Thermodynamics of Stressed Crystals: Stress–Composition Coupling and Its Geological Consequences (Invited)

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The chemical and physical evolution of multicomponent minerals are commonly treated as separate processes. Mineral compositions are typically used to infer pressure–temperature conditions, whereas microstructures are interpreted to reconstruct stress histories. However, these processes are fundamentally coupled: deformation can drive chemical evolution, and chemical changes can, in turn, generate stress. Treating them independently introduces uncertainty in interpreting the rock record and obscures processes governed by chemo-mechanical coupling.

The thermodynamic framework developed by Larché and Cahn[1] provides a rigorous, quantitative basis for describing the chemo-mechanical evolution of stressed, multicomponent crystals. Here, this framework is extended to common rock-forming minerals, including garnet, pyroxene, and feldspar, to quantitatively demonstrate how stress influences mineral composition and, conversely, how chemical evolution can generate stress and induce deformation, even in initially stress-free crystals.

Results show how the composition of multicomponent crystals varies systematically with crystallographic orientation in a fixed stress field. Accounting for this effect refines traditional geobarometry and motivates new "orientation piezometry" approaches, in which combined measurements of composition and orientation across crystal populations can be used to constrain stress. In addition, diffusion of species with contrasting partial molar volumes (e.g., Mg and Ca in garnet) is shown to generate differential stresses on the order of hundreds of MPa, sufficient to fracture crystals and drive recrystallization, as illustrated by examples from the exhumed subduction complex of Holsnøy, Norway.

Together, these results reduce uncertainty in interpreting mineral chemical records, provide new tools for extracting stress information from compositions, and reveal how coupled chemo-mechanical processes govern mineral evolution and microstructural development.

[1] Larché, F. C., & Cahn, J. W. (1985). The interactions of composition and stress in crystalline solids. *Acta Metallurgica*, *33*(3), 331-357.

Mineral Boundary Plane Distributions in Basalt and Their Role in Geological Carbon Sequestration

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Basaltic rocks are promising candidates for geological carbon storage because reactive minerals can immobilise carbon through dissolution and carbonate precipitation. However, predictions of reactivity commonly treat minerals as homogeneous and rarely account for crystallographic anisotropy.

This study quantifies the distributions of grain and phase boundary planes in a natural basalt from Mauna Kea. It evaluates the influence on kinetics during early-stage reactions with wet supercritical CO_2. Electron backscatter diffraction (EBSD) and statistical boundary analysis were used to characterise feldspar, pyroxene, magnetite, and olivine interfaces. The basalt exhibits strong mineral-specific boundary plane orientation anisotropy. Grain boundaries show stronger orientation preferences than phase boundaries, and larger grains exhibit more developed low-energy boundary populations.

Experimental wet supercritical CO_2 dissolution reactions at 150 °C and 9 MPa reveal highly selective dissolution. Olivine dissolves first and remains the dominant reactive phase throughout the longest experimental duration of 7 days. Apatite appears to be the next phase to undergo dissolution, whereas feldspar, pyroxene, and magnetite remain largely unchanged over the experimental timescale of up to 7 days. Dissolution initiates at grain boundaries, phase boundaries, and microcracks before propagating inward, highlighting the importance of interface-mediated dissolution reactions. EBSD-based boundary plane analysis of olivine-feldspar interfaces shows that high-energy orientations adjacent to dominant low-energy planes are preferentially dissolved before more stable boundary populations.

These results show that basalt CO_2 dissolution is governed not only by bulk mineralogy but also by the coupled effects of interface type, interfacial plane crystallographic orientation, and associated interfacial energy. Despite its low abundance, early apatite dissolution may be important for overall reaction kinetics because it can affect permeability. Incorporating evolving boundary plane distributions into reactive-transport models could improve predictions of basalt carbonation and help identify fine-grained, interface-rich basalts suitable for geological carbon storage. By linking crystallographic statistics with reaction experiments, this work provides a microstructural framework for understanding anisotropic reactivity in basaltic systems used for geological carbon storage.

