

A bond valence approach to surface energy and crystal morphology

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The aim of our research is to provide a methodology, which can be applied to investigate the interaction and the reactivity of mineral interfaces with the environment. The underlying principle of our approach is to define the interaction between internal structural parameters and surface parameters in order to obtain an ideal abstract crystal morphology. This abstract crystal morphology can then be used as a reference morphology to different growth morphologies or crystal morphologies predicted by other atomistic simulations.

The internal parameters chosen on behalf of our model are the number of atoms per surface area (reticular density) and the lattice density. The surface parameters are the number of dangling bonds (bond valence deficiency) per surface area or their corresponding surface energy. The internal parameters are determined by the crystal structure type and therefore are invariable. In contrast, the surface parameters are variable due to differences in the chemical compositions of different minerals, even though they may agree in their crystal structure type.

In order to obtain the surface energies of different crystal interfaces, our model uses the bond valence approach of Brown [1]. First we calculate the surface specific bond valence deficiency, then we assign to each bond via its bond length a certain bond energy, which then in its summation over the surface area gives us the surface energy. The main advantage of this approach is, compared to other atomistic simulations, that it does not demand for charged neutral surfaces to obtain the surface energy. Therefore, naturally charged and charged neutral surfaces can be compared likewise, which is a major advantage while comparing different growth morphologies in variably composed solutions.

This performance of our model, its combined approach of internal and interfacial parameters, not only gives results which are in good agreement with literature data, but also enables us to discuss the importance and the occurrence of naturally polar surfaces on behalf of the crystal morphology.

[1] Brown, I.D. (2002), *The chemical bond in inorganic chemistry*. Oxford Science publications.

Gold in sulfide wastes - peat system

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Carbonaceous matter is an effective concentrator of precious metals. We study gold partitioning between sulfide material and peat in a halo around the Ursk tailing pit (Kemerovo region, Russia) with ore cyaniding wastes. The wastes of processed primary ore and ore from the oxide zone are piled up in two 10-12 m piles. Being not fastened, the material has been washed out by floods and rainfalls for more than 50 years. The swampy area downstream of the tailings is burnt by acid mine drainage (AMD) and covered by shed material, with remains of peat mounds rising above.

The shed wastes and peat have been sampled in test pits to 20 cm deep. The gold contents are 0.1 to 3.8 ppm (mean 0.6 ppm) in all wastes, and 1.2 ppb in AMD nearby.

Gold in peat varies broadly, from 0.18 to 155 ppm, mostly 0.18 to 19 ppm. The mean and median values are different (5 and 2 ppm). There are three Au zones in the Ursk halo peat: (1) near the piles and mainstream AMD where the primary and oxide zone ore wastes interlayer (max. 40 ppm); (2) same as (1) but farther from the piles and with higher gold (max. 60 ppm); (3) a perennially wet zone 200 m far from the oxide zone wastes with extremely high gold (40 to 155 ppm).

Peat along the oxide zone wastes bears secondary minerals, namely concentric aggregates of Fe(III) compounds, gypsum, Na-jarosite, framboidal pyrites; barite druses and globules; zinc sulfide; euhedral Hg selenides and sulfides: timmanite (HgSe), onofrite (Hg(S,Se)), cinnabar (HgS).

Gold is high (80 ppm) in material rich in Hg sulfides with Cu, Ag, I, and Se impurities. Submicron and nanoparticles of gold largely cover organic detritus and locally form sheaths over bacterial cells. Native Au particles (to 1.5 μm in diameter, purity 947-1000 ‰), at Cu impurity of 7.5-53 ‰, occur in material cemented with secondary Fe(III) compounds. Cu-gold formation may be mediated directly by bacteria. This process in peat was reproduced in laboratory [1]. Formation of secondary Au in the presence of sulfides is mediated first by iron- and sulfur-oxidizing bacteria and then by thiosulfate oxidizers and sulfate reducers [2].

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[1] Kuimova et. al. (2011). *Lithosphere*. **4**. 131-136. (Published in Russian). [2] Southam et. al. (2009). *Elements*. **5**(5). 303-307.