May 2003 • NREL/CP-520-33576

Conference Paper

The FTIR Laboratory in Support of the PV Program

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Presented at the National Center for Photovoltaics and
Solar Program Review Meeting
Denver, Colorado
March 24-26, 2003

National Renewable Energy Laboratory

1617 Cole Boulevard
Golden, Colorado 80401-3393

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Contract No. DE-AC36-99-GO10337

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The FTIR Laboratory in Support of the PV Program

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ABSTRACT

Fourier Transform Infrared Spectroscopy (FTIR) is a fast, accurate, reliable method for studying molecular structure and composition. Both qualitative and quantitative analyses can be performed on a wide variety of materials. The FTIR spectroscopy laboratory has large-area and micro-reflectance and transmittance capabilities, including automated mapping, in the infrared range from 1.3 to 25 μm. We will examine several examples where FTIR is useful for analyzing semiconductor and photovoltaic-related materials. Although not presented here, FT-Raman and FT-Photoluminescence are additional techniques available to study vibrational modes and emitted radiation of electronic transitions in a wavelength range from 0.8 to 2.5 μm.

1. Crystalline Silicon

Because of its rapid, nondestructive nature, FTIR spectroscopy is used by both in-house NREL customers and industry partners such as AstroPower, Evergreen Solar, and GT Solar as a tool for evaluating crystalline silicon material quality. This routine technique, alone or combined with other measurements such as minority-carrier lifetime and internal quantum efficiency, is an effective means of process control in an industrial setting. It is also an effective means for studying newer materials such as amorphous SiNx deposited on crystalline silicon.

Using FTIR transmittance analysis, impurities in highly resisitive silicon can be detected and quantified. Interstitial oxygen and substitutional carbon concentrations are calculated per ASTM methods F 1188-93 and F 1391-93, respectively. In addition, we can determine absorption coefficients of oxygen precipitates, SiNx, and SiCx vibrations if present. High impurity or precipitate levels usually adversely affect device performance, therefore concentrations must be known for maximizing process control in PV silicon manufacturing [1]. Figure 1 shows a typical absorption spectrum of crystalline silicon.

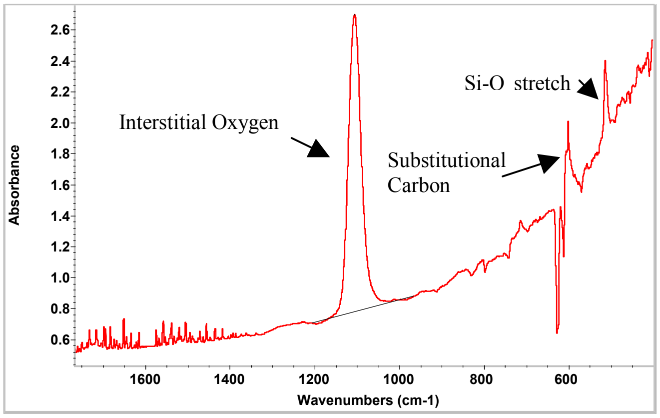

Figure 1. Impurity modes of crystalline silicon.

2. Polymer Analysis

Polymeric materials have widespread use in the PV industry as metallized polymer reflectors, photovoltaic encapsulants, electrochromic devices, desiccant materials and others [2]. Macro or micro reflection absorption or Attenuated Total Reflectance (ATR) can be useful techniques for obtaining infrared data of thick or highly absorbing films or those mounted on reflective substrates.

In reflection-absorption measurements the infrared beam passes through the sample, reflects off the substrate and passes again through the sample at angles ranging from near normal to 60 degrees. This essentially doubles the pathlength of that obtained in a transmission experiment.

For opaque films or those with totally absorbing regions, ATR may be the method of choice. An internally reflecting crystal material with a specific refractive index, length, spectral range, and angle of incidence controls the effective pathlength. Because the pathlength is limited to a few microns, this technique characterizes the surface of the sample and does not penetrate the bulk. Determination of functional groups, as well as comparisons of sample spectra with those of both organic and inorganic commercial library databases, can help identify unknowns or confirm the presence of contaminants. For those materials used as encapsulants for PV modules, FTIR analysis can track spectral changes as a function of weathering to analyze polymer integrity. Figure 2 is an example of polymer coatings on aluminum analyzed in reflectance mode and converted to absorbance to facilitate spectral database searching.

