Towards modelling biogenic magnetite, Fe_3O_4

AMY MONNINGTON[1], DAVID J COOKE[1]
AND COLIN L FREEMAN[2]

[1]Department of Chemical and Biological Sciences, University of Huddersfield, UK (Amy.Monnington@hud.ac.uk)
[2]Department of Engineering Materials, University of Sheffield, UK (c.l.freeman@sheffield.ac.uk)

There is an increasing number of new, exciting and dynamic uses for magnetic nanoparticles (MNPs), including many in the field of medicine (site-specific chemotherapy), technology (spintronics) and industry (ferrofluids). Magnetotactic bacteria produce chains of nanosized magnetite, Fe_3O_4, particles that operate as internal magnets. This biosynthesis of magnetite is the earliest known example of biomineralisation, having first occured some two billion years ago. Despite this, much of the detailed atomistic mechanism by which the process occurs is unknown. Therefore, we have begun to develop an atomistic model for the system, in an attempt to understand the processes involved, particularly the role of the 1-5% Co that is present in the biomineral.

In this work we report initial results for modelling the different surfaces of magnetite, using differing methods. Comparison of the related surface energies produced for these methods, using energy minimisation (METADISE [1]) and molecular dynamics (DL_POLY [2]), identified the {100} surface as the most stable. For all methods, elasticity constants were compared to the data produced from previous studies [3]. Subsequent to this, attachments of simple organic molecules to the magnetite were analysed and modelling of interactions between these molecules and the {100} surface were performed.

Future work will validate the potentials for the interactions between the simple organic molecules and the magnetite surface, enabling us to fit the required organic/ inorganic cross parameters to a system where the stable surfaces are well defined, allowing us to better access the validity of each of the components of the model. This is in the aim of progressing to more complex protein attachments.

[1] Watson, G. W. *et al.* (1996) *J. Chem. Soc. Faraday Trans.* **92**(3), 433. [2] Smith, W. & Forester, T. R. (1996) *J. Mol. Graphics* **14**(3), 136. [3] Doraiswami, M. S. (1947) *Proc. Math. Sci.* **25**(5), 413.

Neodymium isotopic composition of gorgonian corals as reliable tool to reconstruct water mass circulation

P. MONTAGNA[1,2,3]*, M. LOPEZ CORREA[4], S. GOLDSTEIN[2],
M.T. MCCULLOCH[5], A. FREIWALD[6], M. TAVIANI[3],
J.A. TROTTER[5] AND J. RADDATZ[7]

[1]LSCE-CEA, 91198, Gif-sur-Yvette, France
(*correspondence: paolo.montagna@lsce.ipsl.fr)
[2]LDEO, Palisades, NY 10964, USA
[3]ISMAR-CNR, Via Gobetti 101, 40129 Bologna, Italy
[4]GeoZentrum Nordbayern, 91054 Erlangen, Germany
[5]University of Western Australia, 6009 Crawley, Australia
[6]Senckenberg am Meer, Abteilung für Meeresforschung, D-26384, Wilhelmshaven, Germany
[7]IFM-GEOMAR, D-24148 Kiel, Germany

It has recently been shown that intermediate and deep ocean circulation can be reliably reconstructed using the neodymium (Nd) isotopic composition of the aragonitic skeleton of scleractinian deep-water corals [1,2,3,4]. Motivated by these findings, we have investigated the Nd systematics of the high-magnesium calcite skeleton of deep-water gorgonian octocorals. These corals have centennial-scale lifespans and are distributed worldwide, representing potential archives of past oceanic circulation at sub-decadal resolution. Live-collected corals, belonging to the families *Isididae* (genus *Keratoisis*) and *Coralliidae* (genus *Corallium)*, were retrieved from the Atlantic, Pacific, and Southern Oceans as well as from the Mediterranean Sea at water depths between ~500 to ~1300m. Seawater samples from two profiles in the Mediterranean Sea were collected at the same locations and depths as the coral samples in order to compare seawater Nd isotopic compositions with the coral skeletons. The isotopic ratio ($^{143}Nd/^{144}Nd$) was obtained using a VG Sector 54-30 thermal ionization mass spectrometer by dynamic multicollection. The neodymium concentration was analysed along different tracks parallel to the growth bands using a 193nm laser ablation microsampling system connected to a Varian 820 inductively coupled plasma mass spectrometer.

The gorgonian calcite skeletons and the surrounding seawater share equivalent Nd isotopic compositions, which clearly show that these calcite corals are reliable archives of water mass circulation.

[1] van de Flierdt *et al.* (2010) *GCA* 74, 6014-6032. [2] Copart *et al.* (2010) *QSR* **29**, 2499-2508. [3] Colin *et al.* (2010) *QSR* **29**, 2509-2517. [4] Montagna *et al.* (2010) AGU meeting, San Francisco.