Keynote Lecture

X-ray Absorption Spectroscopy and Chemical Speciation: from Archaeology to Biology

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Synchrotron-based X-ray absorption spectroscopy (XAS) is a powerful technique for probing the local structure and electronic environment around a specific atom, and can be applied on matters in any physical state. It is a tool with diverse applications, from defining the coordination sphere around metal ions in metalloproteins, to identifying the pigments used in historical paintings and monitoring their stability. One of such exciting applications was unravelling the new battle of historical shipwrecks on display in the museums around the world. The visible signs of salt precipitation and soft/ acidic wood for the famous Swedish 17th century warship, Vasa, motivated us to explore this conversation challenge with XAS. Analyses of several wood cores from the Vasa and other shipwrecks, including the foremost warship in the navy of Henry VIII, the Mary Rose, showed large amounts of reduced sulfur compounds within the wood. Oxidation processes catalyzed by the active iron ions produce sulfuric acid, causing wood degradation [1, 2]. The important role of X-ray absorption near-edge structure (XANES) spectroscopy in revealing this "sulfur problem" will be discussed.

Meanwhile thiol (-SH) containing molecules play an important role in the detoxification of heavy metals in living organisms. The toxicity of heavy metals such as lead, mercury and cadmium in biological systems is frequently attributed to their strong preference for thiol groups, which can inhibit the activity of cellular enzymes. The tri-peptide glutathione (gamma-Glutamyl-Cysteine-Glycine), the most abundant cellular thiol in the body, is important for protecting organisms against heavy metal ions. Penicillamine (3,3'-dimethylcysteine) and N-acetylcysteine are clinically used for heavy metal detoxification. In this lecture, the critical role of XAS in understanding the structure and bonding of chemical species formed between heavy metal ions and these biologically relevant thiol-containing molecules will be discussed [3].

[1] Sandström, M.; Jalilehvand, F. et al. (2002) Nature 415, 893-7.

[2] Sandström, M.; Jalilehvand, F. et al. (2005) Proc. Natl. Acad. Sci. 102, 14165-14170.

[3] Jalilehvand, F. ; Sisombath, N. et al. (2015) Inorg. Chem. 54, 2160 – 2170.



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