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INFRARED VIBRATIONAL SPECTRA OF CHLORINATED AND HYDROGENATED AMORPHOUS SILICON

S. Kalem, J. Chevallier, S. Al Dallal and J. Bourneix

Laboratoire de Physique des Solides, C.N.R.S., 1, place Aristide Briand, 92190 Meudon-Bellevue, France

Abstract : The infrared spectra of chlorinated and hydrogenated amorphous silicon have been measured. In addition to the hydrogen induced bands at 2110, 1990, 885, 840 and 640 cm^{-1} , we observe two new modes at 545 cm^{-1} (Si-Cl stretching) and 500 cm^{-1} (Si TO modes induced by chlorine). Observation of the 545 cm^{-1} band proves that chlorine acts as a dangling bond terminator. Upon annealing, some of the Si-Cl groups transform into SiCl_4 molecules (SiCl_4 stretching at 615 cm^{-1}). A good agreement is found between the total amount of chlorine determined by electron microprobe analysis and the value estimated from the integrated strength of the Si-Cl stretching mode.

Introduction :

A great deal of attention has been given in the past to hydrogenated amorphous silicon because of its potential application as a solar cell material [1] [2]. More recently, SHIMADA et al. established that fluorine is able to compensate the dangling bonds as hydrogen does [3]. Moreover, MADAN has shown that addition of fluorine in phosphorus doped materials results in a higher doping efficiency and a lower resistivity never achieved in hydrogenated amorphous silicon [4].

Other halogens can be imagined as dangling bond terminators. However, nothing has been reported until now about the role of chlorine in an amorphous silicon matrix. In this paper, we report infrared absorption measurements in chlorinated and hydrogenated amorphous silicon (a-Si : H, Cl) and the first observation of chlorine related bands. We discuss their origin and infer that chlorine acts as a dangling bond terminator. The thermal stability of hydrogen and chlorine was investigated from annealing experiments.

Preparation of a-Si:H, Cl films:

Samples with thickness of 1 μm were prepared on crystalline silicon wafers by glow discharge of a silicon tetrachloride (SiCl_4) and hydrogen mixture. The substrates were held at about 280°C. The power level was 0.2 watt/cm^2 and the growth rate 3 \AA/s . Our films contained 6 to 7% atomic chlorine as determined from electron microprobe analysis and 5% atomic bounded hydrogen as we shall see further. More information on the preparation conditions and properties of the films will be published elsewhere [5].

Absorption spectra :

Figure 1 shows a typical infrared spectrum of a a-Si:H,Cl film in the range 4000-200 cm^{-1} recorded with a PERKIN-ELMER 683 spectrophotometer. The hydrogen induced bands are identified by comparison with purely hydrogenated amorphous silicon [6] :

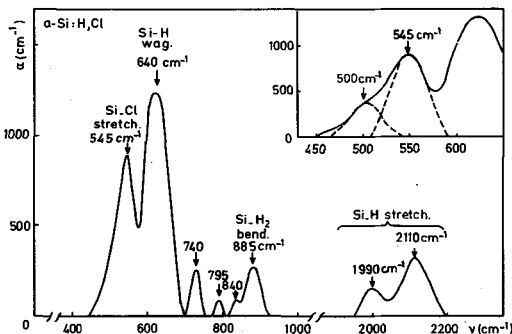


Fig. 1 - Typical infrared spectrum of a a-Si:H,Cl sample.

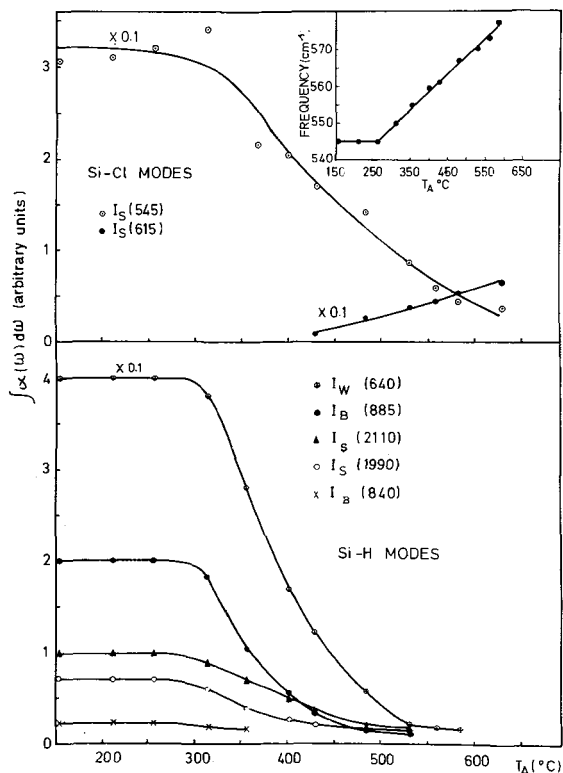


Fig. 3 - Integrated absorption variation of the Si-Cl and Si-H induced bands versus the annealing temperature.

silicon is replaced by hydrogen or chlorine atoms in the various possible configurations around a given silicon atom. We suggest that in unannealed samples, the dominant configurations are SiHCl or (and) SiH₂Cl. As the temperature increases, hydrogen and chlorine are released from such configurations which would favor the formation of SiCl₂ and SiCl₃ types of configurations. Such a view is supported by the following experimental fact. Above 400°C, a new band located at 615 cm⁻¹ appears in our infrared spectra. It is interpreted as the asymmetric Si-Cl stretching mode of SiCl₄ molecules formed in the matrix during annealing. Formation of SiF₄ molecules have also been observed in annealing experiments of a-Si:H,F samples [9].

Bounded chlorine and hydrogen concentrations :

By using an oscillator strength value of 16 cm²/mmole, bond deduced from published absorption data of various chlorosilane gases and local field corrections given by BRODSKY [10], we found 8% atomic bounded chlorine from the integrated Si-Cl absorption band at 545 cm⁻¹. This is in good agreement with the 6-7% determined from electron microprobe analysis. The concentration of bounded hydrogen has been calculated from the integrated absorption of the Si-H wagging band at 540 cm⁻¹ [8]. A value of 5% atomic has been found.

Conclusions :

From the observation of the Si-Cl stretching mode in i.r. absorption, we have established that chlorine is able to compensate the dangling bonds as fluorine and hydrogen do.

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