The magnetic structure of the serpentinized mantle wedge: a magnetic fabric study on the Sanbagawa belt, Japan

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Subduction zones generate megathrust earthquakes and volcanic activities. To minimise the damages caused by them, previous studies have tried to reveal subduction zone conditions (e.g., temperature distribution) through geophysical methods. Magnetic anomalies observed from marine, airborne, and satellite magnetic surveys also offer an accessible proxy for subduction zone conditions. The contribution of the hydrated (serpentinized) mantle wedge to the observed magnetic anomalies should be considered for this because mantle wedge serpentinization forms magnetic minerals. Despite the crucial impacts on the interpretation of the observed magnetic anomalies, the magnetic structure of the serpentinized mantle wedge remains unclear. Here, to reveal the magnetic structure of the serpentinized mantle wedge, we investigate magnetic fabrics of the exhumed mantle wedge serpentinite, collected from the Sanbagawa belt in Japan, by analysing the anisotropy of magnetic susceptibility (AMS), anisotropy of anhysteretic remanent magnetization (AARM), first-order reversal curves (FORCs), and quantum diamond microscopy (QDM). We found that the massive serpentinite above the slab interface is dominated by multi-domain magnetic minerals and shows trench-parallel anisotropy of AMS and AARM with a low degree of anisotropy (up to 4.1). On the other hand, the boundary rocks near the slab interface are dominated by single-domain magnetic minerals and show trench-parallel anisotropy of AMS and AARM with a high degree of anisotropy (up to 6.7). The strong anisotropy of the boundary rocks is caused by an interaction among single-domain magnetic minerals in a chain-like structure. Further studies using focused ion beam-nanotomography (FIB-nT) with micromagnetic modelling will reveal the interaction for a better understanding of the magnetic structure of the serpentinized mantle wedge.

Recent advances in experimental quartz rheology and consequences for the plastic deformation of other silicates (Invited)

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Since the 1960´s, it has been known that crystal plastic deformation (dislocation creep) is an important deformation process in silicates and is responsible for high strain deformation in many earth materials at elevated temperatures. Quartz as one of the most common and ubiquitous minerals in crustal rocks has been frequently used to model the rheology of the Earth´s crust. In order to acquire rheological data, systematic deformation experiments on quartz have been carried out since the mid-1960´s. Some of the most recent advances in experimental quartz deformation have been made by Ghosh et al. (2022, 2024). These results will be presented and reviewed in the context of earlier experiments from the existing literature.

The flow behavior can be described by a dislocation flow law of the form:

$E(dot) = A\ \sigma^{n} / d^{-p}\ e^{-(Q/RT)}$

One interesting result of recent experiments is (consistent with some earlier observations) that the stress exponent n is equal to ≈ 2. For climb-accommodated dislocation creep, a n-value of 3 to 5 would be expected, as it is typically observed and theoretically required in metals. The n-value of ≈ 2 indicates that dislocation creep is not climb- accommodated but other processes dominantly accommodate crystal plastic deformation in quartz. The most important of such processes is grain boundary migration facilitated by disolution-precipitation in the presence of an aqueous fluid, as is demonstrated from microstructures of experimentally deformed polycrystalline quartzite samples. The results are similar to those of wet ice, where n-values of ≈ 2 have been observed, too (Goldsby and Kohlstedt 2001). The lower n-values are consistent with an observed mild grain-size-dependence (low grain size exponents of 1 to 2) of the deformation.

The results from quartz and ice will be compared to other minerals, for example feldspars. It emerges that the expected n-values of 3 to 5 theoretically required in metals cannot be simply applied to silicates and, instead, lower n-values of ≈ 2 are caused by dissolution – precipitation processes in silicates. As a consequence, the rheology of crustal rocks should be modeled with low n-values and low grain size exponents (≈ 0.5 to 1). As grain size exponents are very difficult to determine accurately, it appears more practical at present to carry out an approximate grain size correction utilizing different A-factors in the equation.

