

Orientation-Dependent Structural Phase Transitions and Melting in Shock-Compressed MgO

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Magnesium oxide (MgO) is a prototypical strongly bonded ionic solid and an expected major constituent of rocky planet mantles and gas giant cores, yet its high-pressure phase diagram and shock response remain incompletely understood. Here we combine laser-driven decaying-shock and steady-shock compression with nanosecond x-ray diffraction, velocimetry, and optical pyrometry to investigate phase transitions in single-crystal MgO compressed to 600 GPa and 13 000 K. We observe a pronounced crystallographic orientation dependence in the B1 → B2 transformation pathway and subsequent melting behavior. For compression along [111], the shock-temperature evolution exhibits distinct plateaus consistent with equilibrium B1 → B2 → liquid transitions. In contrast, compression along [110] produces a single temperature discontinuity and diffraction signatures indicative of B2 nucleation from a transient disordered layer at the shock front. The combined thermodynamic and structural data indicate that near-instantaneous disordering can mediate stress relaxation under rapid uniaxial compression. Above 572 ± 24 GPa, all orientations converge to complete melting at $13\,200 \pm 600$ K, constraining the B2-liquid boundary at multimegabar pressures and identifying MgO as the highest-temperature solid measured at planetary interior conditions. These results demonstrate that crystallographic orientation governs phase-transition pathways in strongly compressed ionic solids and provide a benchmark for modeling matter under extreme planetary interior conditions.

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I. INTRODUCTION

The transformation pathways of phase transitions in strongly bonded ionic solids under extreme pressure and strain rate remain poorly constrained by experiment. In particular, whether crystallographic orientation selects among competing solid → solid transition mechanisms, or influences the melt dynamics during the solid → liquid transition under uniaxial dynamic compression has not been systematically investigated.

Magnesium oxide (MgO) provides an ideal system in which to address this question. As a prototypical B1

(NaCl-type) ionic solid that undergoes a reconstructive transformation to the B2 (CsCl-type) structure at multimegabar pressures [1], MgO exhibits multiple theoretically predicted atomistic pathways for the B1 → B2 transition. Because this transformation involves substantial atomic rearrangement and coordination change, its onset pressure, thermodynamic signature, and dynamically selected pathway may depend sensitively on the loading geometry and associated shear stress environment. Understanding how this transition proceeds under shock compression therefore provides a stringent experimental test of high-pressure condensed-matter theory.

Beyond its importance as a model ionic solid, MgO is an expected major constituent of terrestrial mantles and the cores of gas giant planets [1,2]. In Earth's lower mantle, which accounts for nearly half the planet's mass and volume, MgO forms a solid solution with FeO as the second most abundant phase [3,4]. The ambient B1 phase is stable within Earth's mantle but is predicted to transition to the B2 phase at pressures between 300 and 600 GPa, characteristic of large rocky exoplanet interiors [1,4]. This structural transition is expected to influence mantle rheology, planetary differentiation, and core-mantle

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interactions [4–6]. At elevated temperatures, MgO may also exist as an electrically conductive fluid, with implications for planetary magnetic field generation [7]. Despite its geophysical significance, substantial discrepancies persist between theoretical predictions and experimental constraints on the high-pressure phase diagram of MgO [1]. Improved experimental constraints on MgO’s high- P - T phase stability are therefore essential for accurately modeling the formation and evolution of Earth, large rocky exoplanets [8,9], and gas giants [2,10].

Shock compression is a powerful method to reach these extreme conditions. It enables measurements along the Hugoniot curve, which defines the possible thermodynamic states achieved by a material upon shock loading. The Hugoniot states are governed by the conservation of mass, momentum, and energy across the shock front [11]. Phase transitions are one of several mechanisms by which a material subjected to shock compression can accommodate shear strain [12–14]. In the absence of a phase transition, the temperature in a shocked material steadily increases with increasing compression to accommodate the increase in internal energy. However, a change in the phase results in an abrupt change in the otherwise slowly varying Hugoniot curve and appears as jogs or kinks in T vs P (Fig. 1). In the equilibrium view (no kinetic effects), melt initiates where the Hugoniot first intersects the solid-liquid phase boundary. Increasing shock pressure further accesses states along the melt line with coexistence of solid and liquid phases until full melt is achieved. However, when present, time-dependent deformation is predicted to produce

different P - T states [12,15,16] (Fig. 1); which are measurable in our experiments.

Previous shock compression studies on MgO have been limited to uniaxial loading along the [100] axis of single crystals [1,7,17–19]. To investigate whether crystallographic loading direction might contribute to discrepancies between predictions at hydrostatic conditions [19–22] and experimental observations, we conducted shock compression experiments on [111] and [110] single-crystal MgO. These experiments reached hundreds of gigapascals (GPa) and thousands of kelvin (K), while measuring temperature, density, optical properties, crystal structure, and microstructure. Our results place complete melting on the Hugoniot of MgO at 13 200 K and 572 GPa, establishing it as the highest temperature solid known at planetary interior pressures. Notably, we observe a pronounced orientation-dependent response in MgO from 9000–13 000 K and 350–600 GPa.

II. EXPERIMENTS

We use multi-kJ laser pulses at the Omega-EP facility at the Laboratory for Laser Energetics, University of Rochester, to generate either decaying or temporally steady shocks in optically transparent MgO single-crystal samples. Nanosecond (ns) velocity interferometry [23], and streaked optical pyrometry (SOP) [24] were used to determine the shock-front velocity (U_S), reflectivity (R_S), and radiance as a function of time, from which we infer $T_S(U_S)$ and $R_S(U_S)$ [see Figs. 2(b)–2(d), 3(c), and 3(d)]. We use the subscript “S” to denote measurements made at the shock front. Using prior Hugoniot data to relate U_S and P_S , we express $T_S(U_S)$ as a function of pressure, $T_S(P_S)$ [17].

In the decaying-shock geometry, high-power nanosecond laser illumination results in a temporally unsupported shock which uniaxially compresses the MgO up to TPa pressures and 30 000 K, before decaying along the Hugoniot by a factor of 3 in pressure [Fig. 2(a)]. These measurements provide a continuous Hugoniot record from a single shot over an extended pressure range encompassing the predicted stability fields of MgO’s B1, B2, and liquid phases. We present results from three decaying-shock experiments on MgO [110]-oriented samples and four experiments on MgO [111]-oriented samples. We observe pronounced but starkly different $T_S(t)$ thermal anomalies for both orientations, as shown in Figs. 2(c) and 2(d).

