

Sulfur species at chalcopyrite (CuFeS₂) fracture surfaces

SARAH L. HARMER,^{1,*} ALLEN R. PRATT,² WAYNE H. NESBITT,¹ AND MICHAL E. FLEET¹

¹Department of Earth Sciences, University of Western Ontario, London, Ontario, N6A 5B7 Canada

²CANMET Mining and Mineral Sciences Laboratories, 555 Booth Street Ottawa, Ontario, K1A 0G1 Canada

ABSTRACT

Pristine fractured surfaces of chalcopyrite (CuFeS₂) have been studied using Synchrotron Radiation X-ray Photoelectron Spectroscopy and conventional X-ray Photoelectron Spectroscopy. These high-resolution spectra reveal for the first time three distinct contributions to the S 2*p* spectrum. The main symmetric peak is located at 161.33 eV and is likely derived from fully coordinated bulk S atoms. A core-level shifted peak was observed at 160.84 eV and is attributed to surface monomeric species (S²⁻). A second broad contribution at 161.88 eV likely represents surface polymeric species (S_{*n*}²⁻). The data suggest that surface polymers form where S-terminated surfaces such as the (111) plane are exposed during fracture.