How mineralogical transformations impact the rheology of rocks at high pressure and temperature

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INTRODUCTION

The continental crust is a chemically and mineralogically complex layer that accommodates an enormous range of physical processes, from the propagation of seismic waves to the slow creep of rocks over geological timescales. Understanding how the crust deforms, how earthquakes nucleate, and how seismic velocities relate to mineralogy requires accurate knowledge of the physical properties of crustal minerals under the pressure–temperature (*PT*) conditions they experience at depth.

Quartz is one of the most abundant minerals in the continental crust. As such, its mechanical and elastic properties play a key role in the rheology of the crust as a whole. Quartz undergoes two important phase transitions within the pressure and temperature range of the lower crust: the α–β transition and the quartz–coesite transformation. Both transitions involve significant changes in the physical properties of the mineral, with broad consequences for seismic wave propagation, rock strength, and the occurrence of seismic events at depth.

The α–β transition is a continuous, displacive phase transformation occurring at approximately 573°C at ambient pressure, shifting to higher temperatures with increasing pressure. It is associated with strong variations in thermodynamic and elastic properties, such as a dramatic softening of the bulk modulus near the transition (Lakshtanov et al., 2007), which directly affects seismic wave velocities. Velocity contrasts observed in seismic tomography of tectonically active regions, such as the Tibetan Plateau, have been attributed to this transition (Mechie et al., 2004). However, the behavior of the transition and the properties of β-quartz under simultaneous high pressure and high temperature had never been experimentally measured before the work presented in this thesis, leaving a critical gap in the interpretation of crustal seismic data.

The quartz–coesite phase transition, in contrast, is a first-order reconstructive transition occurring at pressures of ~ 2.5–3 GPa, corresponding to depths of approximately 90 km in continental subduction zones. This transition involves a substantial volume reduction of ~ 10%, which can cause mechanical weakening and strain localization. An extreme manifestation of this process is transformational faulting, in which the volume change associated with the transition drives fracture nucleation even under conditions that would otherwise suppress brittle failure. Understanding whether and how this mechanism operates during the quartz–coesite transformation is directly relevant to the question of intermediate-depth seismicity in collisional settings such as the Himalaya or the Alps.

Despite the fundamental importance of both transitions, the experimental study of quartz at true lower-crustal conditions is technically extremely challenging, requiring the simultaneous control of pressure (~ 1–3 GPa) and temperature (~ 600–1400°C) with sufficient precision to collect reliable elastic and structural data. The work presented in this thesis addresses these challenges through a combination of Large Volume Press (LVP) experiments at synchrotron facilities, diamond anvil cell measurements, and deformation experiments with acoustic emission monitoring.

THE α–β QUARTZ TRANSITION: NEW DATA AT CRUSTAL CONDITIOTIONS

Ultrasonic measurements in the Large Volume Press

The elastic properties of quartz across the α-β transition were first investigated at the ID06 beamline of the European Synchrotron Radiation Facility (ESRF, Grenoble), using a large volume press. Experiments were conducted on polycrystalline novaculite samples combining ultrasonic P- and S-wave velocity measurements with simultaneous X-ray diffraction along a pressure–temperature path crossing the α–β boundary at ~ 2 GPa and up to ~ 1300°C.

This approach yielded the first complete dataset of densities, V_p and V_s across the α–β quartz transition at simultaneous *HP*–*HT* conditions (Fig. 1). The results revealed that in the β-field, the bulk modulus (K) is approximately 60 GPa, roughly 30 GPa lower than the ~ 90

