Microbial interactions with engineered metal and metal oxide nanoparticles

M.J. DOKTYCZ[1,2]*, ANIL K. SURESH[1], W. WANG[3], S.D. BROWN[1], B. GU[3], D.P. ALLISON[1,4], D.C. JOY[2,4], J.W. MOON[1], T.J. PHELPS[1] AND D.A. PELLETIER[1]

[1]Biosciences Division
(*correspondence: doktyczmj@ornl.gov)
[2]Center for Nanophase Materials Sciences Division
[3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6445
[4]University of Tennessee, Knoxville, TN

Engineered nanostructures have a central role in energy conservation strategies and economic growth. One of the most significant impacts of engineered nanostructures is for effecting heterogeneous catalysis as required for fuel transformation, energy storage, polymer production and chemical synthesis. The size and composition of the particle affects performance and may similarly affect nanoparticle fate and transport in the environment. Both chemical and biological processes could affect the stability and transformation of nanoparticles in the environment. Our efforts to quantify and characterize interactions between engineered metal and metal oxide nanoparticles and selected microbial species will be presented. Initial studies are focused on defining a standardized approach to identifying and understanding the toxicity of nanomaterials. This approach involves three basic elements. First, the controlled synthesis of selected nanomaterials and extensive characterization of their chemical and physical properties is carried out. Next, multiple measures of bacterial growth and toxicity are performed using a variety of standard organisms. Finally, these studies are followed by investigation of the molecular bases of toxic responses. This basic approach is being applied to the characterization of various nanomaterials including CeO_2, Ag and ZnO nanoparticles. Chemically and biologically based routes to the synthesis of various sizes of nanoparticles have been developed. Dose dependent growth and viability experiments have been performed and are being correlated with genetic-based responses using microarray techniques. The results of these studies are providing a basis for understanding how nanoparticle size and composition influence their interactions with microorganisms, and how microorganisms may alter the fate and transformation of engineered nanoparticles in the environment.

This research is sponsored by the Office of Biological and Environmental Research, U.S. Department of Energy.

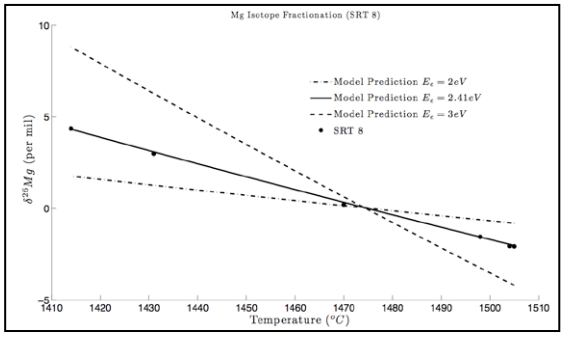
A fundamental approach to isotopic fractionations induced by thermal gradients in melts

G. DOMINGUEZ[1], G. WILKINS[1,2] AND M.H. THIEMENS[1]

[1]Department of Chemistry and Biochemistry, U.C. San Diego, La Jolla, CA 92093-0345
(*correspondence: gdominguez@ucsd.edu)
[2]Department of Mathematics, U.C. Berkeley, Berkeley, CA, 94720-3840

Richter *et al*. [1, 2] have found significant isotopic fractionations of Mg and Ca produced in basalt melts subjected to high-temperature thermal gradients (~1400-1520 °C). These isotopic fractionations were modeled by [1, 2] using an empirical Soret diffusion model.

We consider the diffusion of elements and isotopes from a more fundamental perspective. By treating diffusing species as quantum particles, we derive ratios for the temperature dependent diffusion constants of isotopes of an element as a function of their mass.



The isotopic fractionation of isotopes was modeled using a simple hopping model for the diffusion process. The results of this model for different electronic energies are shown in Figure 1. The optimized electronic energy was then used to predict the isotopic fractionation of Ca isotopes in the same system [2]. We found excellent agreement between the experimental results and our model, indicating that the quantum mechanical approach should be considered for geochemical isotopic fractionations, even at high-temperatures. Additional details of these results and model will be discussed in a forthcoming paper [3].

[1] Richter *et al*. (2008) *GCA*, **72**, 206. [2] Richter *et al*. (2009) *GCA* **73**, 4250. [3] Dominguez *et al*. in prep.