LETTERS

Structure sensitivity of pyrite oxidation: Comparison of the (100) and (111) planes

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ABSTRACT

The interaction of atomically clean (100) and (111) crystallographic planes of FeS₂ with H₂O vapor, O₂, and a H₂O/O₂ mixture was investigated. A combined high pressure/ultra-high vacuum (UHV) apparatus allowed the surfaces to be reacted at environmentally relevant pressures and studied with X-ray photoelectron spectroscopy (XPS) without exposure to the atmosphere. Neither surface exhibited significant reaction in pure O₂. Exposure of FeS₂(111) to H₂O vapor resulted in significant oxidation, but under these same experimental conditions FeS₂(100) exhibited a much smaller amount of oxidation. It is suspected that on FeS₂(100), H₂O only reacted on nonstoichiometric regions (i.e., defects). Both surfaces showed substantial reaction in H₂O/O₂. The amount of FeS₂(100) and FeS₂(111) oxidation in the H₂O/O₂ mixture was more than simply the sum of the reaction observed individually in pure O₂ and H₂O. This result suggests that there is a synergy between H₂O and O₂ in oxidizing pyrite. In all cases, the amount of oxidation that occurred on FeS₂(111) was greater than on FeS₂(100). We believe that this experimental observation is due to a higher concentration of under-coordinated Fe in the outermost surface of FeS₂(111), relative to FeS₂(100).