Point Defects as a Control on the Viscosity Jump in the Lower Mantle

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The viscosity profile of the Earth's lower mantle remains poorly constrained. Existing models yield divergent predictions that often conflict with mineralogical constraints. A key missing parameter in constraining lower-mantle viscosity is the concentration of point defects. Silicon (Si) vacancies are particularly important because they are generally recognized as the rate-limiting factor in diffusion-controlled creep [1]. Diffusion-controlled creep is the dominant deformation mechanism in the lower mantle [2]. However, the constraints on the concentration of Si vacancies in lower mantle minerals are currently very limited. We employed *ab initio* molecular dynamics calculations combined with thermodynamic integration techniques to compute the concentration of Si vacancies in bridgmanite under lower-mantle conditions. Our results show that Si vacancy concentrations decrease by one to two orders of magnitude from the top to the mid-lower mantle, then increase at greater depths. This variation in vacancy concentration induces corresponding changes in lower-mantle viscosity. The magnitude of these viscosity changes exceeds one order of magnitude, and this trend is consistent with the viscosity profiles predicted by many existing models. Furthermore, these findings allow us to constrain the grain size of the lower mantle to about 1 mm and/or the average deviatoric stress is ~1 MPa. However, variations in Si vacancy concentrations alone cannot explain sudden or large changes in viscosity, such as a low viscosity channel below 660 km followed by a sharp increase at 1000 km as suggested in some models (*e.g.* [3]), or other models (*e.g.* [4]) predicting increases in viscosity at about 1000 km. These observations suggest a compositional control for such anomalies. However, the general increase and decrease of viscosity with depth seen in many models is readily explainable by the thermodynamically controlled vacancy concentration and a small increase in grain size.

[1] Ammann, M. W., Brodholt, J. P., & Dobson, D. P. (2009). *Physics and Chemistry of Minerals*, ***36***(3), 151-158.

[2] Reali, R. et al. (2019). *Scientific Reports*, ***9***(1), 2053.

[3] Rudolph, M. L., Lekić, V., & Lithgow-Bertelloni, C. (2015). *Science*, ***350***(6266), 1349-1352.

[4] Lau, H. C. P. et al. (2016). *Journal of Geophysical Research: Solid Earth*, ***121***(10), 6991-7012.

The stishovite to post-stishovite phase boundary Studied by stress cycling experiments in a dDAC

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Stishovite and post-stishovite, the stable forms of SiO2 at mantle conditions, are important mineral phases in the lower mantle, in particular in subduction zone environments, where Mid-Ocean Ridge Basalt (MORB), the crustal component of the subducting slabs, contains up to 20 Vol.% of SiO2. Deeper, where MORB might delaminate from the rest of the subducting slab, it might stagnate at around 600-1000 km depth. Ultimately, MORB will sink toward the base of the mantle, potentially feeding the LLSVPs or other heterogeneities near the CMB. Other scenarii also propose that SiO2 can exsolve into the mantle from the crystallising core, or that SiO2-rich regions can exist as remnants of the magma ocean.

Stishovite and post-stishovite are thus important components of the dynamic mantle, in the regions that are the most crucial to image by seismology and advance our understanding of the dynamics of the Earth's interior.

The stishovite to post-stishovite transition is characterised by elastic anomalies, but its impact on mantle physical properties and seismic wave propagation has not yet been completely understood. For instance previous studies have reported softening of the shear modulus of stishovite near the phase boundary, with strong differences depending on the stress condition of the sample (isostress vs isostrain). Another study has highlighted a strong sensitivity of the phase transition to stress. Hence the real-world physical behaviour of polycrystalline SiO2 across the stishovite to post□stishovite under a cyclic loading, as imposed by a seismic wave in the mantle, could be different to what is expected based on hydrostatic equation of states or classic compression experiments. In addition, non-elastic responses to cyclic stresses, including attenuation, are poorly explored by experiments.

To directly investigate the response of stishovite and post-stishovite to a passing seismic wave, we performed cyclic loading experiments using the dynamic diamond anvil cell (dDAC). We used the dDAC setup available at the synchrotron beamline P02.2, at PETRA III, DESY to simulate seismic waves in stishovite/post-stishovite samples, and followed the evolution of their unit cell and lattice strain using time-resolved X-ray diffraction.

