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Real-Time Atomic Scale Kinetics of a Dynamic Event in a Model Ionic Crystal

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Abstract: The mineral CaF_2 is the archetype of the α fluorite structure and its high-pressure phase transition to γ cotunnite is an ideal test bed for exploring the effects of kinetics. The inter-disciplinary topic of the kinetics of dynamically driven phase transitions is at the forefront of condensed matter physics, both for its theoretical importance and its relevance to technological applications at extreme conditions of pressure and temperature. Here we probe the $\alpha \rightarrow \gamma \rightarrow \alpha$ structural transformations taking place over the nanosecond timescale of a dynamic event, beginning-to-end: from the principal shock Hugoniot state, followed by a quasi-steady off-Hugoniot release state, and finally the unsteady return to near-ambient conditions. We present quantitative, atomic-scale data of the unfolding of the dynamically driven phase transition and its subsequent reversal close to the α/γ phase boundary. Dynamic loading with a two-stage gas gun is coupled with in situ time-resolved synchrotron X-ray diffraction and with continuum scale velocimetry at the Dynamic Compression Sector (DCS), Advanced Photon Source, Argonne National Laboratory. Our results demonstrate the time dependence of phase transitions and highlight the need for modeling of transition kinetics in dynamically driven processes.

Keywords: dynamic compression; kinetics; nanosecond X-ray diffraction; fluorite; phase transition



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1. Introduction

The question of whether phase transition kinetics can affect shock wave propagation has been debated in the field of dynamic compression for over half a century. On the one hand it is accepted that discontinuities in the Hugoniot can be caused by dynamically driven phase transitions. As early as the 1960s, reconstructive phase transitions in silicates, which are sluggish under static compression (sluggish over a pressure range on the order of Gigapascals), were found to occur rapidly under shock compression. This led to the interpretation that shock wave compression is fundamentally different from static compression. On the other hand, instead of very fast reconstructive transitions, another interpretation proposed was crystal lattice deformation and large volume reduction under shock, but without a crystallographic phase transition. Such dynamic studies were all based on the interpretation of continuum scale measurements using velocimetry. With the advent of picosecond/nanosecond X-ray diffraction (XRD) being coupled with shock compression drivers in the last few years, we now have new means to probe phase transitions and their kinetics directly at the atomic scale [1,2].

Shock compression is the primary method for exploring the extreme thermodynamic states of stress and temperature. A single shock compression experiment consists of the measurement of a material's end state achieved by single shock wave compression at constant velocity from a given initial (ambient) state. In a simple shock experiment, the conservation of mass, momentum, and energy are described by Rankine-Hugoniot jump conditions [3,4], which relate the pressure, density, and specific internal energy of the shocked material relative to its initial state. The "Hugoniot" is then defined as a collection of loci of material end states achieved from a given initial state, and in practice it is a collection

of stress-density data points. By definition, the “principal Hugoniot” initiates from ambient conditions, while nonambient initial conditions lead to measuring “off-Hugoniot” states. States following after the initial shock are also referred to as “off-Hugoniot”.

The strain-rate or loading-history dependence of phase diagrams and how to model them remains a key unanswered question. When a material is loaded dynamically through equilibrium phase boundaries, it is kinetics that determines the real time expression of a phase transition. That in turn can play a significant role in the thermodynamic path that the material takes. The material’s end state, in a shock event, may depend on the kinetics of the process that produced this end state. There exists a relationship between the kinetics of a phase transition, the mesoscale structure of a solid, and its constitutive properties. However, the role that kinetics of phase transitions play in a material’s constitutive properties is not well understood. This gap in understanding is due to a lack of experimental data on kinetics, especially quantifiable data at the atomic scale. Our work aims to fill this gap with direct atomic-scale in situ measurements of kinetics of phase transitions occurring during shock events. Such data can then be leveraged in physics-based modelling of kinetics.

In this work we study the kinetics of shock-driven phase transitions using dynamic X-ray diffraction (DXRD). We examine the mineral fluorite or CaF_2 , which at ambient conditions is the archetype of the cubic fluorite structure (α phase, $\text{Fm}\bar{3}\text{m}$, $Z = 4$). Upon static compression to 9 GPa (hydrostatic conditions) or 11–16 GPa (nonhydrostatic conditions), CaF_2 undergoes a phase transition to an orthorhombic cotunnite-type structure (γ phase, Pnam , $Z = 4$) [5–7]. Fluorite is an ideal candidate for the examination of phase transition kinetics because its phase transition is characterized by relatively simple XRD patterns where each phase possesses a distinct set of Bragg reflections. This fact also facilitates the quantitative analysis of XRD patterns, which display coexistence of the α and γ crystal phases.