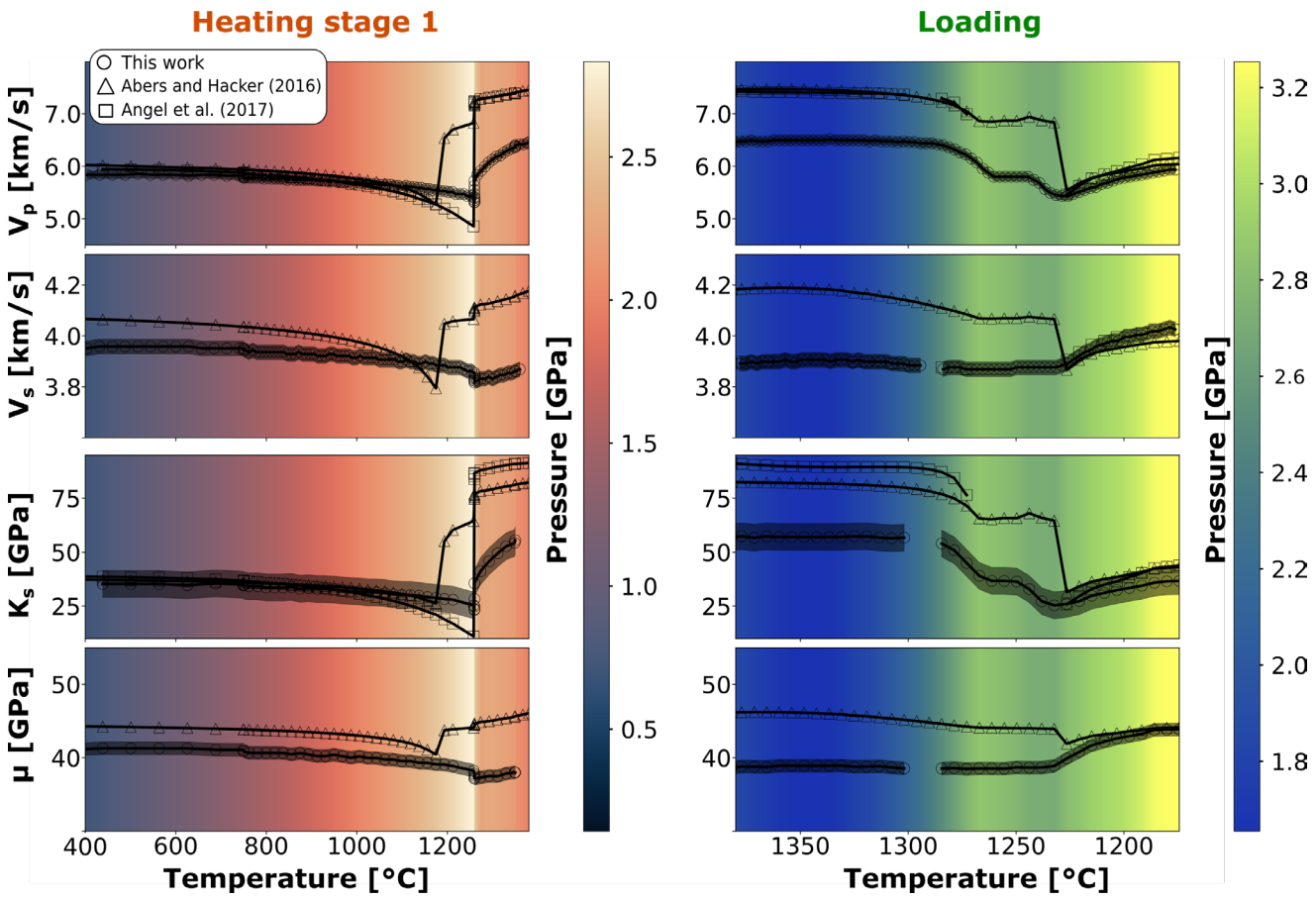

Figure 1 V_p, V_s, bulk modulus (K_s) and shear modulus (μ) from Abers & Hacker (2016) and Angel et al. (2017) compared with the data collected in this study during heating and loading cycles in the LVP press at ID06. In the α field, the experimental data align with the models, while in the β field V_p and K_s are 14% lower than the predictions.

GPa predicted by the equation of state (EoS) of Angel et al. (2017) and the thermodynamic model of Abers & Hacker (2016). These models, upon which the interpretation of crustal seismic data has long relied, were built on data collected either at room pressure or at room temperature, but never at both simultaneously. The new measurements demonstrate that this extrapolation significantly overestimates the stiffness of β-quartz at depth (Mingardi et al., 2025).

Brillouin spectroscopy in a laser-heated Diamond Anvil Cell

To confirm these results with an independent technique, single-crystal X-ray diffraction and Brillouin spectroscopy were performed on a quartz single crystal in a laser-heated Diamond Anvil Cell (DAC) at the Bayerisches Geoinstitut (BGI, Bayreuth). Brillouin spectra were collected across the α–β transition and into the β-stability field, closely reproducing the *PT* conditions of the ESRF experiments (Fig. 2).

