APPLICATION NOTE

FTIR Spectroscopy

AUTHOR

Ian Robertson
PerkinElmer, U.S. LLC.
Seer Green, UK

The Measurement of the Hydrogen Content of Silicon Nitride Dielectric Films on Silicon Wafers

Introduction

Silicon wafers are processed by the addition of dielectric films that are used primarily to isolate circuits from each other and to provide mechanical and chemical protection to the device itself. They are also used as masking materials during the wafer fabrication process. There are a variety of different film substrates, two of the common ones being borophosphosilicate glass and silicon nitride (Si_3N_4). Silicon nitride thin films attract widespread scientific interest across multiple application fields.[1] In addition to the properties required for electronics manufacturing they also provide excellent optical, mechanical, and thermal properties allowing their use in solar cell applications where they serve as antireflection and passivating coatings.[1]

The films are created using a variety of different deposition techniques each of which will affect the quality of the silicon nitride. The process can introduce hydrogen into the film from the silane and ammonia reactants. If there is a high hydrogen content it will affect the film properties and performance. In addition, the nitride film's optical properties depend on the ammonia to silane ratio.

FTIR (Fourier transform infrared) spectroscopy is used widely within the electronics and solar industries for the determination of the chemical properties of materials. This application note describes the FTIR method for the measurement and calculation of the -NH and -SiH content in Si_3N_4 films.

PerkinElmer®
For the Better

Experimental

FTIR measurements can be performed on silicon wafers for a range of applications with measurements possible in either transmission or reflectance. For the measurement of silicon nitride films on silicon wafers the measurements can be performed in transmission with the wafers being positioned in the MappIR system in the PerkinElmer Spectrum 3™ FTIR spectrometer as shown in Figure 1.

The measurement system consists of a PerkinElmer Spectrum 3 FTIR spectrometer and a Pike MappIR (or Mapp300) wafer holder and optical system with automation software. The system is able to analyze a range of wafer sizes from 2 inches up to 8 inches (MappIR) or 12 inches (Mapp300) in either transmission or reflection mode. The automation software allows automated, unattended mapping of the wafer, collecting spectra across the entire wafer according to preset or user-defined mapping arrangements. Data collection is followed by calculations according to the analysis method specified.

Spectra were collected in Transmission mode for 8 inch diameter silicon wafers coated with a silicon nitride film at a spectral resolution of 4 cm^{-1} using 4 scans for data collection. Figure 2 shows the spectra of an uncoated wafer and a wafer coated with a thin layer Si_3N_4 dielectric film.

There are clear differences in these 2 spectra. There are specific spectral bands due to the presence of Si-H and N-H at 2170 cm^{-1} and 3350 cm^{-1} respectively as shown in Figure 3. The calculation deployed in this application note is based on the Lanford and Rand method.[2]

The peak areas are calculated using appropriate baseline regions to account for the spectroscopic baseline effects.

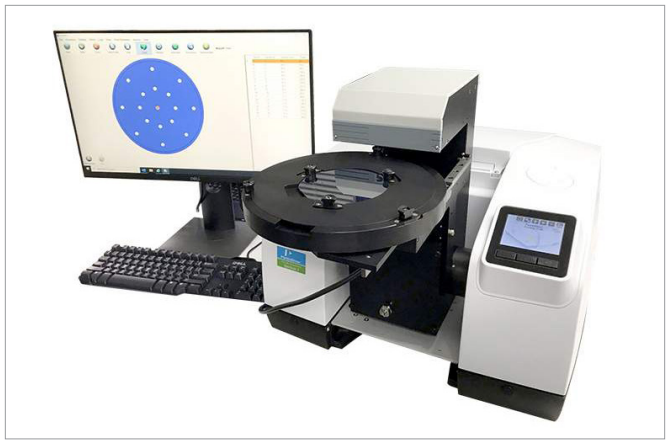

Figure 1. The Spectrum 3 FTIR MappIR System.