3. Amorphous to Microcrystalline Silicon and Related Alloys

Infrared absorption is used to study the material properties of a-Si:H, μc-Si:H, and a-SiGe:H. The regions of interest include Si-H(Ge-H) stretching vibrations from 1880 to 2150 cm^{-1}, SiH$_2$(GeH$_2$) bending vibrations from 760 to 910 cm^{-1}, Si-H(Ge-H) wagging modes around 650 cm^{-1}, and Si-O related absorptions from 1000 to 1200 cm^{-1}.

Additionally, transmittance spectra of these materials grown on crystalline-silicon substrates are used to calculate hydrogen contents using the wag intensity [3]. Transmittance data are converted to absorption coefficients

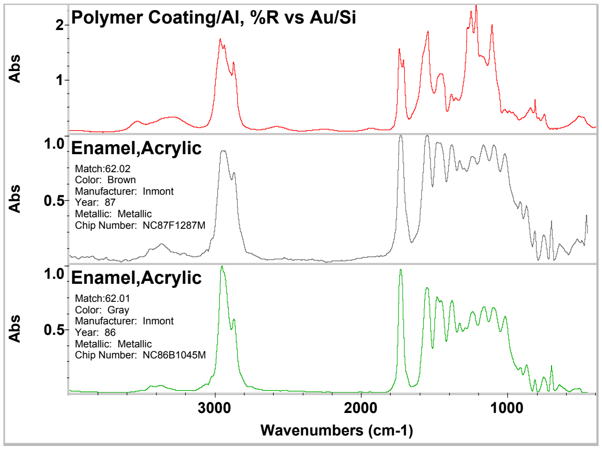

Figure 2. Polymer spectrum and possible match to acrylate group.

and analyzed using a model based on a-Si:H or a-SiGe:H standards calibrated for H content by NRA [4].

In amorphous to microcrystalline films, the study of Si-H infrared bonding configurations are related to microcrystallinity. Also, because films with higher crystalline volume fractions favor increased oxidation, monitoring oxygen-related absorption regions proves to be a valuable exercise in predicting device quality. Figure 3 shows the hydrogen distribution as a function of H-dilution in transition films [5].

As with the above films, hydrogen content and its bonding configuration are also important in silicon-germanium alloys. Incorporating these alloys in tandem devices lowers the band gap and maximizes use of the solar spectrum. Increased Ge-H bonding, detectable by FTIR, produces higher-quality alloys [6]. Figure 4 shows the improvement in Ge-H bonding as a function of lower substrate temperature.

4. Transparent Conducting Oxide Films

Transparent conducting oxides have many applications including thin-film solar cells for the PV industry. In response to increased development efforts, especially in the area of combinatorial growth, the FTIR lab has added large-area reflectance and transmittance infrared mapping capabilities for higher-throughput TCO library characterization. These optical measurements are used to calculate carrier concentration and, hence, conductivity, and can be combined with other measurements to more efficiently optimize material growth parameters [7,8]. Figure 5 is a reflectance map (at 2000cm^{-1}) for a non-uniform 4 x 4 inch Cd_2SnO_4 film.

5. Summary

Because of its versatility and accessibility, the FTIR Laboratory is a valuable contributor to the PV program and enhances its capabilities. We provide support for, and collaborate with, several in-house programs as well as our industry partners.

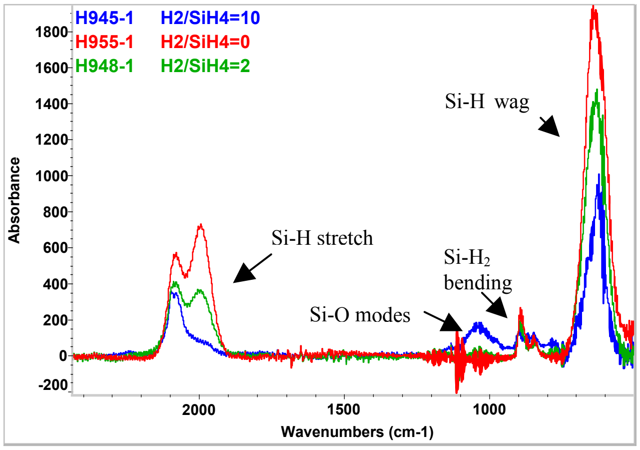

Figure 3. Effect of H-dilution in amorphous to microcrystalline silicon films.

