Trace metals in the Mt. Isa copper ores: Implications for paragenesis

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Trace metals have long been known at the giant (> 8Mt contained Cu) Mt. Isa Copper Orebodies in NW Queensland, Australia, but are poorly understood. Macroscopically all of the copper orebodies are characterised by a primary mineralogy of chalcopyrite-pyrite-pyrrhotite that exhibit a multipart paragenesis. Both pyrite and pyrrhotite are associated with high grade and low grade ores, respectively; although fine grained pyrite pre-dates Cu and is ubiquitous throughout the shale host rock that is also the host to the nearby Pb-Zn orebodies. Cobalt and arsenic are variably concentrated within the low grade Cu ores along with trace quantities of Ni, Sb, Ag, Bi, and In. Examination of Cu ores using the JEOL Superprobe has identified cobaltite, glaucodot, cobaltian-arsenopyrite, arsenopyrite as well as ubiquitous small grains of galena and less common apatite and monazites.

The cobalt sulpharsenides occur as discrete euhedral inclusions within both chalcopyrite and pyrrhotite as well as discrete grains within the silica-dolomite hydrothermal matrix to ore. WDS analyses of chalcopyrite show that the chalcopyrite is practically pure, however, the Co and As abundance in pyrite is significant. Co-As minerals commonly replace the fine-grained pyrite as overgrowths and cement to brecciated grains. Locally, replacement of fine-grained pyrite is near-complete; cobaltian pyrite is surprisingly common around other deposits in the district. The chemical continuum of arsenopyrite and pyrite to cobaltite suggests some metal recycling from the host rocks has occurred during the Cu event suggesting a two stage hydrothermal process:

1) introduction of Cu and Fe (+In) followed by
2) Co-Ni-Bi and recycling of Pb-Ag and As-Sb

Widespread galena replacement throughout the Cu ore is also significant in that it questions: 1) previous bulk lead isotope dating, and 2) the timing of the Cu and adjacent Pb-Zn ores, which are presumed much younger than the post orogenic epigenetic copper ores.

Modelling biomineralization processes

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Nature demonstrates a remarkable ability to control the shape and crystallographic orientation of minerals with the result that the properties of biominerals are often far superior those of manmade materials. Examples include bones, teeth and abalone nacre, which is a thousand times tougher than the pure mineral. Nature's ability to control and manipulate crystal growth with organic molecules has inspired experiments that have attempted to reproduce this control in the laboratory. Complex self organised structures, with a strong resemblance to biological structures, have been grown from solution and selective nucleation of calcite has been induced by ordered organic monolayers. In spite of this success, the factors that control nucleation are poorly understood and simple templating arguments often fail.

Modelling should be able to make a significant contribution to the understanding of biomineralization, however modelling such complex systems is not without its challenges [1]. In this paper we review current models of organic-inorganic interfaces [2] and present results of the crystallization of amorphous calcium carbonate on ordered organic substrates [3]. We illustrate how metadynamics can be used to overcome the timescale restrictions [4] and used to model calcium carbonate nucleation on organic substrates and in contact with an ovocleidin egg shell protein. The contribution of the simulations to our understanding of the role of proteins in biomineralization will be discussed.

[1] Harding *et al.* (2008) *Chem. Rev.* **108**, 4023-4854. [2] Duffy *et al.* (200) *Langmuir* **20,** 7630-7636. [3] Freeman *et al.* (2008) *Langmuir* **24,** 9607-9605 [4] Quigley *et al.* (2008) *J. Chem. Phys.* **128**, 221101