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COMPARATIVE INFRARED VIBRATIONAL SPECTROSCOPY OF CHEMICAL VAPOUR DEPOSITION SiO_2 FILMS

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Abstract: We compare FTIR absorbance spectra due to Si-O stretching, Si-O-Si and O-Si-O bendings in different films of amorphous SiO_2. We study the effect of thermal annealing on these optical structures.

1. Introduction

Amorphous SiO_2 is a very important material in semiconductor devices manufacturing. Nevertheless, in spite of its fundamental importance as dielectric film, very few information about optical, dynamical and structural properties of SiO_2 is at present available. In the present work we apply Fourier transform infrared (FTIR) spectroscopy to the study of vibrational properties of Si-O, Si-O-Si and O-Si-O bonds as function of sample preparation: We compare the cases of thermal oxidation, chemical vapour deposition (CVD) from atmospheric pressure (APCVD) or from low-pressure (LPCVD) and plasma activated SiO_2 films [1].

2. Results and discussion

Accordingly to the structural description of SiO_2 [2], three different effective oscillators are identified in the FTIR spectra: They correspond to the Si-O bond stretching vibration and to the Si-O-Si and O-Si-O bond bending oscillations. The bond stretching and bending are described by a central two-body potential and by a three-body non central (Keating-like) potential, respectively. Following the current literature, we attribute to the Si-O stretching a frequency of 1050 cm^{-1} and to Si-O-Si and O-Si-O bendings a frequency of 450 cm^{-1} and 800 cm^{-1}, respectively. In Table I we summarize the peak parameters for as deposited and annealed films. F is the wave number peak position (in cm^{-1}); H is the peak height (in 10^{-3} absorbance units); FWHM is the full width half medium of the absorbance bands (in cm$-$1). The main conclusions we may drawn are that after annealing the 1050 and 450 cm^{-1} peaks are shifted towards higher frequencies, while the O-Si-O peak is lowered in frequency; the FWHM is strongly reduced in any case and the absorption coefficient is always enhanced. In conclusion, the annealing can be regarded as an ordering process which causes a long-range disorder reduction (*i.e.* a recovering of the crystalline character of the sample); moreover, the statistical distribution of lattice parameters (Si-O bond lenght and Si-O-Si and O-Si-O bond angle) is also reduced and, consequently, FWHM decreases.

Table I

Film type	450 cm^{-1} peak			815 cm^{-1} peak			1080 cm^{-1} peak		
	F	*A*	FWHM	*F*	*A*	FWHM	*F*	*A*	FWHM
dry thermal oxide (1100 °C)	459.0	81	41	806.1	23	69	1080	230	77
APCVD (as deposited) (415 °C)	444.5	33	60	810.0	11	81	1059	128	87
APCVD (annealed) (415 °C)	458.0	60	44	812.0	10	63	1076	182	77
LPCVD (as deposited) (425 °C)	447.5	39	60	815.8	9	65	1057	131	87
LPCVD (annealed) (425 °C)	458.0	70	43	810.0	12	65	1078	206	75
PACVD (as deposited) (380 °C)	447.5	37	59	815.8	9	71	1053	130	93
PACVD (annealed) (380 °C)	458.0	64	43	812.0	11	57	1074	187	75

3. References

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