The data confirmed the LVP findings: in the β-field, V_p ≈ 6.7 km/s and V_s ≈ 3.8 km/s, yielding a bulk modulus of ~ 66 GPa. Notably, the S-wave velocity showed little variation across the transition, indicating that the shear modulus is similar in both phases at these conditions, consistent with room-pressure observations. The convergence of two entirely independent experimental techniques on the same result, using both polycrystalline and single-crystal samples, constitutes strong evidence that existing models substantially underestimate the compressibility of β-quartz at crustal pressures.

Towards a new equation of state

Given these discrepancies, significant effort was dedicated to developing an updated EoS capable of reproducing the new *HP*–*HT* data while preserving the well-established properties of α-quartz. The existing Landau-type model of Angel et al. (2017) describes the total volume and bulk modulus as the sum of a "bare" phase contribution and an excess contribution from the phase transition. Different strategies were explored to modify this framework: varying the power-law exponent of the spontaneous strain for the β-phase, introducing pressure dependencies of the excess properties, and modifying the bare-phase compressibility.

None of the tested variants produced physically consistent results across the full *PT* range. This outcome highlights the fundamental limitation of trying to constrain β-quartz properties indirectly, through room-pressure data and thermodynamic extrapolation, and reinforces the need for targeted *HP*–*HT* measurements along and near the phase boundary at multiple pressures. Future strategies, including new DAC experiments with improved laser heating stability and molecular dynamics simulations based on DFT-derived interatomic forces, are discussed as paths forward.

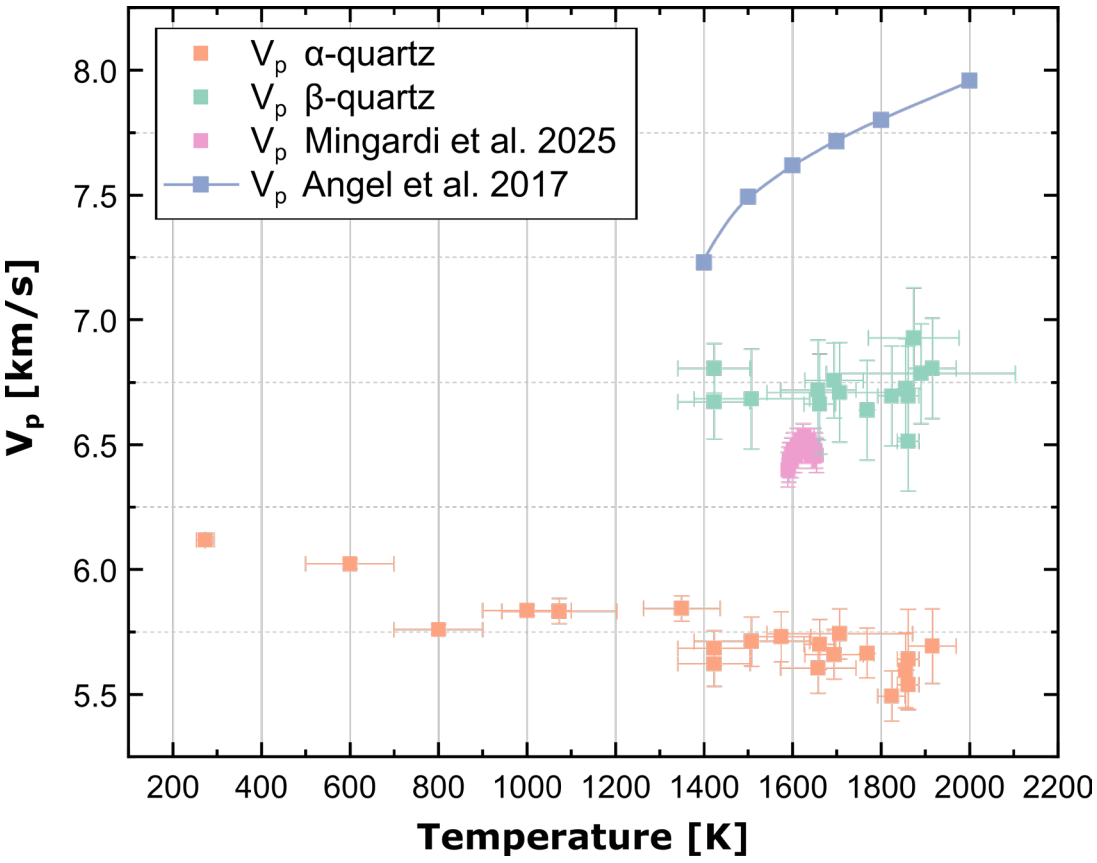

Figure 2 Comparison of V_p collected with Brillouin spectroscopy and multi-anvil ultrasonic technique. The Brillouin data confirmed the LVP findings (here reported as Mingardi et al. 2025): in the β-field, V_p is 6.7 km/s and V_s 3.8 km/s, yielding a bulk modulus of ~ 66 GPa, lower than predicted by the models.