To corroborate the decaying-shock data and further constrain the phase diagram of MgO, we also conducted temporally-steady-shock experiments incorporating, in addition to velocimetry and pyrometry, *in situ* nanosecond x-ray diffraction (XRD) [1] [Fig. 3(b)]. XRD provides a direct probe of the crystal structure, density, and microstructure at a single Hugoniot point. All peaks in the XRD patterns originating from the compressed sample can be assigned to the B1 and B2 phases. Because of the limited

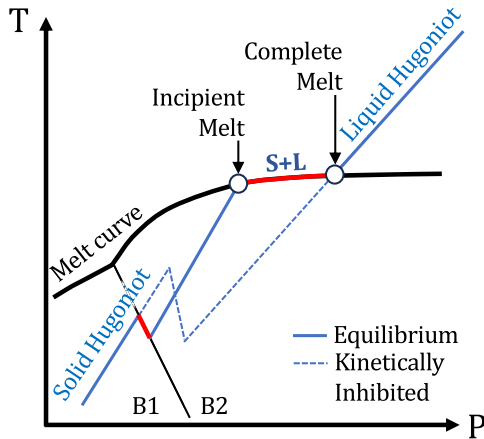


FIG. 1. Qualitative phase diagram of MgO showing the B1, B2, and liquid phases. Our decaying-shock experiments can detect P - T slope changes (red lines) due to phase transitions, constraining the B1-B2 and B2-liquid phase boundaries. Under shock loading, equilibrium melt results in an evolution of solid (S) and liquid (L) phase fractions at P - T states along the melt line. Molecular dynamic simulations have shown that, in kinetically inhibited systems, shear stress can be relieved by the formation of a transient disordered state, with P - T conditions along the low- T extension of the liquid Hugoniot (dashed curve) [12,15,16].

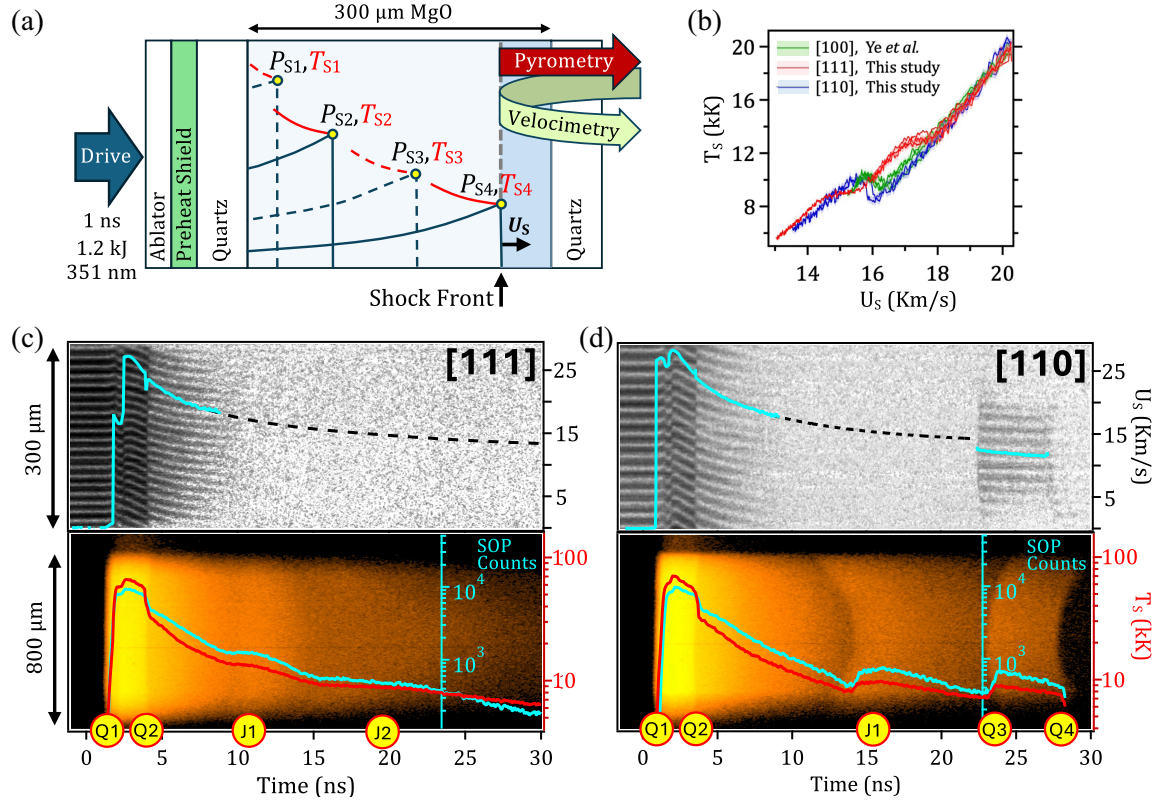


FIG. 2. Decaying-shock measurements of P_S - T_S states. (a) A 1-ns high power laser pulse focused within an 1.1-mm spot uniaxially compressed the target assembly and produced a continuum of shock states, P_S - T_S , throughout the MgO sample. Because the ablation pressure source is turned off rapidly after launching the shock, the Hugoniot pressure states accessed decrease as a function of shock propagation or distance. Four snapshots are illustrated with $P_{S1}-T_{S1} > P_{S4}-T_{S4}$. Behind the shock front, the temperature increases due to an adiabatic release from earlier-in-time higher P_S - T_S states [17]. (b) T_S versus U_S is plotted for three orientations of MgO [17]. Velocimetry (top panel) for (c) MgO [111] and (d) [110] single-crystal samples where fringe movement is directly proportional to the shock speed, U_S . Shock front reflectivity vanishes at $U_S \sim 18$ km/s which requires a model fit (black dashed curve) at later times to determine $U_S(t)$ values (see Ref. [17] and Supplemental Material Sec. S3A for details [25]). Pyrometry data are shown (lower panels) with averaged SOP counts (cyan) and calculated T_S (red) (see Supplemental Material [25] for detailed methodology and additional data). Bottom axis labels denote events: shock entry and exit from quartz layers (Q1 $\rightarrow$ Q2, Q3 $\rightarrow$ Q4), and the observation of $T_S(t)$ jogs in MgO (J1, J2).

signal-to-noise ratio, we cannot resolve the weak scattering from liquid MgO. To determine the shock-pressure distribution in the sample during the XRD snapshot, we interrogate the output from 1D radiation hydrodynamic simulations tuned to reproduce the measured $U_S(t)$ history in the quartz reference plate (see Supplemental Material Sec. S4 [25]). We present results from twelve steady-shock experiments on MgO [111] samples, and nine on [110], taken over the 295–611 GPa pressure range.

