Computer Modeling of Pb Apatites and their Potential for Reducing Pb Levels in Drinking Water

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Due to its resistance to corrosion and maliability lead was the material of choice for water pipes from ancient times until the 20th centurary and many domoestic water supplies are still reliant on legacy lead piping. Over time lead will leach from the pipes into the water supply and if left unchecked can cause Pb levels in drinking water to become dangerously high. Consequently water companies the world over are investigating methods for reducing the levels of Pb present in a safe and economic way that can be applied even when pipes are inaccessable.

One solution being explored is to promote the crystalisation of lead phosphat minerals in the water pipes by adding additional phosphates to the water supply. Here we report on a combined modelling and experimerimental study exploring the Pb-apatite system.

The computer models are based on the atomistic potentials previously fitted by de Leeuw and co workers [1] to study a range of apatite minerals, which we have extended to incorporate the Pb^{2+} ion and were fitted so they reproduce the structure of $Pb_5(PO_4)_3F$ and $Pb_5(PO_4)_3Cl$ as well as $PbCO_3$, $PbCl_2$, PbF_2 and $Pb(OH)_2$ to within 1% of the experimentally determined parameters.

Initially we considered the effect on the unit cell of varying the Pb:Ca ratio and compared this to structure of crystals grown in the lab and found excellent aggreement between the experimental and simulated lattice parameters, thus giving us confidence to use the computer model as a predictive tool and probe how the Pb an Ca will arrange in the structure as a function of Pb content.

Our current work is focused in two main areas. Firstly we are considering the surface properties of the minerlas and whether segregatiuon of Ca or Pb is preferable. Secondly we are probing the mineral water interacebyconsidering the competative adsorption of lead and calcium on calcium and lead rich chloro and fluoro apatitie surfaces.

[1] Rabone and de Leeuw J Comput Chem 27: 253 2006

Magmatic-hydrothermal sutures and clusters of giant porphyry Cu-(Au-Mo) deposits

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Porphyry deposits are the world's major sources of Cu, Mo and Re, and important sources of Au and Ag. They typically form in compressional orogens, either during or after subduction. The transition from extensional tectonism and widespread calc-alkaline volcanism, to a compressional tectonic regime causes inversion of the extensional structural architecture, crustal thickening and shutdown of volcanism, promoting the growth of mid- to upper-crustal intermediate-to felsic magma chambers at major structural intersections. Fractional crystallisation within the magma chamber, possibly coupled with mafic magma underplating, thermal destabilisation and volatile addition, leads to eruptions of hydrous melts and mineralising fluids from the roof of the pluton, producing elongate 'spires' of porphyry that intrude to paleodepths are surrounded and overprinted by of 1-3 km and magmatic-hydrothermal alteration and mineralisation.

Both geochemical and structural processes are fundamental to the formation of clusters of giant porphyry deposits. Several of the world's largest deposit clusters, in terms of contained metal, were localised on major suture zones that developed due to the interaction of arc-parallel and arc-oblique fault systems in the overriding plate. The Eocene—Oligocene Chuquicamata cluster of deposits in northern Chile (Chuquicamata, Radomiro Tomic, Mina Sur, Ministro Hales, Opache and the Toki cluster) was localised along a 25 km corridor controlled by the NNE-trending Mesabi fault and equivalent structures, at its intersection witth the Calama-Olacapato-El Toro NW lineament. The district contains over 93 Mt of fine Cu. In the case of the world's largest porphyry Cu-Mo district, Rio Blanco-Los Bronces (> 200 Mt of fine Cu), at least seven porphyry deposits formed during the late Miocene-early Pliocene along a 12 km long, NNW-trending suture zone, with mineralised centres localised at the intersections between the major NNW-trending structures and cross-cutting NE-trending fault systems. The Paleozoic Oyu Tolgoi district in Mongolia contains at least 1749 t Au and 45.5 Mt Cu in a cluster of eight porphyry Cu-Au deposits aligned along a NNE-trending, 26 km long structural corridor. In each of these examples, conditions that promote repeated magmatic-hydrothermal activity in major upper-crustal sutures were essential for the formation of giant porphyry deposit clusters.