Petrogenesis and geochemistry of the Dajing Cu-Sn-Pb-Zn-Ag Ore Deposit in Chifeng, Inner Mongolia

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The Dajing deposit is the largest tin deposit at the north of North China, which is a fissure-filling hydrothermal ore deposit located at the south of Daxinggan Mountain with Sn, Cu, Pb, Zn, Ag mineralisation. The deposit is controlled by multistage of fracture systems, mainly including NE striking sinistral compresso-shear fractures, a suite of SN striking compresso-shear fractures, and NW striking tenso-shear fractures (with ore veins mainly filling in this group of fractures). The widely outcropped magmatic rocks in the ore district are sub-volcanic rocks. They intruded into the Upper Permian Linxi Group that was formed in the inshore lake basins environment. The sub-volcanic dykes are divided into four main types: aphanophyre, acidic to intermediate rocks (dacite porphyry, rhyolite porphyry and granite porphyry), intermediate to basic rocks (andesitic porphyrite, diabasic porphyrite and basaltic prophyrite) and lamprohpyre, which scattered in the ore district. However, the subvolcanic rocks are dominated by acidic rocks in the central part, and intermdiate to basic rocks in the eastern part. K-Ar bulk isotopic age of the dykes ranges from 155.3 to 177.2 Ma. Wall rock alterations are weak silicification, carbonatization, chloritization and sericitization. They occur on both sides of ore veins.

The acidic rocks in the central are a suit of high-K calc-alkaline dacite with high content of Cu and Sn, while the basic rocks in the eastern are a suit of shoshonitic basalt to basaltic-andesite rocks with high content of Pb and Zn. All the rocks are characterized by enriched LILE and LREE, but acidic rocks have lower REE content with intermediate negative Eu anomaly (δEu=0.56-0.58). All the rocks originated from the same mantle source. They underwent high degree of differentiation and evolution when entered into the secondary magma chamber.

Ab initio molecular dynamics simulation of copper(I) complexation in chloride/sulfide fluids

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Chloride and hydrosulfide are the primary ligands believed to control the transport of copper in hydrothermal fluids. Recent studies of Cu complexation in hydrothermal Cl^-, HS^- solutions have been done using X-ray Absorption Spectroscopy (XAS). However, coordination numbers have a large uncertainty and are strongly correlated with Debye-Waller factors; moreover, it is very difficult to distinguish between chloride and sulfur ligands. *Ab initio* molecular dynamics simulations based on density functional theory enable us to interpret EXAFS results and, potentially, predict stability constants of metal complexes.

In this study, we investigated the species of copper(I) complexes via *ab initio* Car-Parrinello Molecular Dynamics simulations for copper(I) solutions with different hydrosulfide/chloride ratios at 500bar and 600K. Calculations were done using Vanderbilt ultrasoft pseudopotentials and the PBE exchange-correlation functional.

In the absence of Cl-ligands, copper forms a $Cu(HS)_2^-$ complex with a Cu-S bond length of 2.17 Å (vs. an expt. value of 2.15 Å); moreover, the S-Cu-S bond angle is ~162°, in excellent agreement with experiment (150-160°). In the presence of excess chloride, however, we find that Cu forms previously unknown $Cu(HS)Cl^-$ and (minor) $CuCl_2(HS)^{-2}$ complexes. Such complexes would be difficult to resolve from $CuCl_2^-$ or $Cu(HS)_2^-$ using EXAFS. We also explored the complexation of Cu in a low density (0.29 g/cm^3), high T (1273K) fluid (vapour). Here, we find that Cu forms $Cu(HS)_2^-$ (not the neutral CuHS, as expected). We tentatively suggest that charged complexes may be significant in high temperature, low density fluids.

Ultimately, we hope to predict stability constants of metal complexes. To this end, we are testing metadynamics and thermodynamic integration with respect to metal-ligand distances or coordination numbers. Using these techniques, we estimate the free energy difference between $CuCl_2^- + HS^-$ and $CuCl(HS)^- + Cl^-$ to be ~40 KJ/mol.