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Fluorescence XAFS Study of Heterogeneous Samples and Material Composition. FIROUZEH TANNAZI, Illinois Institute of Technology, GRANT BUNKER, Illinois Institute of Technology — Fluorescence XAFS spectroscopy is an appropriate technique for in situ study of the dilute and heterogeneous samples. Application of the standard expressions for calculating the fluorescence radiation from homogeneous samples when applied to inhomogeneous samples can introduce significant errors, which limit the accuracy of this spectroscopic method for determination of material speciation and structure. Hence, development of generalized models are of value. In this study we show that the environmental samples must be treated as heterogeneous samples and also investigate heterogeneity effects, of which particle size is the most important, and their impact on determination of material speciation and structure by XAFS. Our work includes the calculation of fluorescence radiation from arbitrary shaped convex particles by Monte Carlo methods, and adapting and expanding early work on particle size effects from X-ray Fluorescence Spectroscopy to XAFS spectroscopy. We have developed several theoretical models to calculate the fluorescence radiation from heterogeneous samples with arbitrary particle size distributions, compared them and discussed the complementary and importance of heterogeneity effects in each of them. The importance of accounting for these physical effects in interpreting experimental data is emphasized.

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