In our experiments, the sample is uniaxially compressed. While the use of the term “pressure” throughout the paper suggests a hydrostatically compressed state, we cannot rule out the presence of deviatoric stresses which would, in the case of our measurements, and all previous Hugoniot measurements [7,19,51–54], give rise to higher values of longitudinal stress and therefore reported pressure. In the analysis of Fowles [55] using the Lévy-von Mises yield criterion [56] this stress deviation corresponds to two thirds

the yield strength. However, the high pressure strength of MgO is unknown.

III. RESULTS

A. Crystal-orientation-dependent P_S - T_S response

In Fig. 4, the P_S - T_S data averaged over several decaying-shock experiments is plotted against P_S - T_S determined from steady-shock XRD experiments. The evolution of shock temperature differs significantly between the two MgO orientations. We note that the steady-shock temperatures are generally consistent with the decaying shocks, indicating that the orientation-dependent P_S - T_S response is not an artifact of the decaying-shock configuration.

1. MgO [111] decaying shock, and XRD data

For MgO [111], the P_S - T_S data exhibit two distinct temperature plateaus [Fig. 4(a)]. We interpret the onset of

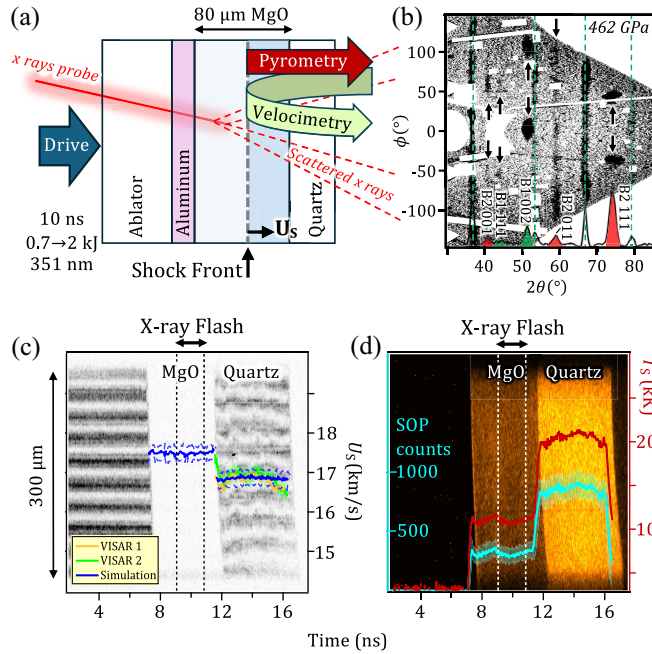


FIG. 3. Measurements of T_S and phase in steady-shock experiments. (a) A 10-ns laser pulse uniaxially-compressed [111] or [110]-oriented MgO single crystal. (b) During shock transit, a 2-ns 8.3-keV x-ray pulse probed the shock-compressed MgO and produced a volume-integrated XRD signal, recorded on image plate detectors in transmission geometry [50]. Here, data are plotted in angular space, with azimuthal angle (ϕ) around the Debye-Scherrer cones (vertical-axis) plotted against diffraction angle, 2θ (horizontal axis). In this view Bragg peaks, such as those from the Ta reference layer (green dashed), appear as vertical lines. The ϕ -averaged lineouts are shown along the bottom axis with arrows indicating the XRD signal associated with the compressed B1 and B2 phases (MgO [110] at 462 GPa). Laue diffraction from the uncompressed quartz windows and other noise features are masked out (see Supplemental Material [25]). (c) Velocimetry measurements constrain sample pressure, and (d) pyrometry data gives a measure of T_S .

the first plateau (points 1 $\rightarrow$ 2) as the B1–B2 transition, and the second (points 3 $\rightarrow$ 4) as the melting transition (incipient $\rightarrow$ complete melt, as in Fig. 1). The phase transition at point 1 corresponds to the predicted B1–B2 phase boundary by Root *et al.* [19]. Here, we observe a temperature plateau instead of the temperature jog predicted by theory. Based on our analysis of MgO [100] data [17], the relatively high optical transparency of the shock state below ~ 400 GPa (optical attenuation length near 1–10 μm) allows thermal emission from higher temperature regions behind the front to reach the detector [Fig. 2(a)]. This contributes to smearing out the temperature anomaly associated with the B1–B2 phase transition. The attenuation length at higher pressures is sufficiently small ($< 1 \mu\text{m}$) that measured thermal emission originates from a small region behind the shock front. Here, we observe a plateau in P_S – T_S , from points 3 $\rightarrow$ 4, as expected

if the shock-induced melting follows the equilibrium behavior.

Steady-shock experiments with *in situ* x-ray diffraction corroborate the interpretation of temperature anomalies in MgO [111] P_S – T_S data as the B1 $\rightarrow$ B2, and melt transitions [Fig. 4(a)]. Only compressed B1-MgO is observed at 295 (20) GPa. The B2 phase first appears at 343(20) GPa, placing the B1–B2 transition between 295(20) and 343(20) GPa. This pressure range aligns with the onset of the low P_S – T_S plateau [point 1 in Fig. 4(a)] and with the predicted equilibrium B1–B2 boundary from Root *et al.* [19].

In Fig. 4(a) *side panels*, we track the evolution of the B2-(001) reflection with increasing pressure. The localization of the XRD signal in the azimuth (ϕ) is characteristic of high orientational order, or microstructural *texture*. For pressures up to 519 GPa (upper left panels), the diffraction signal from the B2 phase is highly localized in ϕ , indicative of large oriented crystallites. At 588 and 611 GPa (upper right panels), the B2 diffraction signal becomes more powderlike (extended in ϕ), which we interpret as grain-size reduction and grain reorientation within the solid-liquid coexistence. A strong reduction in scattered crystalline intensity at 611(31) GPa—compared to B2 scattering at lower pressure—also suggests near complete melt of the B2 phase. This pressure range overlaps with the inferred complete melt conditions from the decaying-shock data.

2. MgO [110] decaying shock, and XRD data

For MgO [110] we observe a dramatically different behavior, evident in the comparison of the pyrometry images [Fig. 2(d)] and T_S vs P_S in Fig. 4(b). Only one large 1300 K temperature jog is observed, followed by a smooth rise in temperature with increasing pressure. The slope of the P_S – T_S measurement after the temperature jog [point 2 $\rightarrow$ 3 in Fig. 4(b)] aligns with the slope of the Hugoniot within the liquid. Our [110] MgO decaying-shock data is similar to the [100]-oriented data reported by Ye *et al.* [17] [Fig. 5(a)] and others [7,18]. A single temperature jog has been observed in other material systems [57] and interpreted as a nonequilibrium response to near-instantaneous shock compression [58]. Our interpretation of the strong orientation-dependent P_S – T_S responses ([111] vs [110]/[100]) is discussed in Sec. IV B.