Here, we couple shock loading with a two-stage gas gun in situ time-resolved synchrotron X-ray diffraction and we probe a structural phase transition over the duration of the full dynamic event, start-to-finish, including the initial principal Hugoniot shock state, release to an off-Hugoniot quasi-steady state, and the unsteady return towards ambient P and T conditions. In two separate experiments we probe the kinetics of the α -fluorite to γ -cotunnite transition in CaF_2 both above and right at the equilibrium phase boundary for an extended period of time of ~ 600 ns.

2. Materials and Methods

The samples consist of finely ground CaF_2 powder compacts with $\sim 72\% \pm 2\%$ theoretical maximum density (single crystal $\rho_0 = 3.18 \text{ g/cm}^3$), 8 mm in diameter, and $\sim 650 \text{ }\mu\text{m}$ in thickness. The phase diagram in Figure 1 illustrates the equilibrium stability region of the α and γ phases.

We performed experiments at the Advanced Photon Source (APS), sector 35 DCS (Figure 2). For dynamic experiments we took advantage of the fact that the X-rays have a time structure; short pulses were delivered every 153 ns, which enabled time-resolved shock experiments. The X-ray pulses (23 keV, pink beam with bandwidth $\sim 450 \text{ eV}$) lasted for $\sim 100 \text{ ps}$, which allowed us to capture essentially instantaneous snapshots of crystal structures at different times during a dynamic event. In dynamic compression (Figure 2), we started with a stack made of the sample and a window transparent to near infrared and hard X-ray radiation. The sample/window stack was impacted by a LexanTM projectile using the DCS 2-stage light gas gun generating a planar shock. The impactor velocities were: $3.554 \pm 0.006 \text{ km/s}$ for the 14 GPa experiment and $4.296 \pm 0.011 \text{ km/s}$ for the 19 GPa experiment. As the planar shock wave travelled through the sample, we monitored both impact time and particle velocity with photonic Doppler velocimetry [8]. Meanwhile, the synchrotron X-ray bunches traversed the sample in transmission and diffracted Debye rings were intercepted on a phosphor detector head coupled to four ICCD cameras resulting in four consecutive images of Debye rings, separated in time by 153 ns. This gave four Dynamic X-Ray Diffraction (DXRD) patterns, each separated by 153 ns in a single experiment.

Each DXRD pattern was corrected for geometric distortion and for phosphor ghosting of the detector, and then was analyzed quantitatively with the technique of Rietveld structural refinements [9].

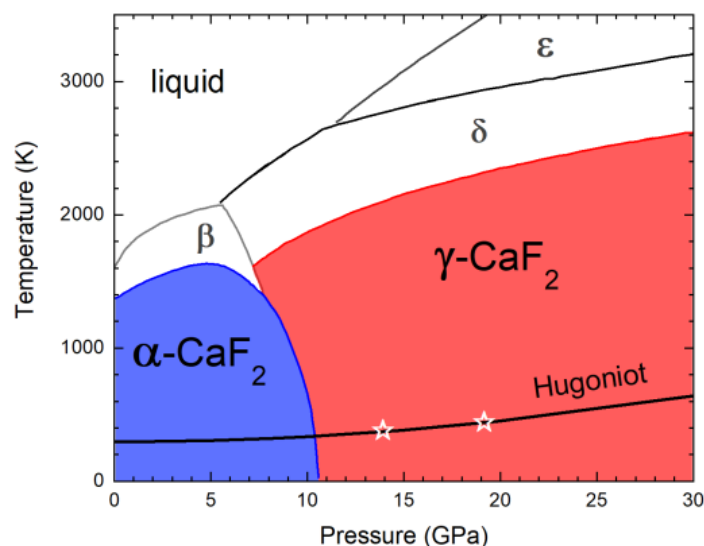


Figure 1. Phase diagram of CaF_2 . The principal Hugoniot is indicated with a black line [2]. The two initial Hugoniot states examined in this work are marked with stars (14 GPa and 19 GPa on the Hugoniot). Phase boundaries are from reference [10], and specifically the α/γ boundary is from DAC data and first principles simulations.

