STRUCTURAL PROPERTIES OF a-Si AND a-Si:H BY EXAFS[1]

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Abstract. - A comparative EXAFS study of the first-shell signals of c-Si,
a-Si and a-Si:H is presented. First-neighbour coordination, distance and
Debye-Waller factor are reported and discussed.

Introduction. - Despite the widespread interest in the characterization of amorphous
Si, both hydrogenated and not, the use of EXAFS technique for studying its structure
has been scarce [1]. This fact contrasts with the considerable amount of work
already done on a-Ge [2]. Possible explanations reside on the more advantageous
energy position of the Ge K-edge from the experimental point of view and on the
greater difficulty in analyzing signals due to light backscatterers.

Quite to the contrary, several diffraction works on a-Si and a-Si:H have
already been performed [3]. It is of great interest, therefore, to compare this
information with the one that can be obtained by EXAFS.

Experimental. - The Si K-edge absorption spectra were taken at LURE (Orsay), using
the beam line equipped with a InSb double-crystal monochromator at ACO storage ring.
The following samples were investigated: two a-Si:H films with different hydrogen
content (14% and 21%, respectively, as determined by the intensity of the Si-H_n
wagging band at 630 cm^{-1}) prepared by glow-discharge; one a-Si film grown by
sputtering; one c-Si sample prepared by evaporation and annealing, that was used as
a model compound.

Data Analysis - The EXAFS signal was extracted by subtracting an atomic-like
polynomial background from the spectra and then normalized using the factor
$[J \cdot (1-8(E-E_o)/3E_o)]^{-1}$ [4]. The origin E_o of k scale was placed in the middle of
the steep rise of the absorption coefficient. The jump J was estimated as the
difference of the mean value μ_o of the absorption coefficient above and below the
white line, both extrapolated at E_o. J/d is proportional to the density of the
sample. A high reproducibility among different measurements on the same sample was
obtained.

EXAFS spectra and their Fourier transforms (FT) are reported in Fig. 1 and 2.
The disappearance of long-range order in the amorphous samples is quite evident.

The signal of the first coordination shell was back transformed into k-space in
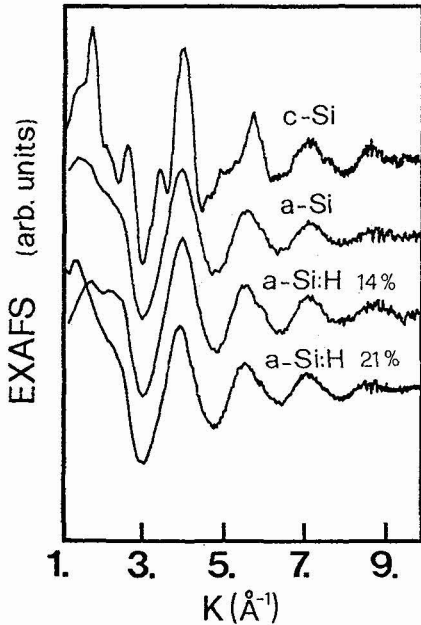order to perform the standard EXAFS analysis. The minimum and maximum of the
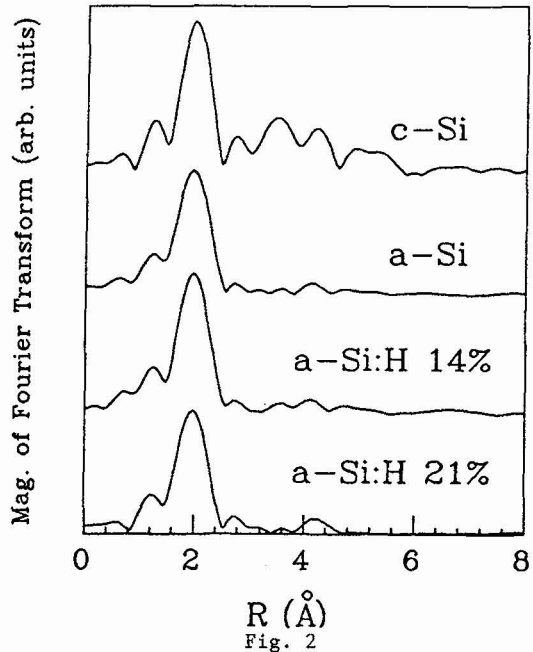
Fig. 1

Fig. 2

filtered region in R-space were placed at the values where the FT reached 30% and 10% of its maximum value, respectively. This procedure was judged the best compromise between the need of eliminating the background or the contribution from higher shells and of retaining maximum information in the filtering procedure.

The filtered signals have been compared by using $Ln(A2/A1)$ technique and by performing a best fit with the c-Si experimental model. Coincident results were obtained which are reported in Table I. The values reported are the average among different independent measurements on the same sample. The errors take into account the uncertainty of the experimental values of the c-Si used as a model.

TABLE I

Sample	ρ/ρ_c	CN_{IR}	CN_E	R($\overset{\circ}{A}$)	$\Delta\sigma^2 (\times 10^{-3} \overset{\circ}{A}{}^2)$
c-Si	1.00	1.00	1.00	2.352	0.
a-Si	0.86(2)	--	0.99(4)	2.34(2)	3.3(7)
a-Si:H 14%	0.94(2)	0.96	0.98(4)	2.35(1)	1.5(6)
a-Si:H 21%	0.85(2)	0.93	0.90(4)	2.36(2)	1.9(7)

Results and Discussion. - In the first column of the Table we report the density of Si atoms as obtained from the magnitude of the jump at the Si K-edge relative to the density of c-Si. The a-Si:H samples exhibit a reduction of ρ/ρ_c proportional to the hydrogen content. Despite the absence of H the sputtered sample too has a low density which is probably due to the presence of voids.

The coordination number CN_E as deduced from the EXAFS analysis is reported in column three, relative to that of c-Si. A relatively high precision ($\sim 5\%$) in the determination of CN_E has been obtained thanks to the accuracy of the analysis. Notice that the sputtered sample exhibits a large coordination almost identical to

that of c-Si, despite its low density. This fact points to the presence of a relativity small number of large voids. Quite to the contrary, the reduction in coordination of the a-Si:H samples closely reflects the presence of hydrogen, which does not contribute to the EXAFS signal. This circumstance can be verified by comparing column three with column two, where the apparent coordination number CN_{IR}, as deduced by the IR hydrogen content, is reported.

The average Si-Si bond distance is reported in column four. In close agreement with previous findings on tetrahedrally bonded amorphous semiconductors, it remains constant and equal to that of c-Si.

Finally, in column five we report the "disorder" factor $\Delta\sigma^2$ i.e. the difference between amorphous and crystalline samples of the variance σ of the bond distance. σ is the result of the static contribution σ_s (i.e. variance of the equilibrium distance), the thermal contribution σ_T and the correlation between the two. The correlation term is generally assumed negligible (it would be exactly zero in the harmonic approximation). For crystalline Si, $\sigma_s=0$ by definition, while σ_T^2 should be $\sim 3.2\cdot10^{-3}\text{Å}^2$ at room temperature, as estimated by using an Einstein model with oscillator frequency equal to 465 cm^{-1}. Assuming that σ_T of the amorphous samples is not far from that of c-Si at room temperature, $\Delta\sigma^2$ then coincides with σ_s^2. From Table I we see that the sputtered a-Si has a strained network with a standard deviation of bond distances of 0.06 ± 0.01 Å (i.e. ~ 2.5%). The presence of hydrogen in the glow-discharge samples relieves part of the strain and reduces σ_s to ~0.04 Å.

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