FROM ELASTICITY TO MECHANICS: THE QUARTZ–COESITE TRANSITION AND TRANSFORMATIONAL FAULTING

The finding that β-quartz is significantly softer at crustal pressures than previously assumed is not only relevant to seismic velocity interpretation, but also raises a broader question: what role do the elastic and mechanical anomalies of quartz phase transitions play in controlling rock strength and faulting at depth? This question becomes particularly interesting for the quartz–coesite transformation, where the volume change is large and abrupt, and where the possibility of brittle failure under otherwise ductile conditions has profound implications for our understanding of intermediate-depth seismicity.

Standard brittle failure is suppressed at great depths by high confining pressure. Transformational faulting has long been proposed as an alternative mechanism capable of nucleating earthquakes in the ductile regime, driven by the interaction of latent heat release, volume change, and strength contrast between the transforming and product phases. These criteria, derived from the study of olivine phase transitions in subducting oceanic slabs (Green & Burnley, 1989; Burnley et al., 1991; Schubnel et al., 2013), were considered to be necessary conditions. The quartz–coesite transition satisfies only the volume change requirement: it releases little latent heat and shows minimal strength contrast between parent and daughter phases (Hunt et al., 2019). Therefore, it was considered unlikely to trigger faulting (Kirby et al., 1996). The experiments presented here were designed to test this assumption directly.

Deformation experiments at PETRA III (DESY)

Deformation experiments were performed at the P61b beamline of PETRA III (DESY, Hamburg) using the Ater-15 six-axis press. Novaculite samples were deformed under differential stress while simultaneously collecting energy-dispersive X-ray diffraction patterns and acoustic emissions (AEs). The six-axis geometry allowed six transducers to be placed on the second-stage anvils, enabling 3D location of acoustic events within the sample in real time. After the experiments, recovered samples were analyzed by SEM imaging, EBSD, and Raman spectroscopy to characterize the microstructures and phase distributions developed during deformation.

The key experimental finding emerges from comparing two experiments performed under different pressure–temperature conditions and, crucially, under different reaction kinetics. In the experiment conducted closer to the equilibrium quartz–coesite boundary, at lower temperature and with sluggish transformation kinetics, the quartz-to-coesite conversion proceeded slowly while the sample was simultaneously subjected to high differential stress. Under these conditions, faulting was observed. In the experiment conducted at a higher temperature, further into the coesite stability field, the transformation kinetics were faster: coesite nucleated and grew more rapidly throughout the sample. Under these conditions, despite similar differential stresses being applied, no macroscopic faulting developed and the sample deformed in a predominantly ductile manner.