Our preliminary results show that at pressure of about 50 GPa, volume strain response to stress in our samples arrives ~15 s later than lattice strain response, when the oscillation frequency is 0.01 s^{-1}. This lag of the volume strain response, however, decreases when increasing the cycling frequency from 0.01 to 0.1 s^{-1}. We will discuss the possible causes of this observation and, in particular, try to discriminate between an elastic or attenuation origin.

Aluminium drives hydrogen incorporation in pyrolitic lower mantle: Constraints from a combined FTIR-ERDA-nanoSIMS analysis

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Hydrogen is present as hydroxyl (OH) defects in the crystal lattices of the nominally anhydrous minerals (NAMs) composing the Earth's mantle. The NAMs comprising the lower mantle: bridgmanite, ferropericlase, and davemaoite, are the three most abundant minerals on Earth, and thus their combined hydrogen solubility exerts a first-order control on the planetary H_2O capacity and overall H_2O cycle. In this study, we equilibrated the three principal NAMs with hydrous melt at the adiabatic geotherm and pressure corresponding to the shallow lower mantle. The H_2O content of the coexisting NAMs is quantified by nanoSIMS using matrix-matched standards characterized by Fourier Transform Infrared (FTIR) spectroscopy combined with Elastic Recoil Detection Analysis (ERDA). Our results show that bridgmanite, ferropericlase, and davemaoite incorporate ~0.03, ~0.16, and ~0.18 wt% H_2O, respectively. Combined with their corresponding crystal chemistry, these data suggest that hydrogen is primarily incorporated via Al^{3+}-H^{+} insertion at the Si^{4+} (octahedral) site in perovskite-type structures and the metal (octahedral) site in ferropericlase. Finally, we refine a maximum H_2O content of 0.058 (0.009) wt% H_2O in a pyrolitic-shallow lower mantle, which is equivalent to ~1.26 (0.2) ocean masses when extrapolated to a chemically homogeneous lower mantle.

Determining Paleo-stress signals using rock magnetism (Invited)

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Stress and shock effects have been experienced through impacts and seismic activities, since the formation of the Earth. From earthquake processes to impact cratering the crust undergoes stress fields from 10^2 to 10^6 MPa, which can have significant effect on rock magnetic signals. Over the past several decades, shock remanent magnetisation has primarily been studied at pressures greater than 1 GPa. From explosive tests to hypervelocity experiments, magnetisation and demagnetisation effects have been observed with respect to distance and intensity. Changes in the bulk magnetic susceptibility and anisotropy of magnetic susceptibility (AMS) in response to high stresses within the elastic, inelastic and plastically deformed rocks have also been found. However, at such high pressures, rocks encounter unavoidable inelastic and thermal effects. Deformed rocks are therefore difficult to use for recovering stress-related magnetic signals, while heating effects result in thermoremanent magnetisation and overprinting the original stress signal.

Attention is drawn to high-pressure ranges because our current understanding of stress effects on magnetic recordings is based on single domain (SD) theory. It is believed that SD grains are generally considered the most reliable and stable magnetic recorders over the geological timescale. However, recent models have shown that single - vortex (SV) grains retain most stable magnetisation under stresses as low as 0.1 GPa, a range previously assumed to be negligible in palaeomagnetic studies.

Until now, most stress and shock magnetic studies have focused on magnetic remanence at high pressures. The effects of stresses within the elastic regime of rocks at low pressures have been ignored.

In this talk, we highlight effects of stress at different strain rates on the anisotropy of magnetic susceptibility (AMS) under different experimental configurations. We show that the AMS may serve a broader purpose than reflecting the alignment of the underlying petrofabric. In particular, we demonstrate that even relatively low stresses can modify magnetic fabrics and influence palaeomagnetic signals, with important implications for the interpretation of palaeomagnetic studies.

