Determination of line tension via pressure profile: a molecular dynamics study

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The oil-water-vapor three-phase systems are investigated by molecular dynamics methods. The line tension has been calculated directly from local pressure profile. In this work, the line tension of decane-water-vapor system is estimated to be around -8.2x10^{-12} N, while the line tension of decane/heptane/toluene multicomponent-oil-water-vapor system has been obtained to 9.1x10^{-12} N. We suggested that the precursor thin film of toluene, which spreads preferentially over the water ahead of the bulk oil, is responsible for the fact that the line tension of decane-water-vapor system have increased from negative to positive values by adding heptane and toluene.

Zn isotope composition of Paleoproterozoic carbonates, banded iron formation and manganese formation

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Previous studies of Zn isotopes in the modern open marine realm demonstrate a consistent biological control of the Zn isotopic composition of the surface ocean. The micronutrient Zn is assimilated in the surface ocean by primary producers and exported to the deep ocean, where it is released by remineralization. Preferential uptake of the light isotopes enriches the surface ocean compared to the source (river-derived Zn in surface ocean, hydrothermal mantle Zn in deep ocean), resulting in a surface-to-deep isotope gradient akin to that of δ^{13}C of dissolved inorganic carbon. Since Zn is incorporated in carbonates without significant isotopic fractionation, Zn isotope ratios of carbonates precipitated in the surface ocean should track fluctuations in primary productivity.

We analyzed the Zn isotopic composition of ~2.2 Ga old shallow and deep marine carbonates, banded iron formation (BIF) and manganese formation (MnF) from the Kalahari Manganese Field in South Africa, which formed in a small rift basin. The δ^{66}Zn (^{66}Zn/^{64}Zn) composition of the carbonate fraction of dolostones mainly ranges from 0.20–0.63‰ (vs JMC-Lyon) and systematically varies with inferred paleo-waterdepth. δ^{66}Zn of BIF samples range from -0.25–0.49‰ and MnF samples from -0.36–0.68‰.

The observed range in δ^{66}Zn cannot be easily explained by analytical artefacts, such as spectral interferences or diagenetic re-equilibration. Hence, we argue that these data represent the composition of the stratified seawater in a Paleoproterozoic rift. Whereas microbial carbonates deposited above the chemocline are enriched (up to 0.63‰) due to the biological pump, deep marine rhythmites are closer to the mantle value (0.2-0.3‰). Upward deepening of the succession, from intertidal microbialaminites to subtidal thrombolites, is accompanied by a gradual decrease in δ^{66}Zn values. The highest Zn isotope values are significantly lower than those reported from Neogene carbonates, which could be due to lack of eukaryotes in the 2.2 Ga old ocean. Eukaryotes have higher Zn requirements than cyanobacteria and, therefore, more efficiently deplete ^{64}Zn in the surface ocean. MnF and BIF likely owe their large variability to formation close to the chemocline, resulting in enriched δ^{66}Zn values if deposited above the chemocline and mantle values if formed below the chemocline. Values depleted with respect to the mantle signature might be due to preferential adsorption of light isotopes by Fe and Mn hydroxides as observed during previous reported experiments.