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Computer simulations and imaging of the effect of calcium on barite crystal morphology

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Barite (BaSO_4) is a major component of inorganic scale that forms in well bores and oilfield pipework, where it can reduce or even halt oil production. Chemical scale inhibitors (SI's) are used to prevent scales forming, and function by inhibition of nucleation and crystal growth retardation. However, for reasons that are poorly understood, these processes are affected by the presence of cations such as Ca^{2+} . We seek to understand why these changes in crystal morphology occur, and thus the mechanism and efficiency of growth inhibition.

In order to understand the structure of barite surfaces at an atomic level and the effect of additives such as Ca^{2+} on these surfaces, a combination of experimental and computer modelling approaches are being used. Environmental scanning electron microscope (ESEM) images of crystals from related experiments are used to constrain simulations, and show morphologies to vary from the classic rhombohedral habit to more complex, multi-faceted structures.

Atomistic simulation programs (GULP and MARVINS) were used to calculate the bulk and surface properties of BaSO_4 using existing empirical potentials. Predicted morphologies exhibit a variation from classic to complex structures with different concentrations of Ca^{2+} , Sr^{2+} and Mg^{2+} modelled on different surfaces of BaSO_4 . These models have enabled the prediction of changes in surface properties, and can be used to interpret preliminary observations of the (001) and (210) barite surface morphologies made using atomic force microscopy (AFM). In-situ AFM flow cell experiments will be used to study surface growth and dissolution processes, in the presence of supersaturated solutions of BaSO_4 . The influence of atomic scale processes on synthetic barite crystal morphology is being investigated using transmission electron microscopy (TEM). Comparison of experimental investigations with predicted crystal morphologies can help to identify the mechanisms of Ca^{2+} incorporation within the barite crystal structure and the effect on barite growth.

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Si isotopic fractionation at the interfaces among Si phases

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Isotopic studies in the fields of earth sciences have usually assumed the equilibria among concerned substances. However, kinetics should be taken into account for rapid crystal growth. A crystallization experiment of Si is suitable to elucidate the interface kinetics because of its simple composition and fast crystal growth rate.

Si isotopic fractionations at the interfaces among three Si phases have been experimentally examined. Crystal growth experiments (Fig. 1) were conducted using the floating zone

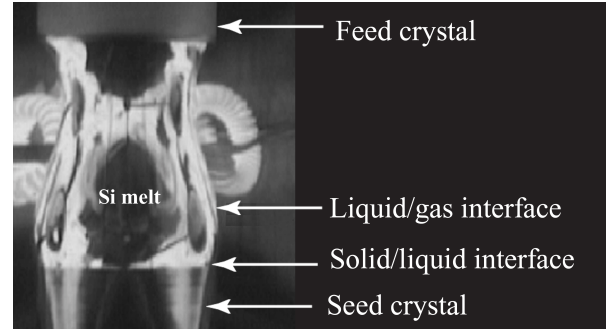


Fig. 1 Interfaces among three Si phases during FZ growth of Si crystal.

(FZ) technique, and the products were then precisely determined for Si isotopic ratios using a SIMS. Previously complicated Si isotopic fractionations were observed at crystal-liquid interfaces [1]. It is concluded that the isotopic fractionation between solid and liquid depends on the equilibrium fractionation factor and growth conditions, especially the degree of supercooling, which might depend on the structure at the crystal surface.

Another possibility for isotopic fractionation is evaporation at the gas-liquid interface. Each Si melt was partially evaporated under several atmospheric pressures of Ar. The Si isotopic fractionation factor under a vacuum is close to the theoretical value of 0.9661 for Si free evaporation. Since there was considerable condensation under 100 kPa of Ar, the evaporation rate was slower than that under vacuum. As a result, the isotopic fractionation was small. It is inferred that the isotopic fractionation factor between gas and liquid depends on the pressure near the interface.

Reference

- [1] Morishita Y., Satoh H. (2003) *Applied. Surface Sci.*, **203-204**, 802-805.