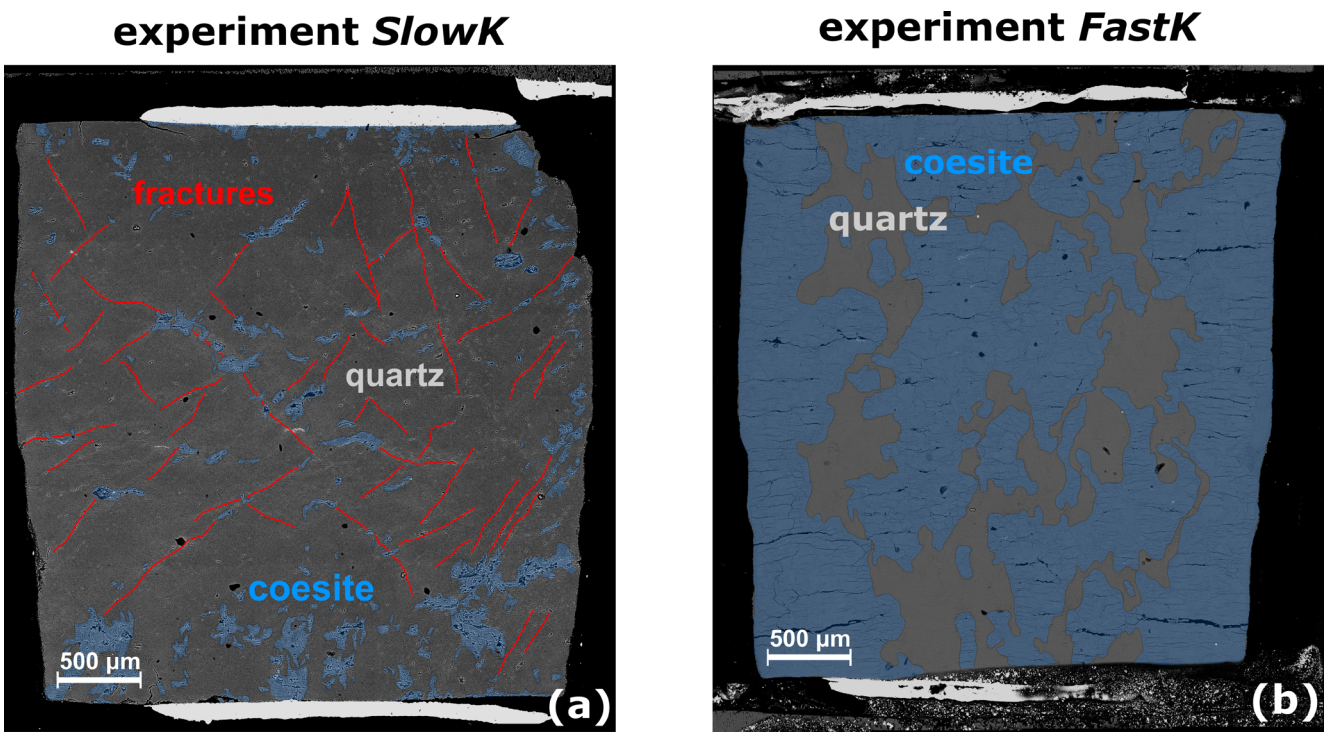

Figure 3 a) *Full SEM mosaic image of specimen at slow kinetics (SlowK). Red lines highlight fractures connecting coesite domains (in blue).* ***b)*** *Full SEM mosaic image of specimen at fast kinetics (FastK). More than 60% of the volume is coesite (in blue), forming vertical domains.*

The contrast between these two experiments is strikingly visible in post-mortem SEM imaging (Fig. 3). The slow-kinetics sample shows a well-developed network of through-going fractures, with coesite concentrated along fault planes and a strong crystallographic preferred orientation of coesite grains consistent with stress-driven nucleation. The fast-kinetics sample, in contrast, shows a more homogeneous distribution of coesite with no macroscopic fractures, reflecting distributed ductile deformation rather than localized failure.

The acoustic emission record reinforces this picture. In both experiments, numerous AEs were recorded throughout the deformation. However, the statistical character of the AE populations differs markedly between the two. The b-value, a parameter describing the relative proportion of large to small events in the magnitude–frequency distribution, widely used in seismology as a proxy for stress state and fracture propagation, evolves very differently in the two cases. In the slow-kinetics experiment, the b-value decreases progressively during deformation, a signature classically associated with the nucleation and growth of a through-going fault in both laboratory and natural seismicity. In the fast-kinetics experiment, b-values remain elevated throughout, consistent with distributed microcracking at the grain scale without coalescence into larger fractures (Fig. 4). The 3D location of AE sources further supports this interpretation: in the slow-kinetics experiment, events cluster progressively along planar structures that correspond to the fault planes visible in the recovered sample, tracing the spatial evolution of fault growth in real time.