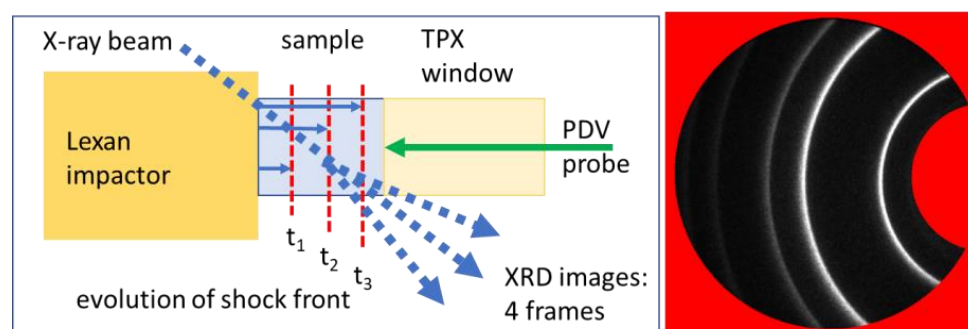


Figure 2. Experimental setup for nanosecond-scale DXRD at the Advanced Photon Source, Sector 35, DCS, and an example ICCD image of the CaF_2 sample showing diffracted Debye rings. Simulations of stress states within the sample (discussed below) were obtained along the path of the X-ray beam.

3. Results

We dynamically compressed CaF_2 to two different principal Hugoniot states: first to an over pressurized state of 19 GPa on-Hugoniot, which was significantly above the $\alpha \rightarrow \gamma$ equilibrium phase boundary. In a second experiment we shock compressed to 14 GPa on-Hugoniot, which was close to the phase boundary and corresponded to just enough stress to induce the forward $\alpha \rightarrow \gamma$ phase transition. Figure 3 shows a set of five DXRD patterns measured on shock compression near the equilibrium phase boundary. Figure 4 shows representative Rietveld full profile structural refinements of XRD patterns at different times during the experiment shown in Figure 3.

When we shock compressed CaF_2 , the DXRD patterns measured over time every 153 ns reflect not only the passage of time, but also the forward $\alpha \rightarrow \gamma$ phase transition, followed by the backwards $\gamma \rightarrow \alpha$ transition which were all caused by the evolving stress conditions in the dynamically compressed sample, due to the interactions of the shock and rarefaction waves. The changing stress states are reflected in the time evolution of the DXRD patterns (Figure 3) since the DXRD measurements probe the entire thickness of

the sample. Those are: the ambient state prior to impact (t-0, α phase); the on-Hugoniot state at 14 GPa (t-1, $\alpha + \gamma$ phases); a somewhat steady off-Hugoniot state at 8–9 GPa set up by a release and reflected shock wave (t-2, $\alpha + \gamma$ and t-3, mostly γ phase); and finally the unsteady release down to near-ambient conditions combined with the arrival of edge waves at 0–5 GPa (t-4, $\gamma + \alpha$).

