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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 FeS_2 with H_2O vapor, O_2, and a H_2O/O_2 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 O_2. Exposure of FeS_2(111) to H_2O vapor resulted in significant oxidation, but under these same experimental conditions FeS_2(100) exhibited a much smaller amount of oxidation. It is suspected that on FeS_2(100), H_2O only reacted on nonstoichiometric regions (i.e., defects). Both surfaces showed substantial reaction in H_2O/O_2. The amount of FeS_2(100) and FeS_2(111) oxidation in the H_2O/O_2 mixture was more than simply the sum of the reaction observed individually in pure O_2 and H_2O. This result suggests that there is a synergy between H_2O and O_2 in oxidizing pyrite. In all cases, the amount of oxidation that occurred on FeS_2(111) was greater than on FeS_2(100). We believe that this experimental observation is due to a higher concentration of under-coordinated Fe in the outermost surface of FeS_2(111), relative to FeS_2(100).