

Determining the effect of ^{57}Fe enrichment on NRIXS-derived force constants

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Non-traditional stable isotopes offer an important avenue of investigation into many Earth processes. Stable isotopes of Fe are regarded with particular interest, as Fe is present in many minerals. As a result, Fe isotope data has now been collected on a wide variety of samples over several decades. Interpreting these data, however, requires robust fractionation factors. Nuclear resonant inelastic X-ray scattering (NRIXS) is used to determine force constants for the Fe-sublattice in Fe-bearing phases. From these force constants, isotope fractionation factors can be derived [1]. This method is particularly appealing as phases do not need to be equilibrated to measure an equilibrium fractionation factor. However, force constants derived from density functional theory (DFT) can be inconsistent with those found by NRIXS, with the NRIXS values generally being greater than the DFT values [1-4].

We are investigating the source of this discrepancy between DFT and NRIXS force constants. NRIXS is restricted to measuring Mössbauer-sensitive isotopes, which for Fe is ^{57}Fe . Natural iron contains only 2.2% ^{57}Fe , so to expedite NRIXS analysis researchers typically dope their samples with ^{57}Fe far in excess of natural abundances. We hypothesize that artificially high ^{57}Fe content could be the source of the inflated NRIXS force constants. To test for this effect, we produced metal (Fe), wüstite (FeO), and fayalite (Fe₂SiO₄) with varying $^{57}\text{Fe}/\text{SFe}$, ranging from 0.02 (natural) to 0.70. We are currently carrying out NRIXS measurements at beamline 3ID at the Advanced Photon Source. These results will allow us to determine whether a correlation exists between ^{57}Fe content and the measured force constants. Results will also inform decisions on the doping level for future NRIXS measurements conducted for isotope geochemistry.

References:

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