observed, then a single intense line appears, consistent with (110) bcc aluminum.
The fcc–hcp and hcp–bcc phase transformations are observed at 216±9 GPa and 321±12 GPa, respectively.
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At higher pressures, the ramp is steeper and small shocks start to form. The aluminum still remains solid.
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A 30-ns ramp pulse held the pressure in the Al constant for over 2 ns at two different pressures where the hcp and bcc phases were observed on OMEGA.
The hcp phase is observed at 311 GPa
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Three lines from the bcc phase are observed at 547 GPa.

The diagram shows a graph with time (ns) on the x-axis and interface velocity (nm/ns) on the y-axis. There are plateaus at 547 GPa, indicating the presence of bcc phase. The diagram also shows the orientation of the bcc (110) and bcc (211) phases at 547 GPa.
Three lines from the bcc phase are observed at 547 GPa
NIF experiments probe two high-pressure phases in a single shot and confirm the bcc phase in OMEGA data.
A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is stable at higher temperatures than calculated by DFT.

Shock observed at Al–LiF interface (100 GPa, 3100 K).
A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is more stable at higher temperatures than calculated by DFT.

The Al in the NIF data is at an elevated temperature state compared to the Al in the OMEGA data as a result of shock heating.
A calculated shock-ramp–compression path for the NIF experiment suggests the hcp phase is more stable at higher temperatures than calculated by DFT.

These data provide key experimental benchmarks for DFT calculations.
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The rolled foils were characterized on a diffractometer beforehand and show (200) plane normals are nearly parallel to the pressure loading axis.

Crystallographic texture is the distribution of grain orientations in a polycrystalline sample. Textured foils diffract into spots rather than continuous rings.
The initial texture of the rolled foils is maintained through the fcc—hcp and hcp—bcc phase transitions.

fcc (111) 216 GPa

hcp (002) 291 GPa

bcc (110) 456 GPa

The preferred orientation in “textured” rolled foils can provide insight into the atomic pathways.

We expect diffraction lines should become more powder-like through phase transformations as atoms rearrange.

Close-packed planes do not randomize through the phase transformations.

- bcc (110)
- hcp (002)
- fcc (111)
The high-pressure texture of the hcp and bcc phases suggests close-packed or nearly close-packed lattice planes remain parallel through both transformations.

Shoji–Nishiyama OR:*  
\{111\}_{\text{fcc}} // \{0001\}_{\text{hcp}}

Burgers OR:**  
\{0001\}_{\text{hcp}} // \{110\}_{\text{bcc}}

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*Orientation relationship

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Kinetics of phase transitions will be studied using time-resolved x-ray diffraction.*

*R. Benedetti et al., YO6.00011, this conference*