Effect of process conditions on the biological selenate reduction and selenium particle production

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Objective and methods

Diverse microorganisms can reduce selenate to elemental Se. Elemental Se particle properties are determined by the Se production mechanism and kinetics. The effect of the used bacterial mixed culture, temperature, Se oxyanion and electron donor concentration on Se particle size, shape, sedimentation rate, and purity was investigated.

Experiments were performed in a pH and T controlled fed-batch system. The feed contained 25mM Se oxyanions and the electron donor was lactate or ethanol.

Results and discussion

SEM pictures of the Se precipitates showed that it was possible to affect the Se particle properties (needles to spheres) by varying process parameters.

The mechanism of Se precipitation was also investigated to determine whether the reaction is direct bio-mineralization or a combination of direct and indirect bio-mineralization. A possible two step mechanism is suggested.

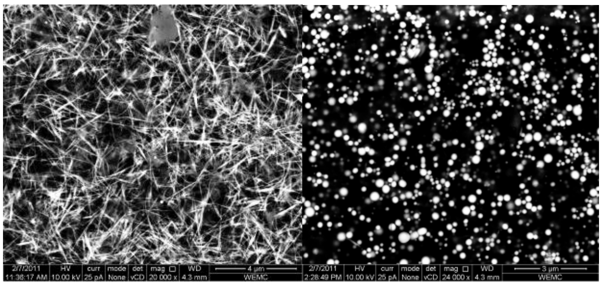

Figure 1: SEM-photos of the Se precipitates. The picture on the left shows Se needles, the scalebar in the lower right corner is 4μm. The picture on the right shows Se spheres, the scalebar in the lower right corner is 3μm.

Atomic environment of Y in silicate melts from molecular dynamics and x-ray absorption spectroscopy

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Trace element partitioning strongly depends on major element composition of the involved phases. Whereas the influence of crystal chemistry is well described by the lattice strain model [1], the role of melt composition and structure is still poorly understood. In experiments with immiscible silicate melts, Schmidt *et al.* [2] observed partitioning of Y and rare earth elements into the more depolymerized (silica-poor) melt, where the tetrahedral network is partially destroyed. An explanation of these findings in terms of atomic-scale structure is still missing.

We performed molecular dynamics (MD) simulations to investigate the local environment of Y as a trace element in different silicate melts of the system CaO-Al$_2$O$_3$-SiO$_2$. The interactions between atoms were described by a new polarizable ion model which also captures many-body effects and was parametrized non-empirically, using density functional theory data as a reference. As a result, we found a systematic dependence of the atomic-scale structure around Y on melt polymerization, which can be quantified by means of the ratio of non-bridging oxygen to the network forming cations Si and Al (NBO/(Si+Al)): Upon increasing NBO/(Si+Al) from 0.0 to 1.9, the coordination of Y by O drops from 7.7 to 6.2, and the average Y-O distance decreases from 2.56Å to 2.46Å. Moreover, using the method of thermodynamic integration, we obtained first results for the exchange coefficient (ratio of partition coefficients) $D_Y^{melt1/melt2}/D_{Al}^{melt1/melt2}$ of Y and Al between two melts.

To validate our structural findings, we performed a joint theoretical and experimental study on extended x-ray absorption fine structure (EXAFS) spectra of Y in silicate melts. These spectra contain information about the coordination of Y and distances to neighbouring atoms. Traditionally, a structural model is refined until the measured spectrum is satisfactorily reproduced. However, for amorphous systems it is often difficult to make an appropriate guess for the structure, and hence we propose a converse approach. We modelled EXAFS spectra by averaging over many MD snapshots, and the agreement with experimental spectra confirms that our model faithfully reproduces the atomic-scale environment of Y.

[1] Blundy & Wood (1994), *Nature* **372**, 452-454 [2] Schmidt *et al.* (2006), *Science* **312**, 1646-1650