Structure of bacterial multiheme cytochromes at the microbial-mineral interface

ALEXANDER JOHS[1]*, LIANG SHI[2], TIMOTHY DROUBAY[2], JOHN F. ANKNER[3], LIYUAN LIANG[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, 1 Bethel Valley Road, Oak Ridge, TN 37831, (*correspondence: johsa@ornl.gov)
[2]Pacific Northwest National Laboratory, Richland, WA 99352
[3]Neutron Scattering Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

Electron transfer by dissimilatory metal-reducing bacteria (DMRB) is facilitated by a series of *c*-type cytochromes associated with the bacterial cell envelope. The outer membrane protein OmcA is located on the cell surface of the dissimilatory metal reducing bacterium *Shewanella oneidensis* MR-1 [1,2]. This 85 kDa decaheme *c*-type cytochrome functions as a terminal reductase that relays electrons generated by the bacteria's metabolism to extracellular acceptors that include solid metal oxides such as hematite (α-Fe_2O_3) [3]. The solution structure of OmcA was determined by small angle X-ray scattering (SAXS) and its interaction with hematite was revealed by neutron reflectometry (NR). SAXS results showed that OmcA is a monomer that adopts a flat ellipsoidal shape with a dimension of 34×90×65 Å. Changes in redox state affect OmcA conformation. In addition, OmcA interacts with small organic ligands known to act as electron shuttle molecules, such as flavin mononucleotide (FMN), resulting in the formation of higher molecular weight assemblies. A model system, developed to study the interaction of OmcA with hematite using NR, shows that OmcA forms a well-defined monomolecular layer on hematite surfaces. This allows OmcA to preferentially interact with hematite in a conformation that appears to maximize its contact area with the mineral surface. Overall, these results provide a structural basis for OmcA mediated redox processes by providing novel insights into its molecular structure and interaction with insoluble hematite and small organic ligands.

[1] Myers et al. (1998), *Biochim. Biophys. Acta* 1373, 237–251. [2] Lower et al. (2009), *Appl. Environ. Microbiol.* 75, 2931–2935. [3] Ross et al. (2007), *Appl. Environ. Microbiol.* 73, 5797–5808.