Molecular Dynamics Simulation of the aggregation of aqueous TiO_2 nanocrystals

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The phenomenon of oriented attachment, in which nanocrystals aggregate along certain preferred directions to form single or twinned crystals, was first observed in experimental studies of the crystallization of colloidal TiO_2 (anatase) [1]. To gain insight into this phenomenon, we used molecular dynamics (MD) to study the aggregation of anatase nanocrystals in the 2-6 nm size range, with shapes dictated by the Wulff construction. In vacuum, the nanocrystals aggregate almost exclusively along preferred crystallographic directions due to multipole interactions [2]. However, the structures of the experimental (aqueous) aggregates are different than those in vacuum, indicating that water plays a role in directing aggregation.

In efforts to understand the role of water, we tested the capabilities of the Bandura-Kubicki potential [3] to reproduce results from density-functional-theory (DFT) studies of the interaction of water with various surfaces of anatase [4]. We find good agreement of the potential with DFT. We performed MD simulations of anatase nanocrystals in water and we will discuss the ordering and dissociation of water around the nanocrystals for both gas and liquid environments. We will discuss possible roles for water in directing nanocrystal aggregation.

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Geochemical reflection of the elements and exploration index ratios

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The geochemical reflections and proximity to the ore zone

Investigation of the geochemical reflection of the elements adjacent to the ore zone is a method for identification of the proximity to the mineralized zone. For this propose, the geochemistry behaviour of the elements must be separate from each others based on the case study and geological conditions. The intensity of the elements mobility or element reflection against the alteration in compared to the unaltered rocks is considered [1, 2, 3]. The ratios of the different elements were calculated to investigate the index ratios. The behaviors of the elements in the ratio must be against each other. The intensity of the ratios reflections was resulted to the identification of the most index ratio. In a case study of polymetal Cu-Zn massive sulphide deposit, Taknar deposit [1], the geochemical reflection of the elements was led to a index ratio for the determination of the proximity to the mineralized zone (Fig. 1).

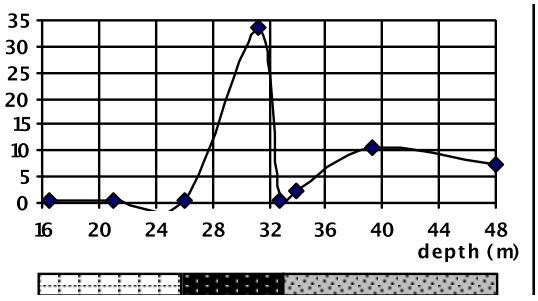

Figure 1: Geochemical reflection of CaO in HW, ore zone & Fw

Conclusion

The geochemical reflection of the elements could be a criterion for planning geochemical exploration pattern recognition.

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