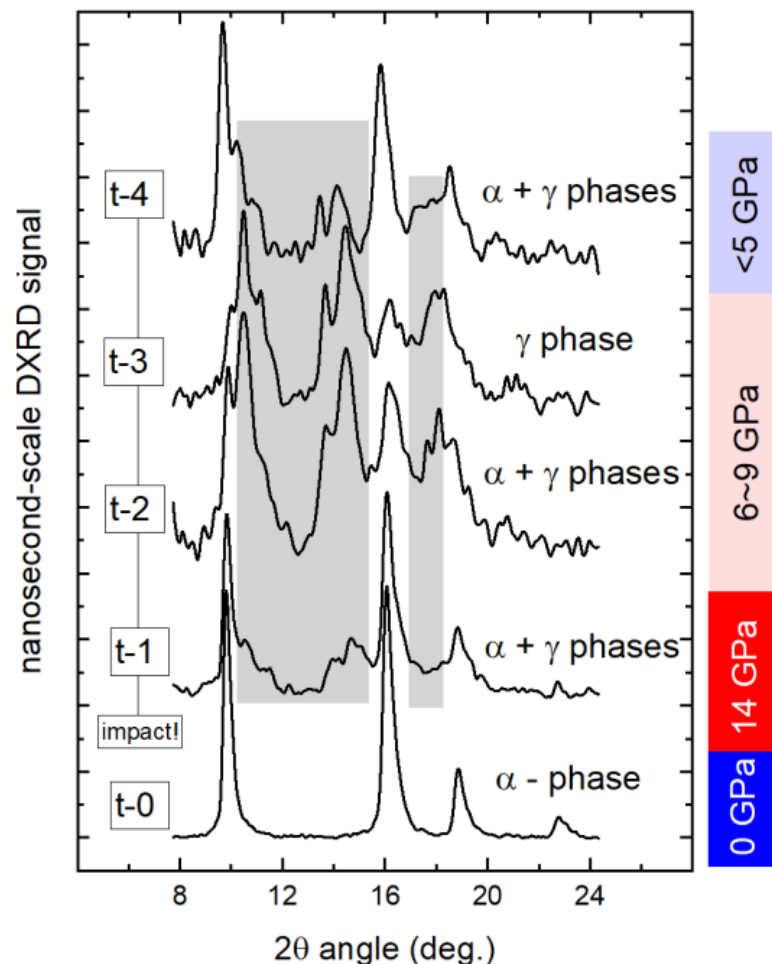


Figure 3. Example results of the DXRD experiments: X-ray diffraction patterns prior to impact (t-0) and after impact (t-1 to t-4). Patterns illustrate the forward $\alpha \rightarrow \gamma$ phase transition and the backwards $\gamma \rightarrow \alpha$ phase transition caused by the evolution of stress states over the time of the dynamic experiment. Grey bands indicate the regions where new peaks of the γ phase appear.

For the purpose of quantitative kinetics analysis, it then becomes useful to describe the stress state in the samples at each point in time throughout each dynamic experiment.

Hence, we use hydrodynamic simulations to model the stress distribution in the sample at every point in time, which determine the spatially integrated stress state in the material as seen by the X-ray beam over the entire ~600 ns dynamic process, start-to-end (Figures 4a and 5a).

The simulations of stress state within the dynamically compressed sample were implemented in CTH [11], a multi-material, Eulerian, finite-volume solid mechanics code developed by Sandia National Laboratories. The materials were all modeled with Mie-Grüneisen equations of state obtained from the literature: Lexan [12], CaF_2 [13], TPX [14]. Our simulations used the Hugoniot of single crystal CaF_2 as input [13]. The compaction behavior of the powder samples was simulated using the P- α model [15] with the Carroll and Holt correction [16] assuming no elastic region and compaction to full density at 1 GPa. The Johnson-Cook model [17,18] was used to represent the constitutive behavior of the

Lexan™ impactor. The constitutive behavior of both the CaF_2 and TPX® were modeled with a simple elastic-perfectly plastic von Mises model. The simulations of stress states within the sample were obtained from stress records of a number of fixed tracers located on a straight line along the angular path of the X-ray beam. The data from numerical simulations were outputted every 2 ns; CTH uses 60% of the Courant limit to define the numerical step. We used a square mesh of 3.3 μm (3000×3000 cells/cm in x and y direction) with an $x = 0$ axi-symmetric boundary condition. The mesh grid was 0 to 6 mm in x and -1 to 3 mm in y direction. All other boundaries were far enough away that their conditions did not affect the simulations results.