The XRD for compression along MgO [110] are also strikingly different from the [111] data. Only compressed B1-MgO is observed at 372(20) GPa, and is highly localized in ϕ (Fig. 4, left lower panels). The B2 phase first appears at 425(20) GPa, placing the B1–B2 transition between 372(20) and 425(20) GPa, approximately 80 GPa higher than [111]. Unlike [111] MgO, the B2-(001) reflection in [110] MgO exhibits a weaker, powderlike texture for the entirety of the probed pressure range [Fig. 4(b), right side panels]. For [110] compression, the B2 onset pressure coincides with the single temperature jog in the decaying-shock data [points 1 $\rightarrow$ 2 in Fig. 4(b)].

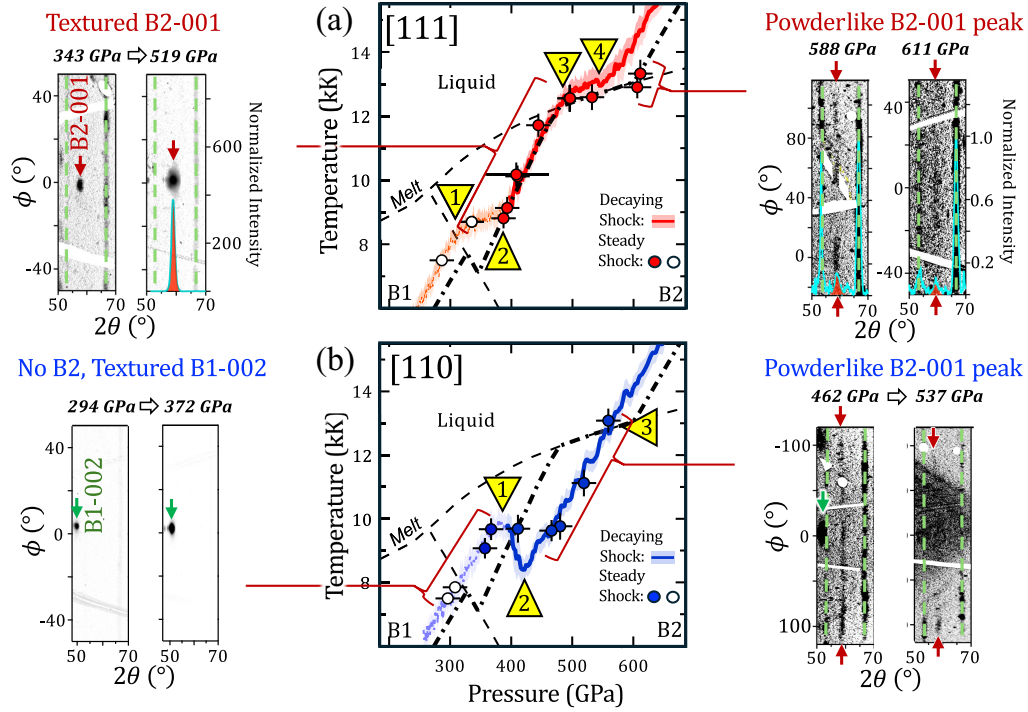


FIG. 4. (a),(b) Predicted stability fields for the B1, B2, and liquid phases are bounded by dashed curves [19]. Determined P_S - T_S states from constant-pressure shock experiments (circular symbols) are overlaid with decaying-shock measurements for [111] (upper, red), and [110] (lower, blue) samples. An equilibrium quantum molecular dynamics (QMD) Hugoniot model from Root *et al.* [19] is shown as the dash-dot black curve. The numbered yellow triangles are discussed in the main text. At lower pressure, the optical attenuation length increases, and measurements of T_S penetrate to include higher- T states beyond the decaying-shock front (transition to faint colors for $AL \gtrsim 1 \mu\text{m}$; see Supplemental Material [25]). For the two lowest pressure steady-shock data (open circles) T_S was not measured but is assumed to equal to the decaying-shock value. (Upper side panels) *In situ* XRD shows ϕ -texture evolution in the B2-(001) reflection (red arrows) for MgO [111], transitioning from highly textured (localised in ϕ ; left images) to powderlike (extended in ϕ ; right images) diffraction at pressures consistent with the onset of melt. A strong reduction in crystalline scattering intensity at 611 ± 31 GPa also suggests near-complete melt. (Lower side panels) The B2-(001) ϕ -texture for MgO [110] is markedly different, characterized by a powderlike distribution at pressures well below the expected melt pressure. A comprehensive summary of XRD data for [111] and [110] samples is provided in Supplemental Material Figs. S1 and S2 [25].

A similar P_S - T_S evolution and XRD texture behavior was previously observed in MgO [100] samples [1]. The bulk pressures and phase assignments for all XRD data from this study, along with the [100] data from Wicks *et al.* [1], are presented in the lower panel of Fig. 5.

B. Experimental constraints on B2-liquid melt

In Fig. 5, the P_S - T_S data for MgO [111] and [110] are plotted along with the previous [100] data [17]. We interpret the complete melt point as the convergence of these three curves at 572 ± 24 GPa and 13200 ± 600 K, where differences due to crystal orientation vanish. Above this pressure, the P_S - T_S curves for all orientations overlap. This point is in good agreement with the end of the second temperature plateau in the [111]-oriented MgO [point 4 in Fig. 4(a)], the loss of shock front reflectivity (see Fig. S10A [25]), as well as the observation of the last B2 XRD signal at $611(31)$ GPa. P_S - T_S values for the three orientations remain in excellent agreement to the limit of

our measurements (~ 1000 GPa and $\sim 30\,000$ K), with no temperature anomalies from 13 000 to 30 000 K (see Supplemental Material Fig. S5D [25]).