Effects of temperature-driven complexion transitions and redox gradients on grain-boundary plane distributions in olivine

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Redox conditions in the upper mantle strongly influence defect populations and transport processes in olivine, while grain boundaries act as fast pathways for diffusion and chemical exchange. Previous experiments demonstrated that metal liners can impose millimetre-scale rim–core

$$fO_2$$

gradients in polycrystalline olivine through defect-mediated grain-boundary oxygen exchange. Here, the potential influence of such redox heterogeneity on grain-boundary plane distributions (GBPD) is investigated and compared with temperature-driven grain-boundary evolution. Three sol–gel Fo90 olivine aggregates are analysed: Ol–Pt, Ol–NiFe–LT, and Ol–NiFe–HT. The samples were hot-pressed for 24 h at 300 MPa at 1200 °C, 1250 °C, and 1300 °C, respectively, followed by refiring treatments. GBPDs were reconstructed from EBSD datasets using stereological methods, with rim regions sampled within 1 mm of the specimen edge and core regions within a 3 mm radius of the centre. The strongest anisotropy is observed in the high-temperature Ol–NiFe–HT sample, which exhibits a pronounced b-plane-dominant distribution with minimal rim–core variation. In contrast, the Pt-lined sample displays only subtle rim–core differences despite the expected strong redox gradient. These observations suggest that temperature-driven grain-boundary evolution, potentially associated with complexion transitions, exerts a stronger control on GBPD than liner-induced redox heterogeneity.

Potential Significance of Iron-Bearing Superhydrous Phase B in the Formation of Mantle Low-Velocity Zones

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Low-velocity zones (LVZs) in Earth's mantle are widely observed; however, their physical origins remain a subject of ongoing debate. In this study, we investigate the origin of seismic low-velocity anomalies by examining properties of iron-bearing, dense hydrous magnesium silicate (DHMS) through first principles simulations. Under high-pressure conditions, the density of superhydrous phase B (ShyB) increases linearly with increasing iron content, whereas its seismic velocities linearly decrease with iron enrichment. This contrasting behavior indicates that iron incorporation markedly enhances the intrinsically high-density and low-velocity characteristics of the ShyB. Our results further demonstrate that the seismic velocities of Fe-bearing ShyB are lower than those predicted by the Preliminary Reference Earth Model (PREM) over most mantle depths. Those finding suggest that Fe-bearing ShyB, as a distinct Fe-rich DHMS, may represent a viable and previously underappreciated mechanism contributing to the development of mantle LVZs (the "410-LVL" and the "800-LVL"). Collectively, this study provides a new physical model and conceptual framework for interpreting the origin of the LVZs in the mantle, with broader implications for the deep water cycle and iron redistribution in Earth's interior.

Comparisons Between the Trace Element Composition and Magnetic Structure of the Cloudy Zone in the Imilac and Odessa Iron-Nickel Meteorites

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Iron-nickel-rich meteorites are relics of differentiated planetesimals from the early Solar System. Due to early differentiation and cores that remained molten for millennia, these planetesimals developed internal temperature–composition conditions capable of generating microstructures with no terrestrial equivalents. Spinodal decomposition induced by part of this cooling process produced nanoscale tetrataenite islands (face-centred tetragonal $Fe_{0.5}Ni_{0.5}$) surrounded by an Fe-rich matrix, referred to as the *Cloudy Zone* (CZ). The CZ exhibits magnetic behaviour comparable to modern rare-earth-element-based (REE) permanent magnets. These powerful magnetic properties have motivated extensive research into tetrataenite synthesis as a REE-free alternative to high-performance permanent magnets. Successful tetrataenite synthesis could provide an energy transition material based in more abundant resources, which will be key in supporting sustainable net-zero goals[1]. Emerging evidence suggests that trace elements may influence the formation, stability, and magnetic behaviour of tetrataenite[2].

We will show analyses of the Imilac (main group pallasite) meteorites using differential phase contrast (DPC) and electron energy loss spectroscopy (EELS). We will also present our correlative workflow to relate EELS and DPC data in order to understand the relationship between compositional variation and magnetic properties and discuss the challenges that arise during this analysis.

