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Constraining atomic dynamics in rock-forming minerals with in-situ X-ray diffraction and its application in silicon isotope fractionation

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The isotope fractionation of silicon is related to many deep earth phenomena. Using in-situ single crystal X-ray diffraction technique and our new *force constants* method, we have determined the equilibrium Si isotope fractionation between various rock-forming minerals. Our results suggest that incorporation of Na helps to enrich heavy Si into omphacite over garnet in eclogite. We found that the omphacite and pyrope garnet in Dabie Mountain eclogites, as well as the kyanite and its host quartz veins, are in equilibrium for Si isotopes, which suggests that the kyanite-bearing Dabie eclogite and the host quartz vein endured the same pressure-temperature condition during their formation. We also found that the Si isotope fractionation between zircon and granite saturates when the granite contains more than 70 wt% quartz, and the equilibrium Si isotope fractionation between zircon and granite at 1000 K is ~0.45‰ for such granites. Newly compiled low temperature diffraction data on epidote also demonstrates that the Si atomic dynamics shows quantum behavior at extreme environments, which has effect on its isotope fractionation.