

# The Influence of Solid Structure and Liquid Composition on Fe-isotope Fractionation Between Solid and Liquid Alloys

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Trace element partitioning between Fe-rich solid and liquid alloys depends on the light-element content of the liquid phase, where light elements (LE) include S, P, Si, C, and O. The “Fe Domain” model is often used to model this dependence, in which the liquid is described as a mixture of Fe and Fe-LE domains [1]. Implicit in this model, is that the bonding environment of iron is modified by the addition of light-elements to the alloy. Phase relations in several Fe-LE systems can also be modeled by invoking differences in bond strength between coexisting bond pairs, e.g., between Fe-Fe and Fe-S pairs in sulfide liquids [2]. These observations suggest that LE-content should play a controlling role on iron-isotope fractionation in systems containing Fe-rich liquid alloys.

We will present the results of experiments in the Fe-Ni-P system, which reveal an important role for both liquid alloy composition and solid metal structure. In the Fe-P system, metallic liquids are isotopically lighter than coexisting solids, and fractionation increases with addition of P to the liquid. Experiments containing ~14 wt% Ni are offset from the Ni-free trend, but broadly parallel with it. The addition of Ni results in the solid phase having a face-centered-cubic structure, in contrast to the body-centered-cubic structure present in our Ni-free experiments. Force constants from the literature for bcc and fcc FeNi alloys confirm that the offset between our Ni-free and Ni-bearing experiments is explained largely by the change in solid structure. Preliminary data in the Fe-S system suggests similar behavior to the Fe-P system, with the largest fractionations comparable to those found by [3]. A single experiment in the Fe-C system shows no resolvable fractionation between solid and liquid metal, but work is ongoing to confirm this result over a wider range of composition.

[1] Chabot & Jones (2003), *MAPS* 38, 1425-1436.

[2] Waldner & Pelton (2005), *Journal of Phase Equilibria and Diffusion* 26, 23-38.

[3] Ni, Chabot, Ryan & Shahaar (2020), *Nature Geoscience* 13, 611-615.