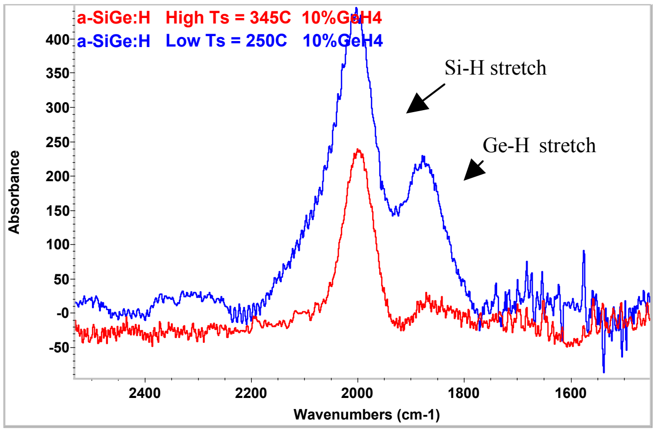

Figure 4. H-bonding in a-SiGe:H.

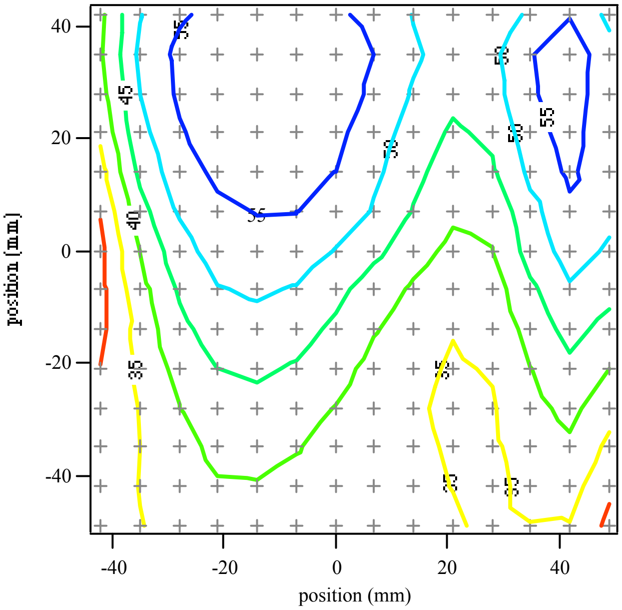

Figure 5. Contour map of the reflectance (at 2000cm^{-1}) for a 4 x 4-inch Cd_2SnO_4 film on glass.

6. Acknowledgements

This work was performed at NREL in the Measurements and Characterization Division of the National Center for Photovoltaics under U.S. Department of Energy Contract No. DE-AC36-99-G010337.

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REPORT DOCUMENTATION PAGE			*Form Approved* *OMB NO. 0704-0188*
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1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE May 2003	3. REPORT TYPE AND DATES COVERED Conference Paper	
4. TITLE AND SUBTITLE The FTIR Laboratory in Support of the PV Program			5. FUNDING NUMBERS PVP3.3101
6. AUTHOR(S) L. Gedvilas, B. Keyes, T. Ciszek, G. Jorgensen, B. Nelson, Y. Xu, and J. Perkins			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) National Renewable Energy Laboratory 1617 Cole Blvd. Golden, CO 80401-3393			8. PERFORMING ORGANIZATION REPORT NUMBER NREL/CP-520-33576
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)			10. SPONSORING/MONITORING AGENCY REPORT NUMBER
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION/AVAILABILITY STATEMENT National Technical Information Service U.S. Department of Commerce 5285 Port Royal Road Springfield, VA 22161			12b. DISTRIBUTION CODE
13. ABSTRACT *(Maximum 200 words)* Fourier Transform Infrared Spectroscopy (FTIR) is a fast, accurate, reliable method for studying molecular structure and composition. Both qualitative and quantitative analyses can be performed on a wide variety of materials. The FTIR spectroscopy laboratory has large-area and micro- reflectance and transmittance capabilities, including automated mapping, in the infrared range from 1.3 to 25 mm. We will examine several examples where FTIR is useful for analyzing semiconductor and photovoltaic- related materials. Although not presented here, FT-Raman and FT-Photoluminescence are additional techniques available to study vibrational modes and emitted radiation of electronic transitions in a wavelength range from 0.8 to 2.5 mm.			
14. SUBJECT TERMS Fourier Transform Infrared; solar cells; spectroscopy; thin films; transparent conducting oxides			15. NUMBER OF PAGES
			16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT UL

NSN 7540-01-280-5500

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298-102