1. Lewis LH, Stamenov PS. Accelerating Nature: Induced Atomic Order in Equiatomic FeNi. Adv Sci. 2024;11(7):2302696. doi:10.1002/advs.202302696.

2. Corrigan CM, Chabot NL, McCoy TJ, et al. The iron–nickel–phosphorus system: Effects on the distribution of trace elements during the evolution of iron meteorites. Geochim Cosmochim Acta. 2009;73(9):2674-2691. doi:10.1016/j.gca.2008.11.045.

Nickel Content of Iron Meteorites

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Iron meteorites sample core material of differentiated asteroids and planetesimals which formed within the first 1—2 Ma of the beginning of the Solar System [1]. Iron and stony-iron meteorite metal that has fully crystallized and cooled slowly will form characteristic Widmanstatten patterns if their bulk Ni abundances are > 6 wt. %. Widmanstatten patterns are a two-phase assemblage of polycrystalline parent taenite (~6—60 wt.% Ni, face-centered cubic crystal structure), and kamacite (5—6 wt.% Ni, body-centered cubic crystal structure) which nucleates and grows along the taenite crystal lattice from ~700—900ºC [2], [3]. Ni is expelled from kamacite into adjacent taenite, and results in a Ni-diffusion gradient from the taenite rim toward the taenite center controlled by cooling rates and the diffusion rate of Ni in solid solution, which forms a characteristic "M-shaped" profile across bands of taenite. Within ~5 μm of the kamacite-taenite rim interface where Ni abundances are 25—50 wt.% Ni, a tetrataenite (TT) forms on the interface, and homogenous "clear" taenite undergoes spinodal decomposition to form a two-phase composite known as the "cloudy zone" (CZ) (Fig. 1), which forms under extremely slow cooling rates (0.5—10^4 K/Ma) [4], and will stabilize from 350ºC into nanoscale high-Ni islands in a low-Ni matrix, and transform via Fe-Ni atomic ordering at 320ºC into ferromagnetic islands of tetrataenite [5].

Recent analyses of Eagle Station pallasites, a rare group of stony-iron meteorites established to originate in the outer solar system [6], has revealed both the occurrence of preserved CZ as well as a new microstructure (unofficially termed "wavy zone" [WZ]) that appears to have replaced former CZ due to thermal alterations, likely a reheating event on the Eagle Station parent body. In this study, we experimentally determine the reheating temperatures and Ni abundances characteristic of WZ formation from natural meteoritic CZ in order to quantify the extent of reheating the Eagle Station pallasites were exposed to. This study also serves to re-evaluate the stability of the CZ spinodal island structure, which has routinely been assumed to erase at temperatures between 350—450 ºC.

[1] M. Bizzarro, J. A. Baker, H. Haack, and K. L. Lundgaard, *Astrophys. J.*, vol. 632, no. 1, pp. 41–44, Oct. 2005, doi: 10.1086/497638.

[2] M. Uehara, J. Gattacceca, H. Leroux, D. Jacob, and C. J. Van Der Beek, *Earth Planet. Sci. Lett.*, vol. 306, no. 3–4, pp. 241–252, Jun. 2011, doi: 10.1016/j.epsl.2011.04.008.

[3] J. I. Goldstein and R. E. Ogilvie, *Geochim. Cosmochim. Acta*, vol. 29, no. 8, pp. 893–920, Aug. 1965, doi: 10.1016/0016-7037(65)90085-2.

[4] J. Yang, J. I. Goldstein, and E. R. D. Scott, *Geochim. Cosmochim. Acta*, vol. 72, no. 12, pp. 3043–3061, Jun. 2008, doi: 10.1016/J.GCA.2008.04.009.

[5] J. F. Einsle *et al.*, *Proc. Natl. Acad. Sci. U. S. A.*, vol. 115, no. 49, 2018, doi: 10.1073/pnas.1809378115.

[6] R. N. Clayton and T. K. Mayeda, *Geochim. Cosmochim. Acta*, vol. 60, no. 11, pp. 1999–2017, 1996.