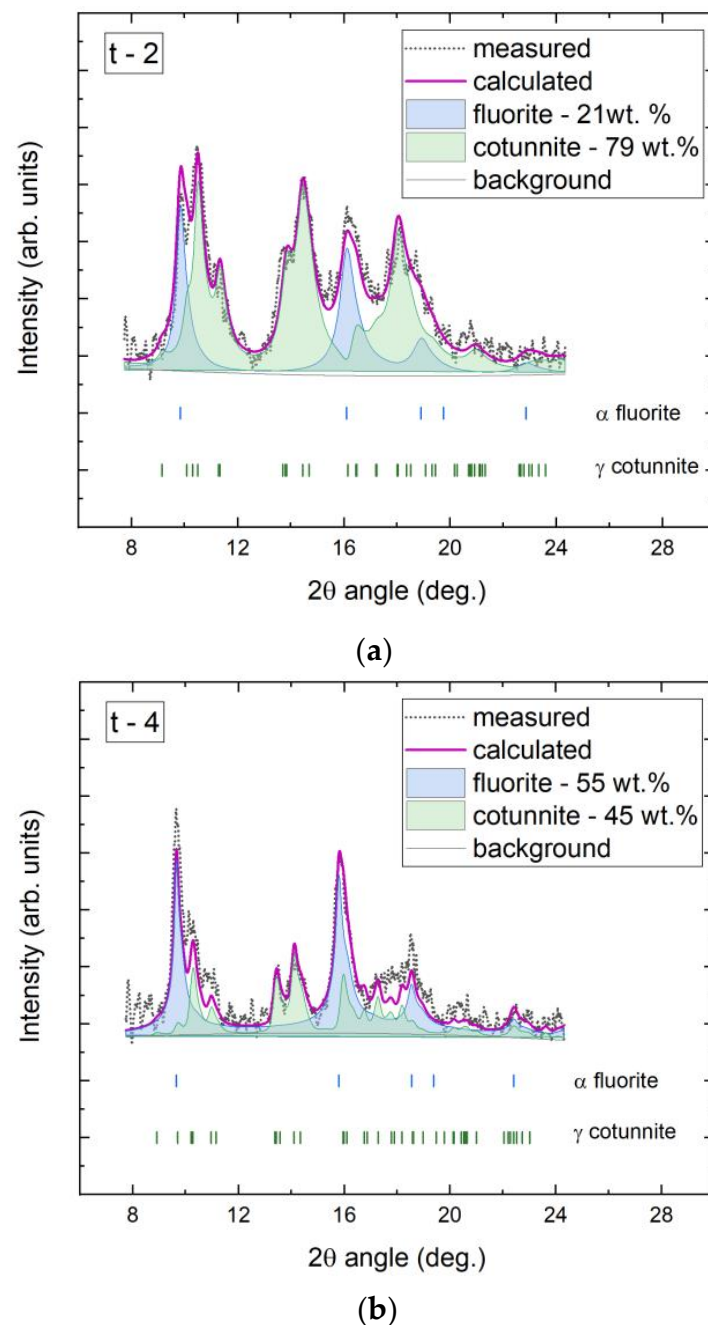


Figure 4. Rietveld full profile structural refinement of XRD patterns in Figure 3 at selected times: (a) at time t-2, and (b) later on at time t-4, illustrating the phase composition of α fluorite and γ cotunnite phases along the measured XRD pattern, the modelled (refined) pattern, background, and Miller indices for the two phases.

