

Quataron concept of nanoparticles formation and crystal growth

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Previously [1, 2] we have described a set of ideas and principles dealing with structural self organization of substance in the nanorange. These ideas have been collectively referred to as the 'quataron concept'. Central in this new concept is the idea that there are specific nanosize clusters arising under non-equilibrium conditions. These clusters cannot be described in terms of known states of substance and represent a separate intermediate phase ('hidden' phase) at the nanolevel. Clusters of 'hidden' phase named as a 'quatarons'.

Quatarons are dynamic structures constantly changing their forms. They are quasi-spherical in shape and have no symmetry restrictions. Quatarons are the basis for all kinds of equilibrium nanostructures from ordinary tetra- and octahedral groupings to the widely known fullerenes or dense dodecahedral and icosahedral clusters, colloidal, fractal particles. In particular, quatarons are fullerenes predecessors.

Physically quatarons are pre-crystallization clusters of the 'transient' phase. It has been found that clusters more than ~1.2 nm in size can become potential centers of crystallization. Only such clusters contain a minimal number of atoms necessary for crystal nucleation. At the same time, crystals grow by smaller clusters (quatarons), which are transformed to 'two-dimensional' nuclei already on the growing crystal surface. Quatarons are ideal as growth units: chemical composition of quatarons is the same as that of crystals, topologically quatarons are close to structural modules of crystals, variability of the structure allows quatarons to join any crystal surface. As a result we have to revise a number of outdated ideas on crystal growth theory.

Quatarons as objects which properties are determined by quantum-mechanical laws, on the one hand, and laws of classical physics, on the other hand, determine the originality of the nano-state of matter. Uniqueness of quatarons consists in that they bear lines of live organisms and live matter. In particular they as well as live cells are capable to divide at achieving certain sizes. Their role as nano-reactors of concentration and synthesis of new compounds, including biomolecules of the elementary elements of live matter is unique [3].

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[1] Askhabov (2004) *Russ. Miner. Soc.* **4**, 108-123.

[2] Askhabov (2005) *Physics of Solid State* **47**, 1186-1190.

[3] Askhabov (2008) *Doklady Biological Sciences* **418**, 50-52.

Arsenic mobilization in acid mine drainage from the Tinto Santa Rosa Mine, Iberian Pyrite Belt, Spain

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The waters and sediments of the acidic discharge of the Tinto Santa Rosa abandoned mine in the Iberian Pyritic Belt (SW, Spain) were studied to characterize the natural processes controlling arsenic attenuation in acid mine drainage waters.

Variation in water composition and pH from the acid mouth downstream was characterized by a pH decrease, accompanied by a systematic decrease in ferrous iron, total iron, As(III), As(V) and total arsenic concentrations. This evolution indicates that along the stream As(III) and Fe(II) were respectively oxidized to As(V) and Fe(III), and the latter precipitated as schwertmannite ($\text{Fe}_8\text{O}_8(\text{OH})_{5.5}(\text{SO}_4)_{1.25}$), goethite (FeOOH) and jarosite ($\text{KFe}_3(\text{SO}_4)_2(\text{OH})_6$), which partially sorbed the aqueous As(V).

The total arsenic content associated with the bed-stream sediments was determined by total acid digestion. Results showed a high arsenic content in the solids, present mainly in its pentavalent state based on arsenic K-edge XANES analysis. Least-squares fitting (LSF) of XANES spectra yielded evidence of changes in As speciation along the stream and in depth in the sediments. Comparison of the sediment mineralogy, arsenic concentration, and arsenic speciation showed that the highest arsenic concentrations were associated with sediments made up mainly of schwertmannite.

Reactive transport modelling coupling advective flux and the main chemical reactions observed in the field was performed using the PHREEQC code [1]. Despite the simplicity of the considered model, the kinetic expressions of the processes related to arsenic attenuation reproduced well the observed arsenic mobilization data along the Tinto Santa Rosa acid discharge.

[1] Parkhurst & Appelo (1999) *Water Res. Res. Investigations Report* **99**, 4259.