The P_S - T_S and XRD data for MgO [111] are closely aligned with the equilibrium QMD calculations of Root *et al.* [19]. We provide an experimentally constrained B2-liquid melt line using a Simon-Glatzel fit,

$$T(\text{K}) = 12931 \pm 293 \left(\frac{P(\text{GPa}) - (525.5 \pm 4.8)}{310^{+49}_{-29}} \right)^{0.162 \pm 0.021}. \quad (1)$$

The fit with uncertainty is plotted as the bold black curve in Fig. 5, with gray shading to denote the uncertainty in the fit. This empirical relation has been used to describe the melting behavior of other oxides including SiO_2 [57] and MgSiO_3 [65]. We use the B1-B2-liquid triple point to constrain the fit at lower pressures. The triple point is taken as the intersection of an experimentally derived

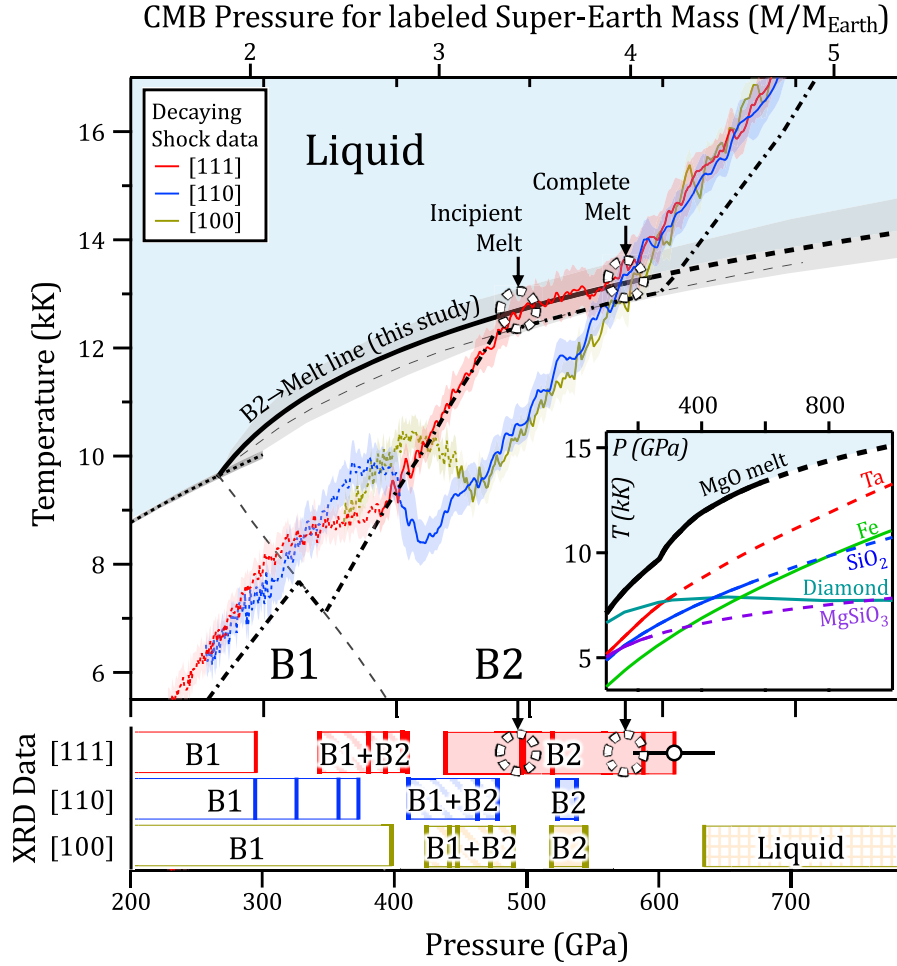


FIG. 5. P - T phase map of MgO. Upper Panel: P_S - T_S data for MgO [110] and [111] are shown as blue and red curves, with [100] data from Ref. [17] in green. Predicted B1, B2, and liquid stability fields are outlined by grey dashed curves [19]. The equilibrium QMD Hugoniot model from Root *et al.* [19] is shown as the dash-dot black curve. A low-pressure B1-melt fit [59] is shown as a dotted black curve. Pressure (bottom axis) is related to core-mantle boundary (CMB) conditions for labeled Super-Earth/Earth mass ratios (top axis) [60]. Our experimentally constrained B2 melt line (thick black curve) places complete melt at 572 ± 24 GPa and $13,200 \pm 600$ K. Inset: MgO melt line compared against the melt line of other materials [57,61–64]. The solid portion of the curves are constrained by experiment, which are then extrapolated to high pressure (dashed). Lower Panel: XRD-derived structural ranges for MgO [111], [110], and [100], where each vertical line represents an experimental structural measurement shown in Fig. 4, or Ref. [1] for [100] data.

B1-liquid melt line [59] and the B1-B2 phase boundary from Root *et al.* [19], which occurs at 9635 K and 266 GPa. At higher pressures, the fit is constrained by the P_S - T_S plateau in the MgO [111] data [points 3 $\rightarrow$ 4 in Fig. 4(a)] which we interpret as the solid-liquid coexistence. The uncertainty in the fit reflects the uncertainty in the average P_S - T_S data.

To our knowledge, at these extreme pressures, MgO has the highest recorded melt temperature of any known material, including metals such as iron and highly refractory Ta, other prototypical magnesio-silicate rocks MgSiO_3 , SiO_2 , and strongly covalently bonded diamond [Fig. 5(a), inset]. This illustrates that chemical intuition based on bonding characteristics at ambient conditions may be misleading at extreme pressures.

B2-MgO adopts a denser, more highly coordinated structure than B1-MgO (8 vs 6). This enhanced packing promotes robust ionic bonding and a mechanically stiff lattice that resists melting [66], with substantial Coulombic attraction between Mg^{2+} and O^{2-} ions opposing thermal disordering. The combination of high pressure, increased lattice binding energy, and persistent ionic character contributes to the exceptionally high melting temperature of the B2 phase and to the steeper slope of the MgO melting curve above the B1-B2-liquid triple point.

IV. DISCUSSION

The stark differences in the P_S - T_S states, and XRD texture for compression of [110] samples compared to

[111] samples in Fig. 4 is puzzling: *Why is the observed shock temperature so different when we shock compress MgO along different high symmetry axes?* We argue that these observed orientation-dependent responses are related to phase transition mechanisms and the ability for shear stress to be relieved over the rapid shock-compression timescales.

A. Crystal orientation-dependent B1 $\rightarrow$ B2 phase transition pathways

The conventional understanding of solid-solid phase transformation atomistic pathways involves the transition of atoms from an ordered parent phase to an ordered daughter phase, facilitated by lattice strain and atomic shuffles. Applied to MgO, each transition pathway is characterized by the orientation of the daughter B2-phase relative to the parent B1 phase. By measuring the orientation relationship (OR) between specific crystallographic planes and directions within both phases using diffraction techniques, the atomistic transition mechanism can be experimentally constrained [1,13].

