

Laboratori Nazionali di Frascati

LNF-87/52

A. Filipponi, F. Evangelisti, A. Balerna and S. Mobilio:
**AMORPHOUS HYDROGENATED ALLOYS: A COMPARATIVE EXFAS
STUDY OF $a\text{-Si}_{1-x}\text{C}_x\text{:H}$, $a\text{-SiN}_x\text{:H}$ AND $\text{Si}_{1-x}\text{Ge}_x\text{:H}$ AT THE Si K-EDGE**

Estratto da:
SIF - Conf. Proc. "Synchrotron Radiation at Frascati" Vol. 5, 143 (1986)

Servizio Documentazione
dei Laboratori Nazionali di Frascati
P.O. Box, 13 - 00044 Frascati (Italy)

AMORPHOUS HYDROGENATED ALLOYS: A COMPARATIVE EXAFS STUDY OF
 $a\text{-Si}_{1-x}\text{C}_x\text{:H}$, $a\text{-SiN}_x\text{:H}$ AND $a\text{-Si}_{1-x}\text{Ge}_x\text{:H}$ AT THE Si K-EDGE

A.Filipponi, F.Evangelisti
Dip. di Fisica, Università "La Sapienza" di Roma, Roma, Italy

A.Balerna and S.Mobilio
INFN, Laboratori Nazionali di Frascati, Frascati, Italy

In recent years amorphous hydrogenated Si alloys have been the subject of several electrical and optical studies. However, structural investigations are scanty⁽¹⁻⁴⁾.

Their structure is generally described within the continuous random network model, but also simple assumptions like random mixing or chemical ordering must be verified. Moreover, the relation between these alloys and the corresponding crystalline phases should be investigated.

Samples of $a\text{-Si}_{1-x}\text{Ge}_x\text{:H}$, $a\text{-Si}_{1-x}\text{C}_x\text{:H}$, $a\text{-SiN}_x\text{:H}$ at various concentration were deposited from a glow-discharge in binary gas mixtures of SiH_4 , CH_4 , GeH_4 and NH_3 respectively.

All samples were characterized by IR, optical and ESCA spectroscopies.

The Si K-edge absorption spectra were measured at LURE (Orsay) using the X-ray beam of ACO.

Two pure $a\text{-Si:H}$ samples with different hydrogen content (14%, 21%) were prepared in order to have model compounds in the limit $x=0$. A $a\text{-Si}$ sample prepared by sputtering and a $c\text{-Si}$ (evaporated and recrystallized) completed the series of silicon samples. Polycrystalline $a\text{-SiC}$ powders were used as model compound for the Si-C bond.

As an example, we show in Figs. 1 and 2 the Fourier transforms of the $a\text{-Si}_{1-x}\text{C}_x\text{:H}$ and $\text{SiN}_x\text{:H}$ data.

Standard EXAFS analysis applied to the silicon samples gave the following evidences:

- a) The Si-Si bond distance remains constant in all samples and equal to $2.35 \pm 0.02 \text{ \AA}$.
- b) In the two $a\text{-Si:H}$ samples the Si-Si coordination number was found small

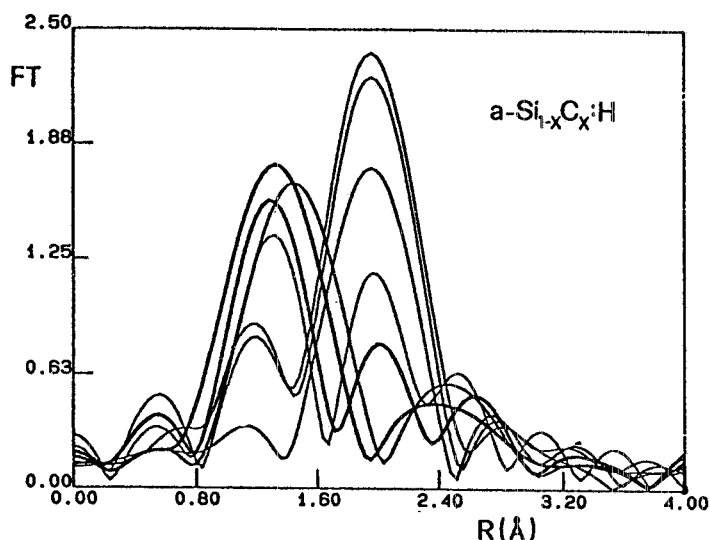


Fig. 1

ler than in the crystal by 4% and 10%, respectively, in close agreement with the number of H atoms bonded to Si as found in the IR spectra.

c) The static disorder parameter (bond length variance) is $(3.7 \pm 0.6) \times 10^{-3} \text{ \AA}^2$ in the a-Si sample. The introduction of hydrogen in a-Si:H relaxes the strain in the network and reduces the disorder parameter to $(1.3 \pm 0.5) \times 10^{-3} \text{ \AA}^2$ and $(2.0 \pm 0.6) \times 10^{-2} \text{ \AA}^2$ for the two samples.

As for the alloys, the following results were obtained:

a) In a-Si_{1-x}Ge_x:H and a-SiN_x:H, all first-neighbour distances were almost constant and independent of the concentration. In the a-Si_{1-x}C_x:H systems, the Si-Si bond-length was found constant, while the Si-C distance exhibits an expansion from 1.80 Å at $x \sim 0.5$ to 1.89 Å (i.e. equal to that of c-SiC) at $x \sim 0.9$.

b) The relative first-shell composition as derived from EXAFS shows that in a-SiN_x:H a tendency to form stoichiometric clusters exists at large x values.

c) At high x values a second shell contribution is detected in a-Si_{1-x}C_x:H and a-SiN_x:H samples. In the a-SiN_x:H case it is totally composed of Si atoms, while it is mainly formed of C in a-Si_{1-x}C_x:H alloys.

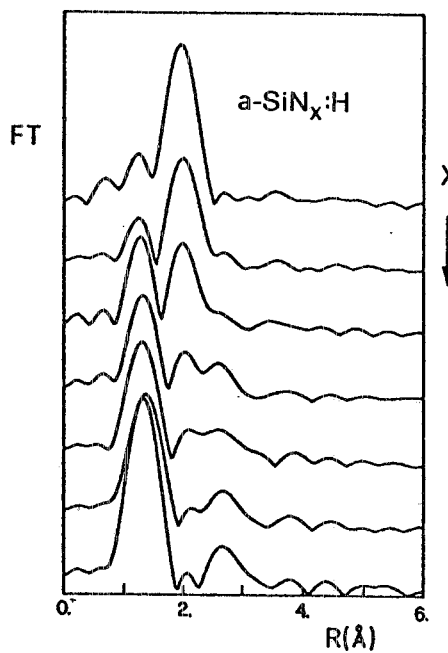


Fig. 2

References:

- (1) L.Incoccia, S.Mobilio, M.G.Proietti, P.Fiorini, C.Giovannella and F.Evangelisti, *Phys. Rev.* B31, 1028 (1985).
- (2) F.Evangelisti, M.G.Proietti, A.Balzarotti, F.Comin, L.Incoccia and S.Mobilio, *Solid State Commun.* 37, 413 (1981).
- (3) S.Minomura, K.Tsuji, M.Wakagi, T.Ishidate, K.Inoue and M.Shibuya, *J. Non-Cryst. Solids* 59-60, 541 (1983).
- (4) R.Bellissent, A.Chenevas-Paule, P.Lagarde, P.Bazin and D.Raoux, *J. Non-Cryst. Solids* 59-60, 237 (1983).