Lattice Dynamics from X-ray Total Scattering

V. Petkov, S. J. L. Billinge, V. Levashov, M. F. Thorpe

Department of Physics and Astronomy and Center for Fundamental Materials Research, Michigan State University, East Lansing, MI, U.S.A.

Introduction

It has been known for a long time that x-ray diffraction data contain information about the lattice dynamics of materials in the form of thermal diffuse scattering (TDS).[1] As early as the 1950s people were determining the phonon density of states and atomic force constants experimentally from the TDS determined from x-ray measurements on single crystals.[1] Recently we[2] and others[3] showed that the TDS that is present in *powder diffraction* measurements can be used to obtain force constants with reasonable accuracy. This development is potentially very interesting for two reasons. First, powder measurements are relatively straight-forward and quick, allowing phonon densities of states to be measured as a function of temperature, composition, and even pressure. Second, this allows the lattice dynamics of materials, which are difficult to crystallize as large single crystals, to be studied.

In order to study the possibility of using powder diffraction to study lattice dynamics we have undertaken a study of a number of simple fcc metals. At the MU-CAT ID-6 beamline we measured the total scattering diffraction from pure lead powder. These data are being analyzed to obtain force constants for lead and thereafter phonon dispersion curves and densities of states to compare with literature values.

Results and Discussion

Lead powder was measured in flat-plate transmission geometry on the MU-CAT ID-6 beamline at room temperature using 40-keV x-rays. The data are corrected for detector deadtime, absorption, and multiple scattering; backgrounds are removed and the data are normalized to obtain the sample dependent total scattering intensity. This is shown if Fig. 1. Notice the pronounced temperature diffuse scattering under the Bragg peaks, especially at high momentum transfer, Q. The TDS is pronounced because Pb is so soft; even at room temperature the atoms are undergoing large amplitude vibrations. The data are Fourier transformed to real-space to obtain the atomic pair distribution function (PDF), which is shown in Fig. 1(b). Plotted over the data is a line calculated using a central force potential. The agreement is reasonably good, but a number of discrepancies exist. The experiments will be repeated at low temperature over a wider Q-range to improve the real-space resolution of the measurement and to obtain the temperature dependence of the displacement amplitudes. This may also reveal evidence for anharmonicity, which results in a T-dependent phonon density of states.

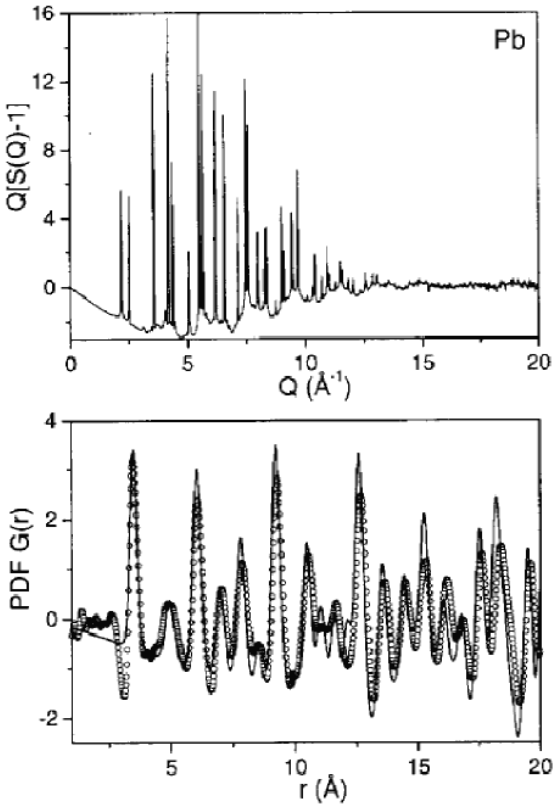

FIG. 1.

Acknowledgments

The authors would like to acknowlege the assistance of Doug Robinson. Research at MSU is supported by DOE through grant DE-FG02-97ER45651.

The MU-CAT sector is supported by the U.S. DOE-BES through the Ames Laboratory under Contract No. W-7405-ENG-82. The APS is supported by the U.S. DOE-BES under contract No. W-31-109-ENG-38.

References

[1] B.E. Warren, *X-ray Diffraction*, (Dover, New York, 1990).

[2] I-K. Jeong, Th. Proffen, F. Mohiuddin-Jacobs, and S.J.L. Billinge, J. Phys. Chem. A **103**, 921 (1999).

[3] D. Dimitrov, D. Louca, and H. Röder, Phys. Rev. B **60**, 6204 (1999).