Theoretical calculations have identified two primary energetically favorable mechanisms for the B1 $\rightarrow$ B2 transformation in MgO: the Buerger's mechanism [67,68] and the Watanabe-Tokonami-Morimoto (WTM) mechanism [69,70]. The Buerger's mechanism (BM) involves compression along one of the $\langle 111 \rangle$ directions of the B1 unit cell, accompanied by expansion in all orthogonal directions of the B1 phase (see Ref. [1], and Supplemental Material, movie 1 [25]). The WTM mechanism requires a combination of two cooperative motions: the sliding of atoms within alternate (001) layers, followed by expansion in the [110] direction (see Ref. [1], and Supplemental Material, movie 1 [25]).

Here we employ a forward diffraction model (see Sec. S5B), originally applied to XRD data from shock compressed MgO [100] single crystal samples [1], to determine the consistency of our XRD data with the proposed WTM and BM mechanisms. We find that our MgO [110] XRD data [Fig. 6(a)] can be reproduced by the forward model only when the WTM mechanism is active, resulting in the formation of six orientational variants. This conclusion is consistent with a similar analysis of MgO [100] samples [1]. In contrast, for the [111] data [Fig. 6(b)], the texture in ϕ (diffraction intensity distribution around the Debye-Scherrer cones) can only be explained by the forward diffraction model for the BM mechanisms, with a single orientational variant present. To interpret these orientation-dependent responses, we need to consider how uniaxial compression results in deformation along specific crystallographic planes.

Uniaxial loading along the [111] axis applies the required compressive strain along a single $\langle 111 \rangle$ direction within the B1 unit cell, consistent with the conditions needed to activate the Buerger's mechanism during the B1 $\rightarrow$ B2 transition. In contrast, under compression along

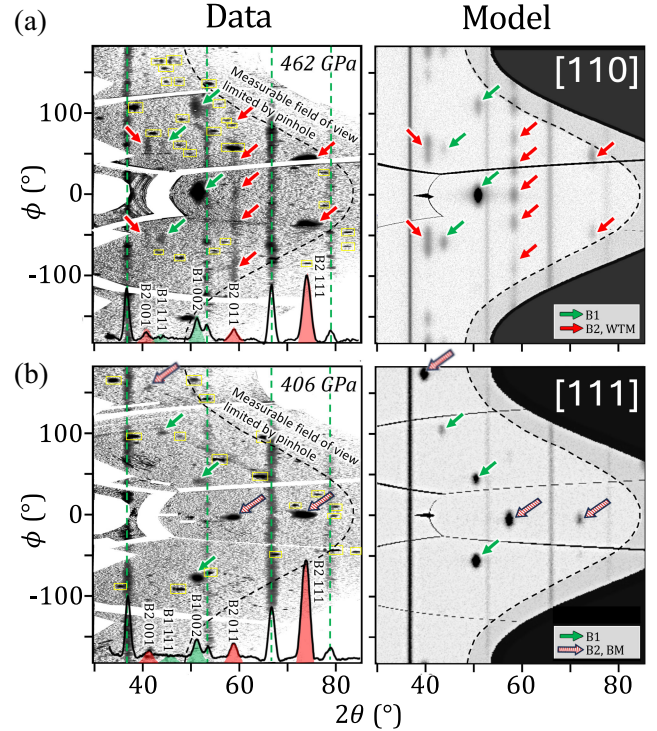


FIG. 6. Experimental (left) and simulated (right) diffraction patterns for (a) MgO-[110] at 462 GPa, and (b) for MgO-[111] at 406 GPa. For both shots the diffraction consists of signal from the compressed B1 phase (green arrows), and the transformed B2 phase (red arrows). By employing a forward diffraction model, we find that the XRD data are consistent with the WTM defined B1 $\rightarrow$ B2 pathways for [110]-oriented MgO, and for [111]-oriented samples only the BM mechanism is active. For both MgO orientations the ϕ -averaged lineouts are shown along the bottom axis with arrows indicating the reflections associated with the compressed B1 and B2 phases. Laue diffraction from the uncompressed quartz windows (yellow squares) are masked out (see Sec. S5A).

the [100] and [110] orientations, the resolved stress along $\langle 111 \rangle$ is insufficient to activate the BM pathway (see Supplemental Material, movie 1 [25]), so the alternative WTM pathway is required to facilitate the B1 $\rightarrow$ B2 transition. Because compression along [111] provides the specific stress state required for the Buerger's mechanism, it naturally explains the lower B2 onset pressure (295–343 GPa) observed in our [111] XRD data.

B. Single- T_S jog for MgO [100] and [110]: Evidence for transient disordered states

Next, we consider two proposed kinetically driven material responses to explain the single P_S - T_S jog observed within [110] and [100] data: (i) a *superheated solid*, where the solid material surpasses the melt line before undergoing bulk melting [57,58,71], and (ii) a *disordered solid or liquidlike state*, where a thin ($\sim \mu\text{m}$ -thick) disordered layer, at temperatures below

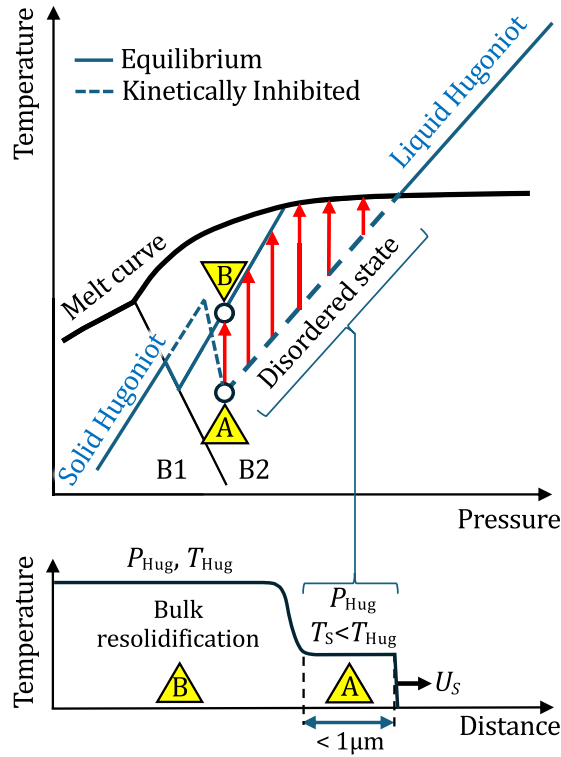


FIG. 7. Following NEMD simulations of shock-compressed single-crystal systems [12,15,16], we interpret the single T_S - P_S jog in [110] and [100] is a result of disordered or liquid-like formation within a sub- μm thick layer at the shock front. This is followed by recrystallization and a release of energy related to B2 chemical bond formation (points A $\rightarrow$ B). The release of this excess energy satisfies the Hugoniot jump conditions and leads to a rise in the bulk temperature [16]. The disordered P_S - T_S states follow the extension of the liquid Hugoniot, as described in simulations of shock-compressed SiO_2 by Shen *et al.* [16].

equilibrium melt, forms at the shock front before recrystallizing back to the solid [12,15,16] (see Fig. 7). Our diffraction results cannot distinguish liquid from disordered or amorphous material, so we use the term “disordered” inclusively.

