

Constraining elemental partitioning and isotope fractionation of mantle minerals with *in-situ* single crystal X-ray diffraction

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The elemental and isotopic composition of the mantle provides important constraints to the earth's interior structure and dynamics. Conventional analyses to constrain the elemental and isotopic behaviors are usually carried out on samples quenched from high P-T experiments, which is intrinsically slow as multiple experimental run charges are required to capture different P-T conditions. Single crystal X-ray diffraction is a promising method to constrain the chemical composition of mantle mineral *in-situ* at high P-T conditions. We have developed a synchrotron-based single crystal X-ray diffraction setup that is compatible with high pressure diamond anvil cell and laser/resistive-heating. Our setup features *in-situ* operation in which one sample is used for the measurement at multiple P-T conditions, so as to improve the efficiency. Using this setup, we are able to determine the *in-situ* evolution of the elemental composition of minerals with pressure, temperature and time, which paves the way for the determination of major elemental partitioning at relevant mantle conditions. By combining the *in-situ* diffraction measurements and first-principle calculations, we have also developed a force-constant approach to constrain the isotope fractionation β -factor of silicon in mantle minerals.