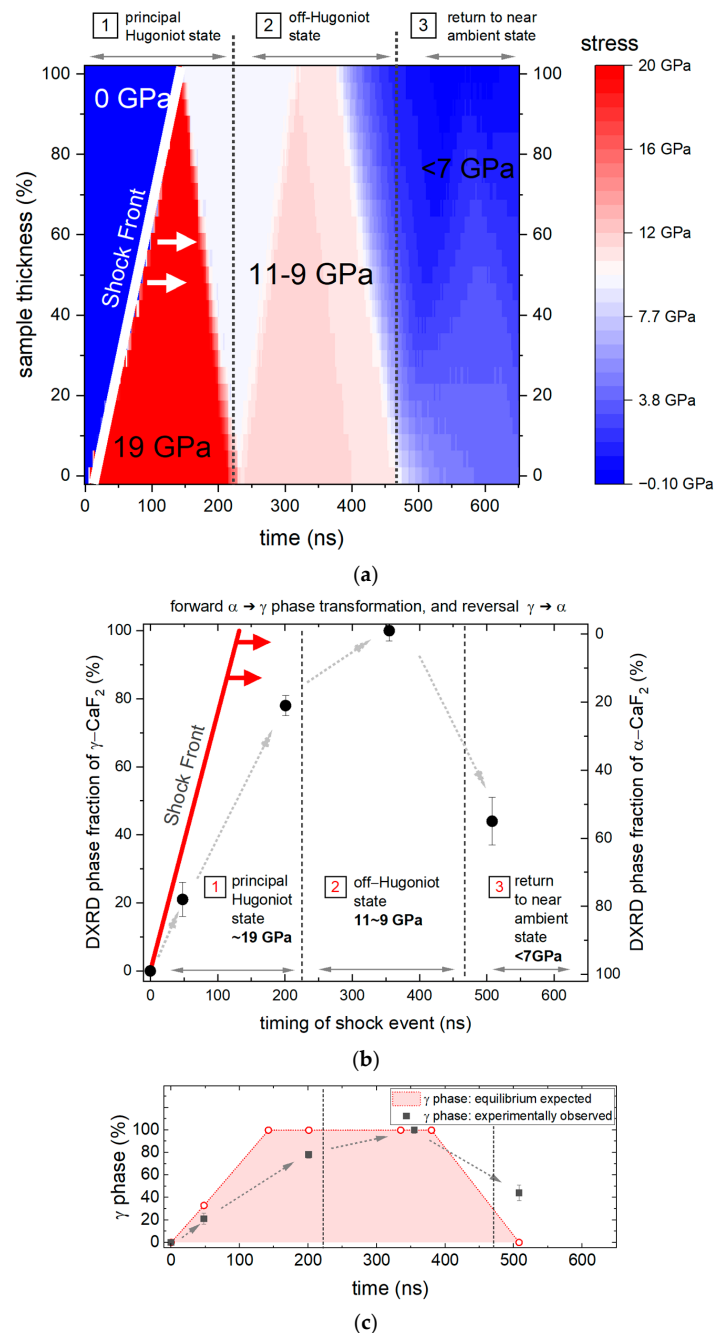


Figure 5. Dynamic compression to an over pressurized principal Hugoniot state (~19 GPa) and the corresponding kinetics of the $\alpha \rightarrow \gamma \rightarrow \alpha$ phase transitions. (a) Hydrodynamic simulations of the stress distribution in the dynamically compressed sample, along the path of the X-ray beam over the entire ~600 ns shock event, start-to-end. At any point in time, a hypothetical vertical line drawn across the figure gives the stress distribution in the sample, as seen by the X-ray beam at that instant. (b) Kinetics of the $\alpha \rightarrow \gamma \rightarrow \alpha$ phase transitions: quantitative fractions of α and γ -CaF₂ phases. Fractions were obtained from Rietveld refinements of the four DXRD snapshots collected on dynamic compression to 19 GPa. (c) Comparison of experimental vs. equilibrium expected percentage of γ phase, assuming a scenario where the phase transition was instantaneous and started at a stress of at least 9 GPa (vs. 10.5 GPa on the phase diagram) to account for simulation uncertainties, shock heating, and the negative Clapeyron slope of the $\alpha \rightarrow \gamma$ phase transition. In all panels, the timescale axes are identical and vertical dashed lines are placed at the same time marks. Numbers 1, 2, and 3 identify the three stress regions discussed below: 1—principal Hugoniot state; 2—off-Hugoniot state, and 3—return to near-ambient conditions.

Next, we analyzed each XRD pattern with the quantitative method of Rietveld [9] structural refinements (Figures 4, 5b,c and 6b,c). We used the Rietveld full-profile structural refinements to analyze the fractional contributions of the two CaF_2 crystal phases in each DXRD pattern measured in these experiments. This allowed us to quantify the percentage of contribution of the $\alpha\text{-CaF}_2$ and $\gamma\text{-CaF}_2$ phases at each stage of the dynamically driven phase transition. Finally, we compared, in Figures 5c and 6c, the percentage of γ phase measured experimentally versus that expected from the equilibrium phase diagram when considering a sufficient stress state to induce an instantaneous $\alpha \rightarrow \gamma$ phase transition.