Both the superheated- and the disordered-state interpretations result in a single P_S - T_S jog, as observed in the [110] and [100] decaying-shock data, but they fundamentally differ in predictions of the high-pressure, post-jog phase: complete melting in the superheated model and persistence of bulk solid in the disordered-state case. Previous experimental observations of a single P_S - T_S jog in shock-compressed fused silica and α quartz were interpreted as evidence for a superheated solid, with the low- T jog point taken as a proxy of the melt line [57,58,71]. However, those studies lacked the complementary structural data needed to confirm bulk melting, and the superheated solid interpretation.

Transient disorder or liquidlike formation at the shock front has been proposed in nonequilibrium molecular dynamics (NEMD) simulations as an alternative stress-relieving

mechanism under shock compression, where conventional plasticity is insufficient [12,15,16]. This behavior was observed in simulations of shock-compressed α quartz and fused silica [16], and other materials [12,15], at P_S - T_S conditions along a low- T extension of the liquid Hugoniot (see Fig. 7). Recrystallization behind the shock front releases energy by the formation of chemical bonds as the solid phase forms. The release of this excess energy satisfies the Hugoniot jump conditions and leads to a rise in the bulk temperature (points A $\rightarrow$ B, Fig. 7).

Our combined P_S - T_S and structural data provide compelling evidence for transient disordered state formation during shock compression of MgO [110] and [100] samples. In our experimental geometry, thermal emission is measured from a $\sim$ sub- μm -thick layer behind the shock front, defined by the (pressure-dependent) optical attenuation length [1,17]; Fig. S9. This length is comparable to the expected thickness of the disordered layer [16]. We observe P_S - T_S states at pressures above the temperature jog that fall along the low-temperature extension of the liquid Hugoniot, with no further temperature anomalies at the expected equilibrium melt line [Fig. 5(a)]. This behavior is consistent with NEMD simulations [15,16].

Our XRD experiments probe the volume-integrated structure of the $\sim 60 \mu\text{m}$ -thick shock-compressed region—well beyond one optical attenuation length—making them sensitive to phases further from the shock front. We observe crystalline diffraction at pressures above the temperature jog in both MgO [110] and [100] samples [Fig. 4(b) and Ref. [1]], including weak texture in the high pressure, post-jog B2 signal [Fig. 4(b)], consistent with polycrystalline growth from a disordered state. The persistence of crystalline diffraction at pressures above the temperature jog is inconsistent with the superheated solid $\rightarrow$ catastrophic bulk melting model [57,58,71].

Based on the [110] P_S - T_S and XRD data, we propose that a disordered layer at the shock front forms at $\sim 385 \text{ GPa}$, corresponding to the onset of the temperature jog [point 1 in Fig. 4(b)]. Between 385 and 570 GPa (complete bulk melting pressure), the measured T_S reflects the disordered state rather than the bulk temperature. A summary of our experimental results is shown in Table I.

As described in Sec. IV A, uniaxial compression along $\langle 111 \rangle$ directly facilitates the shear-stress relieving transformation from B1 $\rightarrow$ B2 via the Buerger’s pathway at $\sim 330 \text{ GPa}$. For this reason, we propose, the [111]-oriented samples do not exhibit the signatures of a disordered layer formation at the shock front. Conversely uniaxial compression along the $\langle 110 \rangle$ and $\langle 100 \rangle$ directions does not activate the B1 $\rightarrow$ B2 via the Buerger’s pathway. Therefore shear stress levels in the crystal continue to build with increasing pressure until a critical level is reached ($\sim 400 \text{ GPa}$) where shear-induced mechanical disordering at the shock front results in near instantaneous stress relaxation [12].

TABLE I. Summary of experimental observations. Data from MgO [100] are taken from Ref. [17] (#) and Ref. [1] (*). Buerger's mechanism (BM); Watanabe-Tokonami-Morimoto (WTM).

MgO crystal orientation	P_S - T_S onset of first jog	P_S - T_S onset of second jog	Pressure onset of B1 $\rightarrow$ B2 transition	Pathway for B1 $\rightarrow$ B2 transition	Transient disordered phase
[111]	320 GPa 8600 K	490 GPa 12 700 K	295–343 GPa	BM	No
[110]	380 GPa 10 000 K	...	372–415 GPa	WTM	Yes
[100]	#410 GPa 10 500 K	...	*397–425 GPa	*WTM	Yes

We note the pronounced difference in ϕ -texture for the B2 peaks between the [110] and [111] samples (Fig. 4). The B2 XRD signal for the [111] samples are highly localized, consistent with large oriented crystallites, while the B2 peaks for the [110] samples exhibit a mixed texture + powderlike distribution. The latter, we propose, is a result of the physical model described in Fig. 7, where B2 nucleation occurs from the disordered or liquidlike state (powderlike XRD) and from unmelted or nondisordered B1 grains (textured XRD). We speculate that the near-hydrostatic environment of the disordered layer facilitates the B1-B2 transformation, which explains the consistency in pressure of the P_S - T_S jog with the B2 onset. This effect, for large strain solid-solid transitions, was first predicted by Levitas *et al.* [72] but, to our knowledge, was never observed experimentally.

C. Implications for material science

Although NEMD simulations have long predicted transient shear-induced disordering or melting across diverse materials [12,15,16,73–76], experimental evidence has been lacking. Such direct temperature measurements, made possible by pyrometry through a transparent sample, are rare under high-strain-rate, anisotropic shock loading.

In previous decaying-shock studies reporting continuous shock-front temperature data, nonequilibrium behavior has been variously interpreted. For example, the single temperature jog in MgO [100] [7,18] and in fused silica or quartz [57,71] has been ascribed either to superheating [18,57,58,71] or to a solid-solid phase transition [7]. Our [110] MgO data identifies this jog to be consistent with the formation of a transient disordered state; an interpretation not considered in these previous studies, which underscores the importance of complementary bulk structural probes.

