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Anisotropic surface energies and adsorption behaviors of scheelite crystal

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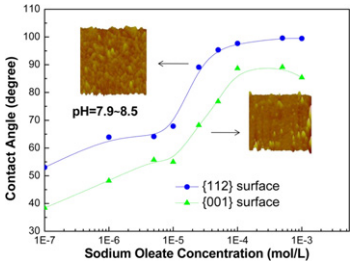
HIGHLIGHTS

- Anisotropic surface energies of scheelite were calculated by DFT calculations.
- Two predominantly cleavage planes, e.g. {1 1 2} and {0 0 1} surfaces were confirmed.
- Anisotropic adsorption behaviors oleate molecules at two surfaces were observed.
- Anisotropic adsorption behaviors were interpreted based on AFM and MD simulations.

GRAPHICAL ABSTRACT



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ABSTRACT

Anisotropic surface broken bond densities and surface energies of six surfaces of scheelite were calculated with density functional theory (DFT). The calculation results show that its surface energy is directly proportional to its surface broken bond density. {1 1 2} and {0 0 1} surfaces are the two predominant cleavage or exposed planes. The prediction of morphology is well consistent with our experimental observations based on XRD. Anisotropic adsorption behaviors and wettability of these two surfaces after being immersed in sodium oleate and DDA solutions were studied by means of contact angle measurement, AFM and flotation test. The contact angle values at a given NaOl concentration decreased in the order {1 1 2} > {0 0 1}. As for DDA, similar wettability for the two surfaces was observed. The results were interpreted by AFM and interaction energies for the adsorption of surfactants on each surface calculated in accordance with molecular dynamics (MD) simulation.

1. Introduction

As an important ore mineral of tungsten, scheelite $CaWO_4$ is commonly associated with other calcium-bearing minerals in mineral ore deposits, such as calcite $CaCO_3$, apatite $Ca_{10}(PO_4)_6F_2$ and fluorite CaF_2, from which it shall be separated by means of flotation as a result of the increasing need to process low-grade complex ores. It is well established that flotation is a surface-chemistry based process for separation of fine ores that takes advantage of the differences in wettability on mineral particle surfaces. However, most calcium minerals possess very similar surface properties, semi-soluble nature and similar responses to various known families of collectors such as fatty acids [1,2]. To separate these calcium-containing minerals from each other by means of flotation still remains a thorny problem.

Most calcium minerals show a remarkable variety of habits in nature crystals [3], particularly calcite and scheelite, and hence exhibit several anisotropic exposed surfaces which may possess different physicochemical characteristics. Generally, the exposed mineral surfaces in the flotation slurry will be both cleavage planes because of the crushing of the mineral and expressed surfaces in its crystal morphology [4]. Since the challenge for flotation separation is that the separation has to be based on subtle differences on the

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