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Thermal conductivity of deep earth minerals using high pressure-temperature time-resolved powder X-ray diffraction at European XFEL

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Large scale dynamics within the Earth are the result of cooling. Heat is transported towards the surface by large scale convection in the mantle and in the core, and by conduction across the thermal boundary layers at the core–mantle boundary and the lithosphere. There is a range of estimates for the thermal transport properties, e.g. thermal conductivity (k) in the lower mantle ranges between 4 and 16 W/m K, [i] resulting from a lack of consensus on how to represent the pressure (and temperature) dependence of k; different models yield very different extrapolations.[ii]

A three-pronged approach is here established to study thermal conductivity of deep earth minerals at CMB conditions.

(i) Generating high-pressure and high-temperature states of matter in a diamond anvil cell (DAC) and resolving crystallographic changes in the sample via powder XRD. HED at European XFEL is the only facility at present that has sufficiently high X-ray energy coupled with MHz pulse trains to perform time resolved measurements of heat flow in high pressure samples heated by XFEL pulse trains. The femtosecond FEL pulses generate a unique thermal disturbance in bulk matter at a definitive time point, providing an idealized starting point for thermal relaxation. The AGIPD detector at HED allows for easier determination of relaxation dynamics and heat flow.

(ii) Powder XRD analysis can be carried out by utilising the different timescales of XRD and X-ray absorption, whereby XRD is immediate and occurs before any subsequent unit-cell expansion due to X-ray absorption. The first X-ray pulse is used to collect a diffraction image of the unexcited state of the sample. The next X-ray pulse probes the heated state of the sample 222 ns after first excitation (at 4.5 MHz), before heating the sample again and the step is sequentially repeated.

(iii) Finite element modelling studies allow the determination of thermal parameters such as thermal conductivity and expansivity. Utilising volume change with temperature in a sample, which can be extracted from the diffraction data, a primary model can be made. Temperature dependent thermal conductivity is fitted to the data. Beam energetic data is integrated into the Finite element modelling to dynamically model the fluctuations in the intensity of energy pulses.

[i] (Goncharov et al., 2009, Lay et al., 2008, Hofmeister, 2007, Hofmeister, 1999, Brown, 1986, Kieffer, 1976)

[ii] Goncharov et al., 2009, Hofmeister, 2007, Brown, 1986).