Predictive Modeling of Chemically Complex Earth-Forming Materials via Deep-Learning-Driven Atomistic Simulations (Invited)

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Understanding the structure, dynamics, and evolution of Earth's interior requires quantitative knowledge of how Earth-forming materials behave at high pressure and temperature. Properties such as density, elasticity, and thermodynamics are needed to build mineralogical models that explain seismic observations and to understand how elements are redistributed during chemical differentiation. Thermal conductivity and viscosity, in turn, control how heat and mass are transported through the deep Earth and therefore influence its long-term evolution. However, measuring these properties directly remains extremely difficult, especially for chemically complex materials under extreme conditions. Although ab initio atomistic simulations can provide highly accurate results, they are still limited to relatively small system sizes and short timescales, making it difficult to connect atomic-scale behavior to the macroscopic properties we seek to understand.

In this presentation, I will introduce our recent work on developing an efficient deep learning-based atomistic simulation framework for studying chemically complex Earth-forming materials under extreme conditions. After being trained on high-accuracy quantum-mechanical data, this approach can predict material properties with near-ab initio accuracy at only a fraction of the computational cost, making it possible to study larger systems over longer timescales than conventional ab initio methods. I will first present benchmark results on standard test systems, including rMD17 and water, and compare its performance with existing machine-learning approaches. I will then show applications to the Fe–Si phase diagram under inner-core conditions and to the partitioning of highly siderophile elements between silicate melts and liquid iron alloys under core-formation conditions. These results demonstrate how scalable atomistic simulations can provide a quantitative picture of the crystal structure of Earth's inner core and the origin of volatile elements, paving the way for a high-throughput workflow to study Earth forming materials

Liquid immiscibility in the Fe-O-S ternary system at high pressure and temperature

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The recent InSight mission provided seismological data from Mars used to reconstruct its interior structure and composition. These studies suggest the Martian outer core density must contain very large concentrations of light elements, possibly a mixture of S, O, C and H. Similar data for the Moon is expected from the Farside Seismic Suite mission. The light element content of liquid cores impact their internal crystallization and convection, which in turn effect heat flow and generation of a magnetic dynamo. Accurately determining core compositions will clarify both the origin of Mars and the Moon as well as their evolution. Compositional constraints are achieved by comparing measured properties of candidate materials (e.g. density) with geophysical observations. Direct experimental measurements are arguably the best means to accurately study these Fe alloy melt systems. Whilst the density of several light element bearing systems have been measured before, to our knowledge no studies have measured the density of oxygen bearing melts under appropriate conditions despite this being a likely core component. This is especially true of the Martian core, which requires approximately 50 mol% light elements, of which sulphur is likely to be the largest component. Since metal-silicate equilibration experiments have demonstrated that oxygen solubility in Fe melts dramatically increases with sulphur content, a sulphur-rich core will also be oxygen-bearing.

Researchers wishing to experimentally measure the density of melts in the Fe-O-S system face a problem, in that an immiscibility field exists within the system at low pressure in which the system will exsolve into oxygen-rich and oxygen-poor melt phases. Density measurement techniques require a single melt phase, therefore the boundaries of the immiscibility field must be constrained experimentally over a range of pressures and temperatures before density measurements can be conducted with confidence. Additionally, if a planetary core were to exist with the composition and under the conditions that correspond with the immiscibility field of the Fe-O-S system, these melts would density separate and stratify. Since this has not been observed within the Martian core, the immiscibility field boundary provides further limits on core composition.

We have performed a series of quench experiments within a multi-anvil apparatus at high pressure and temperature with compositions within this immiscibility field. The quenched immiscible melts produced in these experiments are analysed for composition on an SEM, which define the boundaries of the field.