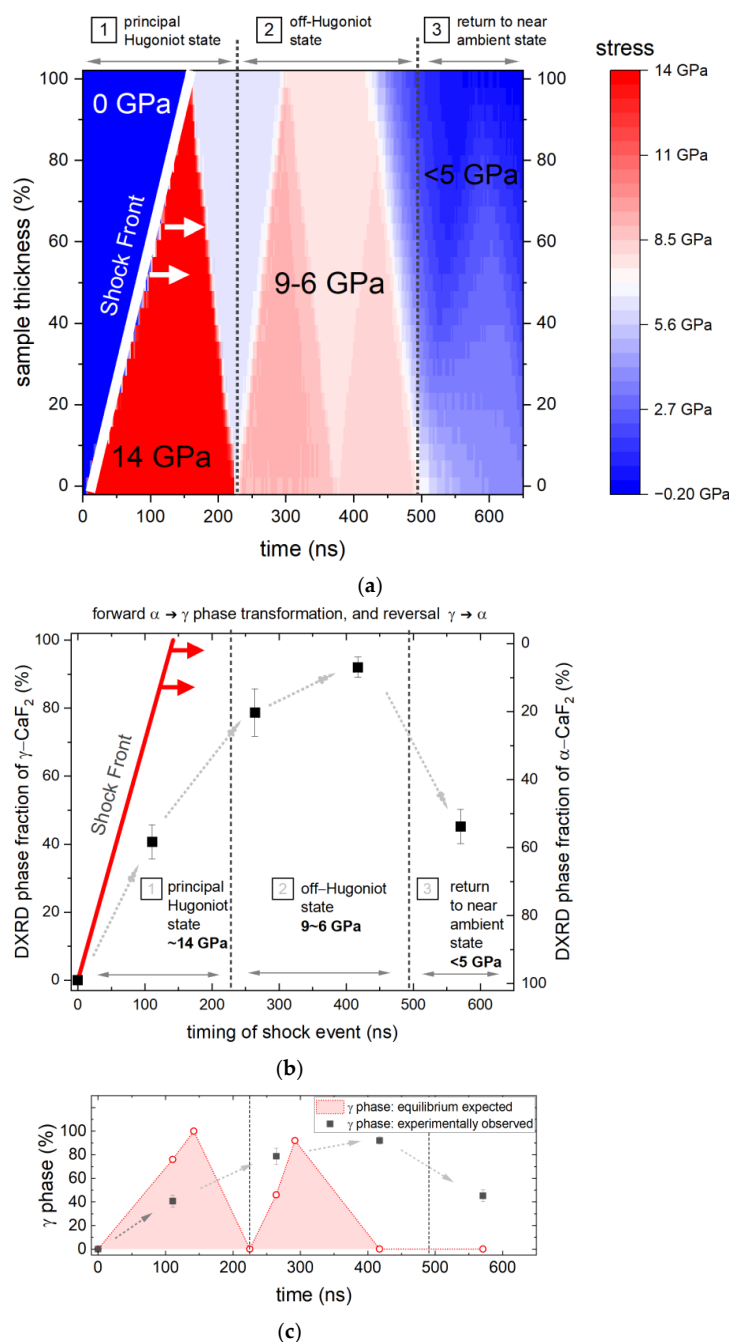


Figure 6. Dynamic compression at the edge of the equilibrium α/γ phase boundary (principal Hugoniot state of ~14 GPa) and the corresponding kinetics of the $\alpha \rightarrow \gamma \rightarrow \alpha$ phase transitions. (a) Hydrodynamic simulations of the stress distribution in the dynamically compressed sample along the path of the X-ray beam over the entire ~600 ns shock event, start-to-end. At any point in time, a hypothetical vertical line drawn across the figure gives the stress distribution in the sample, as seen in

the X-ray beam at that instant. (b) Kinetics of the $\alpha \rightarrow \gamma \rightarrow \alpha$ phase transitions: quantitative fractions of α and γ -CaF₂ phases. Fractions were obtained from Rietveld refinements of the four DXRD snapshots collected on dynamic compression to 19 GPa. (c) Comparison of experimental vs. equilibrium expected percentage of γ phase, assuming a scenario where the phase transition is instantaneous and starts at a stress of at least 9 GPa (vs. 10.5 GPa on the phase diagram) to account for simulation uncertainties, shock heating, and the negative Clapeyron slope of the $\alpha \rightarrow \gamma$ phase transition. In all panels the timescale axes are identical and vertical dashed lines are placed at the same time marks. Numbers 1, 2, and 3 identify the three stress regions discussed below: 1—principal Hugoniot state; 2—off-Hugoniot state, and 3—return to near-ambient conditions.

4. Discussion

To obtain an atomic-scale picture of the full dynamic event beginning-to-end, we measured, in real time, the kinetics of the unfolding forward $\alpha \rightarrow \gamma$ and backwards $\gamma \rightarrow \alpha$ phase transitions. Specifically, we used DXRD in two different dynamic events to quantify how long the phase transition needed to begin, to complete, and finally to revert (Figures 4 and 5).

The results of hydrodynamic simulations (Figures 5a and 6a) allowed us to distinguish three stress state regions over the course of the dynamic event. Each region has distinctive characteristics: (1) simple on-Hugoniot state where stress is either 0 or 19 GPa (14 GPa for the second case), followed by (2) a somewhat steady state hovering at the phase boundary (or an under-pressurized stress state for the second case), and finally (3) the unsteady release back to near-ambient conditions mixed-in with the arrival of edge effects at the tail end of the 600 ns-long dynamic process. Under-pressurized refers to a stress state below the α/γ equilibrium phase boundary.

The four ICCD images, separated by 153 ns, probe the sample in the stress states described above. Hence, we captured four instantaneous XRD snapshots of the structure in the dynamically compressed sample (Figures 5b and 6b). We examined the atomic-scale kinetics of $\alpha \rightarrow \gamma \rightarrow \alpha$ phase transition across the entire shock process: (1) the on-Hugoniot shocked state, which induces a first $\alpha \rightarrow \gamma$ phase transition, (2) a quasi-steady state generated from a release and shock wave reflection, and finally (3) the unsteady release back to near-ambient conditions and the reverse $\gamma \rightarrow \alpha$ structural phase transition.