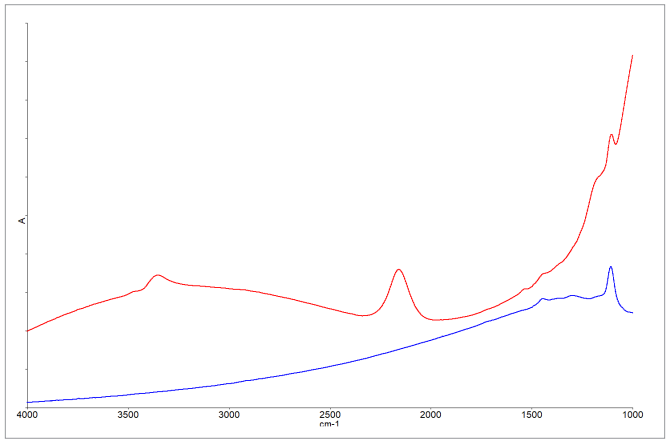

Figure 2. Spectra of Uncoated Silicon Wafer (blue) and Wafer with Si_3N_4 film (red).

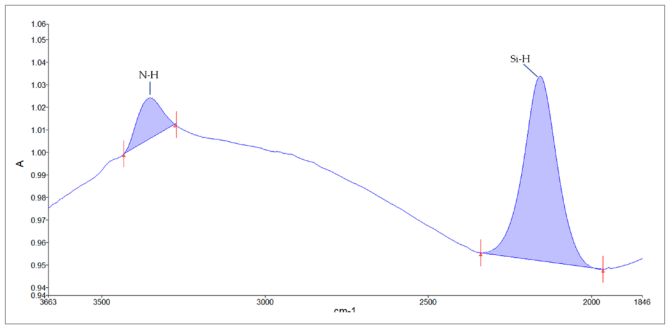

Figure 3. Spectral ranges used for the Si-H and N-H concentration calculations.

Calculations

Calculation methods from paper "The hydrogen content of plasma-deposited silicon nitride.", Lanford and Rand.[2]

Number of Si-H bonds/cm^3 =K1 x (peak area of Si-H)/thickness

Number of N-H bonds/cm^3 = K2 x (peak area of N-H)/thickness

Where K1=1.36 x 10^{17} and K2=1.904x 10^{17}

K1 and K2 Values from literature.[2] K2/K1=1.4 and accounts for relative absorption coefficients of Si-H and N-H

Si-H % =(Si-H atom)/[(film density x 3.035 x 10^{22}) +(Si-H atom)+(N-H atom)]

N-H % =(N-H atom)/[(film density x 3.035 x 10^{22}) +(Si-H atom)+(N-H atom)]

Calculations

Film Thickness 8500A

- Si-H bonds/cm^3 =K1 x (peak area of Si-H)/thickness
  = 1.5744 x 10^{22} bonds/cm^3
- N-H bonds/cm^3 =K2 x (peak area of N-H)/thickness
  = 0.4883 x 10^{22} bonds/cm^3
- Si-H%=(Si-H atom)/[(film density x 3.035 x 10^{22}) +(Si-H atom)+(N-H atom)]
  =1.5744 x 10^{22}/[(2 x 3.035 x 10^{22}) + 1.5744 x 10^{22} + 0.4883 x 10^{22}]
  =19.36%
- N-H%=(N-H atom)/[(film density x 3.035 x 10^{22}) +(Si-H atom)+(N-H atom)]
  =0.4883 x 10^{22}/[(2 x 3.035 x 10^{22}) + 1.5744 x 10^{22} + 0.4883 x 10^{22}]
  =6.00%

Conclusion

FTIR spectroscopy utilising the MappIR system has been demonstrated to be a fast and easy method for the determination of the hydrogen content of silicon nitride films. This method could be deployed in investigations into the film deposition process in order to optimize the film properties for the material's application in either semiconductors or solar cell devices.

References

1. Alain E. Kaloyeros *et al 2020 ECS J. Solid State Sci. Technol.* 9 063006.
2. William A Lanford, M J Rand, Journal of Applied Physics, volume 49, 1978, pages 2473–2477.

PerkinElmer, U.S. LLC.
710 Bridgeport Ave.
Shelton, CT 06484-4794 USA
(+1) 855-726-9377
www.perkinelmer.com

12137