Light Element Exsolution in Fe-Si-C-(H) System in Planetary Liquid Cores

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Light elements are thought to be essential components of liquid cores in terrestrial planets and play a key role in core formation, chemical evolution, and the long-term evolution of planetary interiors. In multicomponent Fe-light element systems, when multiple light elements coexist in liquid iron, their solubilities are mutually constrained, forming an anti-correlated solubility relationship, referred to here as simultaneous solubility. When the concentration of light elements exceeds the simultaneous solubility limit, light element exsolution may occur from Fe-rich liquids. Here we investigate the simultaneous solubility and exsolution behaviour of light elements in the Fe-Si-C-(H) system using multi-anvil press quench experiments combined with machine-learning force field molecular dynamics simulations.

High-pressure and high-temperature quench experiments were conducted at 9-21 GPa and 1400-2200 °C, corresponding to Mercury core-relevant conditions. The results show that C and Si exhibit anti-correlated solubilities in Fe-rich melts, defining a simultaneous solubility limit recorded by quenched samples. We also observed light element exsolution, with elemental Si, diamond, and graphite identified as the exsolved phases. Specifically, large diamond grains near the top side of the recovered sample indicate elemental C exsolution during high P-T equilibration. Their accumulation near the top of the sample chamber is likely related to gravitational segregation. By contrast, fine-grained elemental Si and C within the quenched Fe-rich melt record further exsolution during cooling, indicating that the Si-C simultaneous solubility decreases as temperature decreases.

We further extended the P-T range toward Earth core conditions using molecular dynamics simulations with a MACE machine-learning interatomic potential trained for the Fe-Si-C system. Two-phase simulations of Fe-Si liquid coexisting with solid diamond were conducted at 90-330 GPa and 4100-5500 K to investigate carbon solubility in diamond-saturated Fe-Si melts. The results show that carbon solubility increases with temperature, whereas pressure has a comparatively weaker effect, indicating that temperature is the dominant control on carbon solubility under the investigated conditions. These results suggest that, in the Fe-Si-C-(H) system in reduced planetary liquid cores such as those of Mercury and Earth, simultaneous solubility provides a compositional constraint on the range of Si and C contents that can coexist in Fe-rich liquids. Light element exsolution may occur during cooling when this solubility limit is exceeded, providing new insight into light element redistribution during planetary core evolution.

Phase relations of subducted sediments to near the core-mantle boundary

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Sediments are transported into the deep Earth through subduction zones. While their phase relations are relatively well understood at pressures below 28 GPa (e.g. *Ishii et al., 2012*), their higher-pressure behaviour remains unknown. Furthermore, sediments can undergo partial melting during the early stages of subduction, leaving behind a refractory 'restite'. The high-pressure phase relations of such restite compositions, are entirely unconstrained.
In this study, we explore the minerals assemblages of a typical subducting clay and its restite after 50% melt extraction at 3 GPa and 800 °C. We conducted laser heated diamond anvil cell (DAC) experiments up to pressures of 123 GPa and multi anvil experiments up to 30 GPa. The diamond anvil cell experiments were conducted along a hot subduction geotherm for the restite composition and a cold subduction geotherm for the clay composition. The multi anvil experiments were conducted at 1600 °C for both compositions to promote crystal growth in these dry systems. The DAC samples were analysed both in situ and ex situ using synchrotron XRD. The multi anvil samples were characterised using laboratory-source XRD, scanning electron microscopy (SEM) and electron probe microanalysis (EPMA).
Phase assemblages recovered from both methods at the same pressure conditions were consistent, implying the chemical compositions obtained from the multi anvil experiments also apply for the DAC samples.
From 25-80 GPa, all experimental run products with a clay composition exhibit stishovite, new aluminous phase and calcium-ferrite type phase. We observe no NAL at high pressure, but an additional Ti-rich perovskite phase in the restite composition. Due to an absence of Potassium in the restite composition, K-Hollandite is not observed. For the Clay composition, K-Hollandite is absent above 40 GPa.
Our results extend the pressure range of the stable phase assemblages of sedimentary compositions significantly and highlight the importance of compositional control on future high pressure sedimentary phase relation studies.

Ishii, T., Kojitani, H., & Akaogi, M. (2012). High-pressure phase transitions and subduction behavior of continental crust at pressure–temperature conditions up to the upper part of the lower mantle. Earth and Planetary Science Letters, 357, 31-41.