First, we discuss the dynamic compression toward an on-Hugoniot state of ~19 GPa (Figure 4), i.e., the over-pressurized case. This initial stress state was much larger than the pressure necessary to generate the phase transition, as illustrated in the phase diagram (Figure 1). On initial impact (Figure 5, region 1, 19 GPa) the kinetic delay of the transition was already clear, and the growth of the γ phase was slower than the motion of the shock front through the material. The white diagonal line on Figure 5 is useful to illustrate that if the phase transition were instantaneous, then the γ phase percentage data points would fall directly on that line. Note that phase percentage points to the left of the white line would mean that the phase transition moves faster than the shock front which would, of course, be unphysical. The kinetic delay of formation of the γ phase points led to a kinetic delay in growth of the γ phase or possibly to the existence of an incubation time, similar to what we found in our previous work [2]. As stress states decreased to the ~9–11 GPa range (Figure 4, region 2), the material hovered at the equilibrium α/γ phase boundary and this was enough to keep driving the $\alpha \rightarrow \gamma$ phase transition forward (Figure 5b,c). The percentage of γ phase increased to a complete transition (~100%) around 350 ns, this was likely because of the energy supplied by the over pressurized state achieved at the beginning of compression (Figure 5b,c). The reverse phase transition $\gamma \rightarrow \alpha$ was noted at 500 ns and possibly before that, as the material was subjected to uneven stresses of 0–7 GPa at the tail end of the experiment (Figure 5, region 3).

To measure the kinetics of the same transition, but closer to the equilibrium α/γ phase boundary, we shock compressed CaF_2 on the Hugoniot to 14 GPa in a second experiment (Figure 6). This stress state allows us to minimize the consequences of over-pressurizing while it was just enough to generate the $\alpha \rightarrow \gamma$ phase transition, since the phase boundary was at 10.5 GPa (Figure 1). On initial impact, the kinetic delay of the transition was again present, and the transition was slower compared to the first experiment (Hugoniot state of ~ 19 GPa). The lower on-Hugoniot state provided less energy for overcoming the activation energy barrier and hence the transition was slower than in the first experiment (Figure 6, region 1, 14 GPa). However, as the stress state decreased to the 8–9 GPa range, (Figure 6, region 2) the phase transition—surprisingly—continued to progress. This occurred in stress conditions where we would rather expect the material to revert to the α phase based on the established equilibrium phase boundary (Figure 6b,c). Again, the percentage of γ phase grew all the way to 90% or an almost complete transition, around 400 ns. The reverse phase transition $\gamma \rightarrow \alpha$ started somewhere later than 400 ns, as the material found itself in a region of uneven stresses at <5 GPa. Unlike Figures 5c and 6c, it also showed two peaks in the phase fraction plot purely due to the evolution of the stress state. We interpret this as competing forces at work: reverting and converting. That combined with the inherent latency of the transition could also be a reason that the phase fraction stayed higher than predicted by an instantaneous transition.

Dynamic compression was accompanied by modest shock-induced heating. We estimated that, for a single crystal of CaF_2 , the shock temperatures were 375 K at 14 GPa and 445 K at 19 GPa on-Hugoniot (Figure 1). The heating effects are larger in a porous sample [19]. However, even a 30% increase in temperature (which is unlikely in the present experiments) would still not be enough to drive the material over the $\alpha \rightarrow \gamma$ phase transition boundary, especially in the second experiment (see phase diagram and in Figure 1).

It is straightforward to conclude that it is the delayed kinetics of the $\alpha \rightarrow \gamma$ phase transition that drives the transition forward even in an under pressurized state (Figures 5c and 6c). This kinetic delay is also responsible for the slow reverse $\gamma \rightarrow \alpha$ structural phase transition, in a P-T region where, according to the static phase diagram, only the α phase should exist. The time interval between single data points (153 ns) does not allow us to rule out the possibility that the transition might experience a slowdown before reverting towards growth on a shorter timescale. This would depend on the rate of growth of the transition compared to the rate at which stress states change within the material.

5. Conclusions

We established the real time kinetics of the forward $\alpha \rightarrow \gamma$ and backwards $\gamma \rightarrow \alpha$ phase transitions in CaF_2 during a complete dynamic compression event, beginning-to-end. The DXRD technique allows to quantify how long the phase transition needs to begin, complete, and finally to revert. We distinguish three time intervals corresponding to three stages in the dynamic process over ~ 600 ns: simple on-Hugoniot compression, followed by a somewhat steady and under-pressurized stress state, and finally the unsteady release back to near-ambient conditions accompanied by the arrival of edge effects. Over these three stages, we follow the initial $\alpha \rightarrow \gamma$ phase transition in CaF_2 , the continued transformation to (almost) pure γ phase in off-Hugoniot under-pressurized conditions, and finally the slow backwards $\gamma \rightarrow \alpha$ -transition. Our results are the first atomic-scale report demonstrating the quantification of a dynamic process beginning-to-end with a structural phase transition that is kinetically delayed on initial shock and that continues to be kinetically delayed in underpressurized conditions. We also find that the reverse phase transition displays both hysteresis in the stress domain coupled with a kinetic delay in time. Our findings illustrate the time dependence of phase diagrams and highlight the need for modeling of kinetics in a variety of dynamically driven processes.

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