Laboratori Nazionali di Frascati

LNF-87/53

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Estratto da:
SIF - Conf. Proc. "Synchrotron Radiation at Frascati" Vol. 5, 147 (1986)

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SPHERICAL WAVE ANALYSIS AND MULTIPLE SCATTERING EFFECTS IN HYDROGENATED AMORPHOUS SILICON

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The lack of data at low k in the EXAFS spectra is one of the main limitations of the technique when amorphous materials are investigated. Typically only the first shell distance and coordination are obtained. Low k values are not available because in this region multiple scattering effects are thought to be relevant (XANES region). Recently this assumption has been questioned. It has been shown[1] that single scattering theory can be well applied down to the XANES region (down to k=1.5 $Å^{-1}$) provided that a full curved wave theory of EXAFS is used. On the other hand it has been shown[2] that, after a carefull subtraction of the EXAFS signal, multiple scattering effects can be revealed in the region above 1.5 $Å^{-1}$ thus gaining information on the three and four body correlations.

We have investigated the possibility of extending EXAFS data analysis to the low k region in amorphous silicon in order to get next-nearest neighbour distance and coordination and isolate multiple scattering contribution to the absorption coefficient.

K-edges spectra of glow-discharge amorphous silicon were recorded at LURE (Orsay) using the ACO storage ring. The EXAFS signal was extracted subtracting an atomic like polinomial background to the data in the range k=1.5-9.5 $Å^{-1}$. With a simple analysis in terms of Fourier transform (FT) only the first coordination shell contribution has been detected (Fig. 1).

The first peak inverse FT was fitted to a theoretical first shell EXAFS calculated in the spherical wave approximation[3] (SWA) to obtain the structural parameters: coordination number N, distance R and Debye-Waller factor. To avoid systematic errors the theoretical spectrum has been fourier-filtered in the same range as the experimental one, before the fitting. An excellent agreement was obtained (Fig. 2).

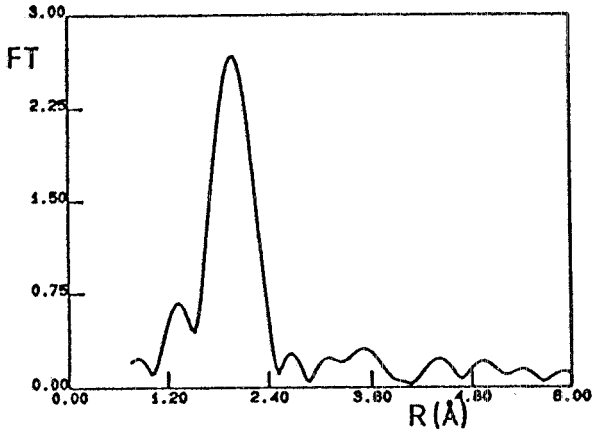

Fig. 1 - Fourier transform of the EXAFS signal of a-Si:H.

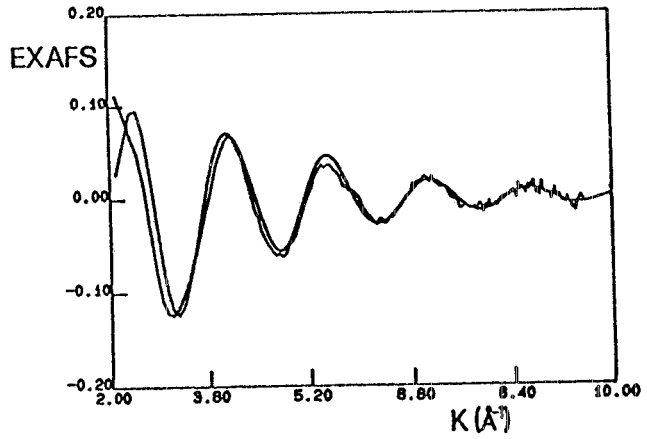

Fig. 2 - Experimental EXAFS and Theoretical first shell signal.

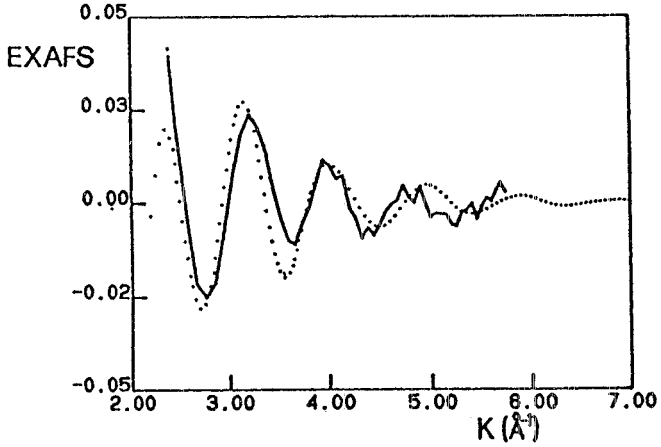

Fig. 3 - Comparison between the residual spectrum (——) and the theoretical EXAFS calculated from X-ray diffraction (···).

The phase shifts used were calculated in the muffin-tin approximation from a potential of a 17-atoms cluster, with diamond geometry, allowing a 10% overlap of the spheres.

The unfiltered SWA spectrum with the best fit parameters was then subtracted from the experimental data. The residual spectrum (Fig. 3) consists of a high frequency signal which could be due both to multiple scattering effects and/or to a contribution from higher shells.

A three path multiple scattering theoretical spectrum was calculated for a tetrahedron of 5 atoms; this spectrum has a slightly higher frequency and lower amplitude then the residual spectrum, thus showing that no multiple scattering effects have been detected. On the other hand an excellent agreement has been found between the residual spectrum and a theoretical EXAFS spectrum calculated using the radial distribution function (RDF) available from X-ray diffraction data (Fig. 3).

This result shows that a carefull EXAFS data analysis in the SWA approach can reveal the RDF beyond the first coordination shell, quite to the contrary of what is generally believed for such amorphous systems.

References:

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