III-02

Anomalous dispersion applied to a tin-mordenite powder sample at the ESRF

Anette Frost Jensen
Dept. of Chemistry, University of Copenhagen, Universitetsparken 5, Lab 4, Copenhagen, Denmark

Poul Norby
Chemistry Department, Brookhaven National Laboratory, Bldg. 555A, Upton, NY, U.S.A.

Jean-Louis Hodeau
Laboratorie de Cristallographie, Centre National de la Recherche Scientifique, BP 166, 38042 Grenoble, France

Heinz Graafsma
European Synchrotron Radiation Facility, BP 220, 38043 Grenoble Cedex, France

Åke V. Kvick
Experimental Division, European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France

J.-E. Jorgensen
Aarhus University, Denmark

Applications of anomalous dispersion in materials science crystallography is a rapidly developing field, which has benefited tremendously from the increasing availability and quality of x-ray synchrotron sources in the past decade. At the European Synchrotron Radiation Facility (ESRF), we have at the Materials Science Beamline recorded powder diffractograms of the zeolitic ionic conductor, tin mordenite, at 47 incident photon energies in the range from 29.008 keV to 29.708 keV, bracketing the Sn K-absorption edge at 29.2 keV. The purpose of this study is to determine the Sn atomic positions and the Sn-Sn interatomic distances that cannot be revealed by traditional crystallographic techniques due to a disorder over several sites of the tin ions. (Knudsen, N., Krogh-Anderson, E., Krogh-Anderson, I. G., Norby, P., Skou, E. *Solid St. Ionics*. **61**, [1993] 153). The sample also contains grains of tinoxide, SnO_2, which complicates the analysis and eliminates a normal EXAFS analysis as a possibility to determine interatomic distances. In order to solve the problem, we use the newly developed diffraction anomalous fine structure (DAFS) technique. (Pickering, I. J., Sansone, M., Marsch, J., George, G. N. *J. Am. Chem. Soc.* **115**, [1993], 6302. Stragier, H., Cross, J. O., Rehr, J. J., Sorensen, L. B., Bouldin, C. E., Woicik, J. C. *Phys. Rev. Lett.* **69**, [1992], 3064). This method in principle allows extraction of site-specific absorption spectra, so that despite crystallographic disorder and multiple phases, interatomic distances and valence states of the probe atoms can be determined reliably. We will present the first results of this work.