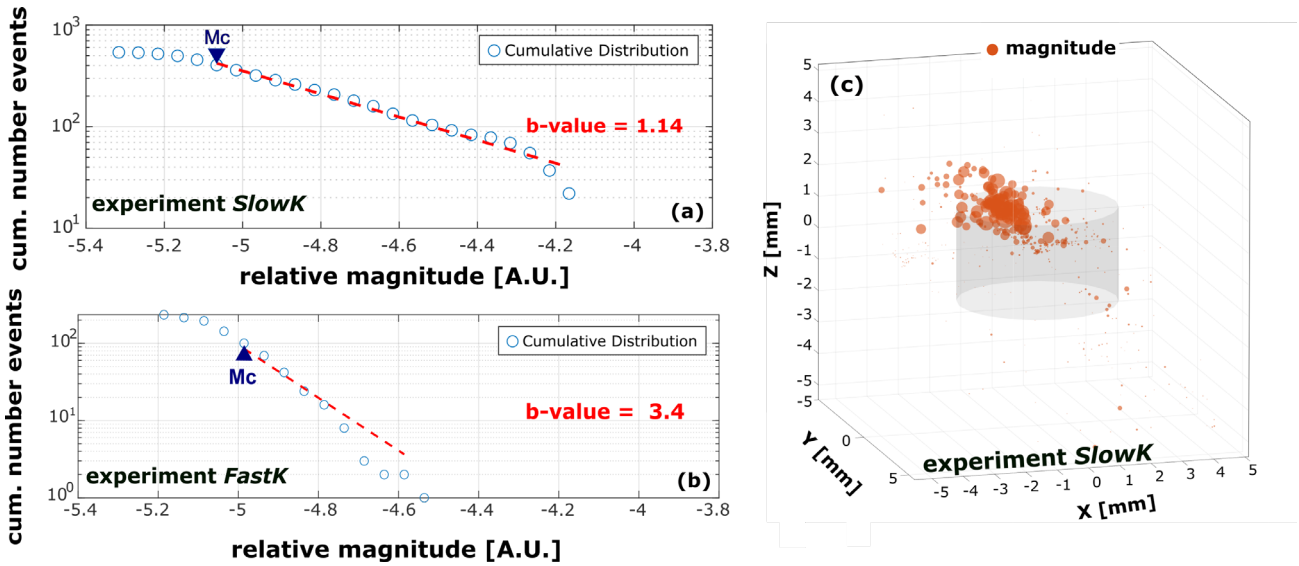

Figure 4 *AE magnitude distribution (b-values) for the slow kinetics experiment SlowK* ***(a)*** *and the fast kinetics one, FastK* ***(b)****.* ***c)*** *AE hypocenter location for experiment SlowK. Largest AEs hypocenters plot within the sample and align along a fault plane that cross-cuts the sample.*

A volume-driven faulting mechanism

Taken together, the microstructural observations, the AE statistics, and the spatial distribution of acoustic sources paint a coherent picture: when the quartz–coesite transformation proceeds slowly, near the equilibrium boundary, the local stress perturbations generated by the ~ 10% volume reduction of the transformation are not rapidly dissipated by the surrounding transforming material. Instead, they accumulate around newly formed coesite grains, concentrating stress in a way that (in a sample already under high differential stress) is sufficient to nucleate fractures. These fractures then propagate and coalesce, ultimately producing sample-scale faults. When kinetics are fast, the transformation front advances too quickly for these stress concentrations to build up and localize; deformation remains distributed and ductile.

This mechanism operates without significant latent heat release and without a meaningful strength contrast between quartz and coesite. Volume change alone is sufficient to drive the instability, provided the kinetics are slow enough for stress to concentrate. This result substantially broadens the conditions under which transformational faulting can occur, well beyond what the classical olivine-derived framework would predict. In continental subduction zones, quartz-bearing crustal rocks reach depths of ~ 90 km under conditions that closely resemble those of the slow-kinetics experiment: near-equilibrium transformation, cold temperatures in the slab core, and large accumulated deviatoric stresses. The present results suggest that, under these natural conditions, the quartz–coesite transformation is a viable trigger for intermediate-depth seismicity, a mechanism that does not require the thermodynamic conditions previously considered essential, and that may operate wherever crustal quartz is subducted to sufficient depths.

CONCLUSIONS

This thesis presents the first experimental investigation of quartz elastic and mechanical properties under true lower-crustal *PT* conditions, addressing two interconnected problems in crustal geophysics.

On the elastic side, β-quartz at ~ 2 GPa and ~1300°C has a bulk modulus approximately 30% lower than predicted by existing models. This finding, confirmed by two independent techniques, calls for a revised EoS for quartz and for caution in interpreting seismic velocity contrasts in the crust as signatures of the α–β transition. On the mechanical side, transformational faulting can occur during the quartz–coesite phase transition driven by volume change alone, without substantial latent heat release or strength contrast. Faulting is controlled by reaction kinetics: slow kinetics promote brittle behavior, while fast kinetics lead to ductile weakening. These two results, taken together, highlight how the phase transitions of a single, abundant mineral can exert a profound and previously underestimated influence on the elastic and rheological behavior of the continental crust – from the propagation of seismic waves to the nucleation of earthquakes.

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