The structural evolution of mercury sulfide precipitate: an XAS and XRD study

JOHN M. CHARNOCK,^{1,2,3,*} LESLEY N. MOYES,² RICHARD A. D. PATTRICK,³ J. FREDERICK W. MOSSELMANS,¹ DAVID J. VAUGHAN,³ AND FRANCIS R. LIVENS²

¹CLRC Daresbury Laboratory, Warrington, Cheshire WA4 4AD, U.K.

²Department of Chemistry, University of Manchester, Oxford Road, Manchester M13 9PL, U.K. ³Department of Earth Sciences, University of Manchester, Oxford Road, Manchester M13 9PL, U.K.

ABSTRACT

We investigated structural changes during precipitation of HgS from sulfidic solutions using Xray absorption and X-ray diffraction techniques. The results show that initially an unstable low Hg coordination complex forms that is probably chain-like in structure, with one sulfide atom at 2.35 Å and one at 2.97 Å. This is rapidly transformed to a four-coordinate mercury sulfide compound that initially forms as clusters with the local ordering characteristics of cubic metacinnabar. However, during aggregation the black Hg-S precipitate loses its initial longer-range ordering and becomes pseudocubic. As it ages, the pseudocubic structure transforms to a cubic structure, and then to stable crystalline metacinnabar. This study provides clear evidence that the precipitation and formation of metal sulfides is a complex multistage process.