Previous studies that invoked a superheating interpretation of the temperature jog treated the low- T_S point as a proxy for the equilibrium melt curve [57,58,71,77,78]. Our observations in MgO show that the termination of the jog occurs well below the melt curve, implying that melt curves inferred previously under the superheating assumption could be underestimated. Therefore, our results motivate revisiting previously published melt curves for

other geologically relevant materials, including SiO₂ [57,58,78] and Mg₂SiO₄ [77].

D. Implications of MgO melt on gas giant core crystallinity

In Fig. 5 we provide an experimental constraint of the MgO B2-liquid melt curve. This has direct implications for

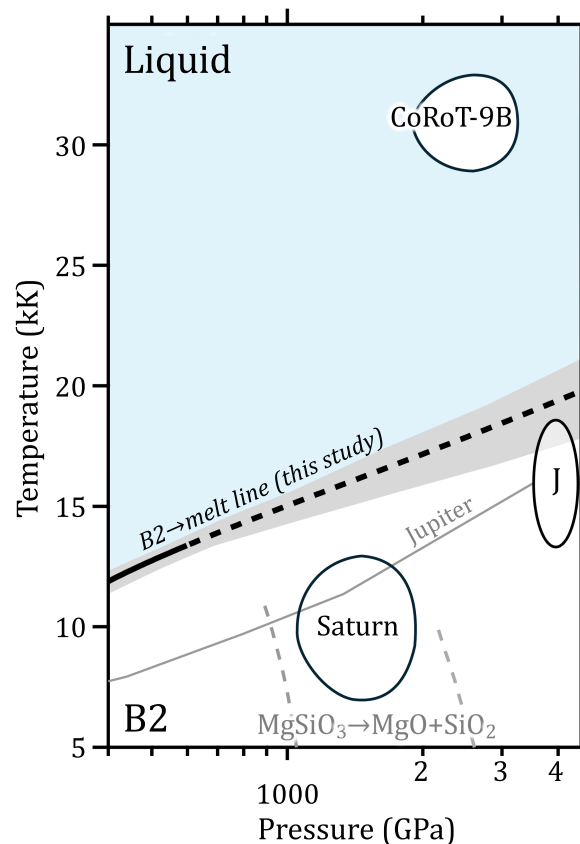


FIG. 8. Extended melt curve with the calculated core envelop conditions for Saturn and Jupiter (J) [82], and “hot-Jupiter” exoplanet CoRoT-9B [10]. The solid grey curve represents Jupiter’s interior path [83]. Calculated conditions of MgSiO₃ dissociation into MgO + SiO₂ are shown as the dashed grey curves [79,80].

our understanding of the cores in Jupiter, Saturn, and other gas giants. Along with ice, MgO is expected to be a major core component of gas giants such as Jupiter and Saturn [2], where extreme pressure enables the dissociation of MgSiO_3 into MgO and SiO_2 [79,80], or a melting-related demixing instability in MgSiO_3 resulting in a mixture of solid MgO and liquid SiO_2 [81]. Figure 8 shows an extrapolation of our MgO melt curve compared to the predicted core envelop conditions for Saturn [82], Jupiter [82], and exoplanet CoRoT-9B which was modeled by Zhao *et al.* [10] as a “hot-Jupiter.” Our MgO melt line suggests that crystalline MgO may exist in the cores of Saturn and Jupiter but a highly conductive liquid MgO would exist in the core of CoRoT-9B.

V. CONCLUSIONS

We have investigated the response of single-crystal MgO to dynamic compression up to 600 GPa and 13 000 K using combined shock thermodynamics and *in situ* nanosecond x-ray diffraction. At high pressures, all orientations converge to complete melting at 572 ± 24 GPa and 13200 ± 600 K, defining the B2-liquid boundary at multi-megabar conditions. At shock pressures below melt, our measurements reveal that crystallographic orientation governs the pathway of the $\text{B1} \rightarrow \text{B2}$ reconstructive phase transition under uniaxial shock loading. Compression along [111] activates the Buerger mechanism and produces a shock-temperature evolution consistent with equilibrium solid-solid and solid-liquid transitions. In contrast, compression along [110] and [100] delays the $\text{B1} \rightarrow \text{B2}$ transformation by ~ 80 GPa and yields a single temperature jog accompanied by diffraction signatures consistent with B2 nucleation from a transient disordered layer at the shock front.

Recent theoretical studies predict that anharmonic phonon-phonon interactions can stabilize the B1 phase [20–22,84,85] up to ~ 465 GPa [21] under shock compression. In contrast, we find that [111] compression triggers the $\text{B1} \rightarrow \text{B2}$ transition at ~ 330 GPa, consistent only with quasiharmonic approximation (QHA) predictions [19–22,86] (see Supplemental Material Fig. S22 [25]). Because the QHA neglects explicit temperature dependence, this discrepancy implies reduced levels of anharmonic stabilization. These findings challenge current high-temperature phase stability models and provide essential constraints for planetary-interior phase diagrams.

More broadly, our findings demonstrate that crystallographic orientation can control phase-transition kinetics under dynamic loading, with measurable consequences for shock thermodynamics and microstructural evolution. Such orientation-dependent nonequilibrium behavior is expected to be relevant across a wide class of materials subjected to extreme strain rates, including metals, ceramics, and planetary materials. The ability to experimentally resolve transformation pathways under these conditions provides a framework for testing atomistic simulations of

high-pressure phase transitions and for refining models of matter under extreme compression.

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All authors were involved in discussions related to experimental design, data analysis, and interpretation. J.K.W. was the PI for the NLUF project. J.K.W., R.F.S., and Z.Y. designed and conducted the experimental campaigns. Z.Y. analyzed the decaying shock data with guidance from M.M., R.F.S. and S.S. analyzed the steady shock data. S.S. developed the forward diffraction code. F.C., J.H.E., M.M., S.S., J.W.S., and Z.Y. provided feedback on the data analysis methodology. R.F.S., F.C., J.H.E., M.M., S.S., Z.Y., and J.K.W. collectively developed the interpretation of the data and the preparation of the manuscript. The LLNL AnalyzeVISAR, AnalyzePXRDI, and HEXRD code were used to analyze the data. J.H.E., M.M., and S.S. developed analysis tools for XRD image processing. The authors declare that they have no competing interests.

DATA AVAILABILITY

The numerical data underlying the figures are provided in the Supplemental Material [25]. The complete raw experimental data cannot be made publicly available because their release is subject to facility and institutional data-management policies. The data are available from the corresponding author upon reasonable request.

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