Fractionation of Si isotopes during core formation from first principles calculations

Piotr M. Kowalski*[1] and Sandro Jahn[2]

[1]Forschungszentrum Jülich GmbH, Institute of Energy and Climate Research - IEK-6: Nuclear Waste Management, D-52425 Jülich, Germany (*correspondence: p.kowalski@fz-juelich.de);
[2]GFZ German Research Centre for Geosciences, Telegrafenberg, D-14473 Potsdam, Germany.

Recently, we have developed an efficient ab initio based computational approach to predict equilibrium isotope fractionation factors between chemically and structurally complex crystalline solids, fluids and melts at high T and P [1,2]. Our method has been successfully applied to "non-traditional" stable isotopes of light elements such as B and Li, which are important geochemical tracers widely used in petrology. We have shown that we are able to correctly reproduce the experimentally observed fractionation sequences: fluid-tourmaline-mica for B and staurolite-fluid-mica-spodumene for Li isotopes with a computational uncertainty comparable to the experimental error. Moreover, with the calculations we explained the discrepancy between the results of in-situ experiments and measurements on natural samples [2].

With this well tested methodology we investigate here the Si isotope fractionation between silicate melt and liquid metal under the extreme P-T conditions of Earth's core formation (P~25 GPa, T~3000 K) that are not yet accessible to experiment [3]. The equilibrium Si isotope fractionation factors between these materials are of great interest as they are needed to understand the origin of the difference in the isotopic signatures observed between the Bulk Silicate Earth (BSE) and Chondrite meteorites [3]. It has been proposed that the observed difference reflects the fractionation of Si isotopes between silicate melt and iron-rich metal during the formation of Earth's core [4]. We will present a comparison of our predictions with the available experimental data and discuss the effect of the pressure-induced changes in the melt structure on the fractionation of Si isotopes. Our results shed new light on the origin of the excess of the heavy Si isotopes in BSE and may also help to further constrain the silicon content of the Earth's core.

[1] Kowalski, P. M. and Jahn, S. (2011) *Geochim. Cosmochim. Acta* **75**, 6112-6123. [2] Kowalski, P. M. Wunder, B. and Jahn, S. (2013) *Geochim. Cosmochim. Acta* **101**, 285-301. [3] Shahar, A. *et al*. (2011) Geochim. Cosmochim. Acta **75**, 7688-7697. [4] Georg, R. B. *et al.* (2007) *Nature* **447**, 1102-1106.

Characteristics of metal bearing phases in MSWI residues from Poland

P. Kowalski[1]*and M. Michalik[1]

[1]Institute of Geological Sciences, Jagiellonian University
ul.Oleandry 2a, 30-063 Krakow
(*correspondence: p.kowalski@uj.edu.pl)

Mineralogical characteristic of MSWI (municipal solid waste incineration) residues is important, especially in time of ongoing changes in municipal waste management system in Poland. These changes leads to significant reduction of the amount of landfilled raw wastes. A way to achieve this goal is construction of nine incineration power plants with assumed slags production around two hundred thousand tons per year. The increasing slag production makes that it is essential to take a closer look into this material in terms of possible environmental pollution.

The aim of this study is mineralogical and chemical characteristics of the metal-bearing phases of the MSWI residues. Slags were collected from two the biggest incineration power plants in Poland. One of them is oriented to incineration of non-hazardous municipal waste and the other on industrial and hazardous municipal wastes.

Slags from incineration of wastes are non-consolidated, grainy materials, containing large amount of amorphous phase, mostly composed of Si-rich glass.

Metals in slags are present in several forms:

1. As large fragments which are mixed with slags grains and part of uncombusted materials (rock fragments, glass and ceramics),
2. In form of metallic inclusions in glass or minerals,
3. As a component of mineral and amorphous phases.

Metals in form of metallic inclusions are monometallic (mainly Fe, Al, Pb, Zn, Cu) or in form of alloys (Fe-Ti, Fe-Ni, Fe-Cu, Cu-Sn+Pb and Cr-Fe). Metals in minerals are concentrated mostly in form of oxides (mainly Fe and Al oxides) and in silicates, aluminosilicates and sulfates (e.g. Cu). The content of metals in glass varies in wide range. High concentration of them is connected with presence of metallic inclusions inside the glass. Content of metals in slags varies within broad range – e.g. Cu from 330 to 4900 ppm, Zn from 1500 to 4700 ppm, Pb from 50 to 6300 ppm and Cr from 300 to 600 ppm in municipal slags and from 2000 to 2500 ppm in industrial slags. These concentrations could be potentially hazardous and further studies about leaching potential and mobility of these metals are needed.

DOI:10.1180/minmag.2013.077.5.11