Characterization of Interstitial Oxygen in 200 μm Thick Silicon Wafer by Micro-FTIR System

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Abstract Interstitial oxygen (Oi) content of a silicon wafer is an important material characteristic for single crystal photovoltaic applications. Interstitial oxygen in silicon is typically measured by infrared absorption or so-called FTIR technique. However, the accuracy of FTIR measurements becomes debatable when the wafer thickness is getting thinner and thinner. In this work, we propose to construct a Micro-FTIR system based on a commercial FTIR spectrometer (Bruker Tensor 27). This home-built Micro-FTIR system offers F/2 optics, 900 μm spatial resolution, and 12x12 mm^2 scan area for FTIR mapping. We also develop our own method to characterize the Oi content of silicon wafer in various thicknesses, ranging from 200 μm to 2 mm. We believe that this Micro-FTIR system and the analysis method may turn into a powerful tool to investigate the defects in silicon single crystal wafer and 2D emergent materials in the near future.

Micro-FTIR system setup

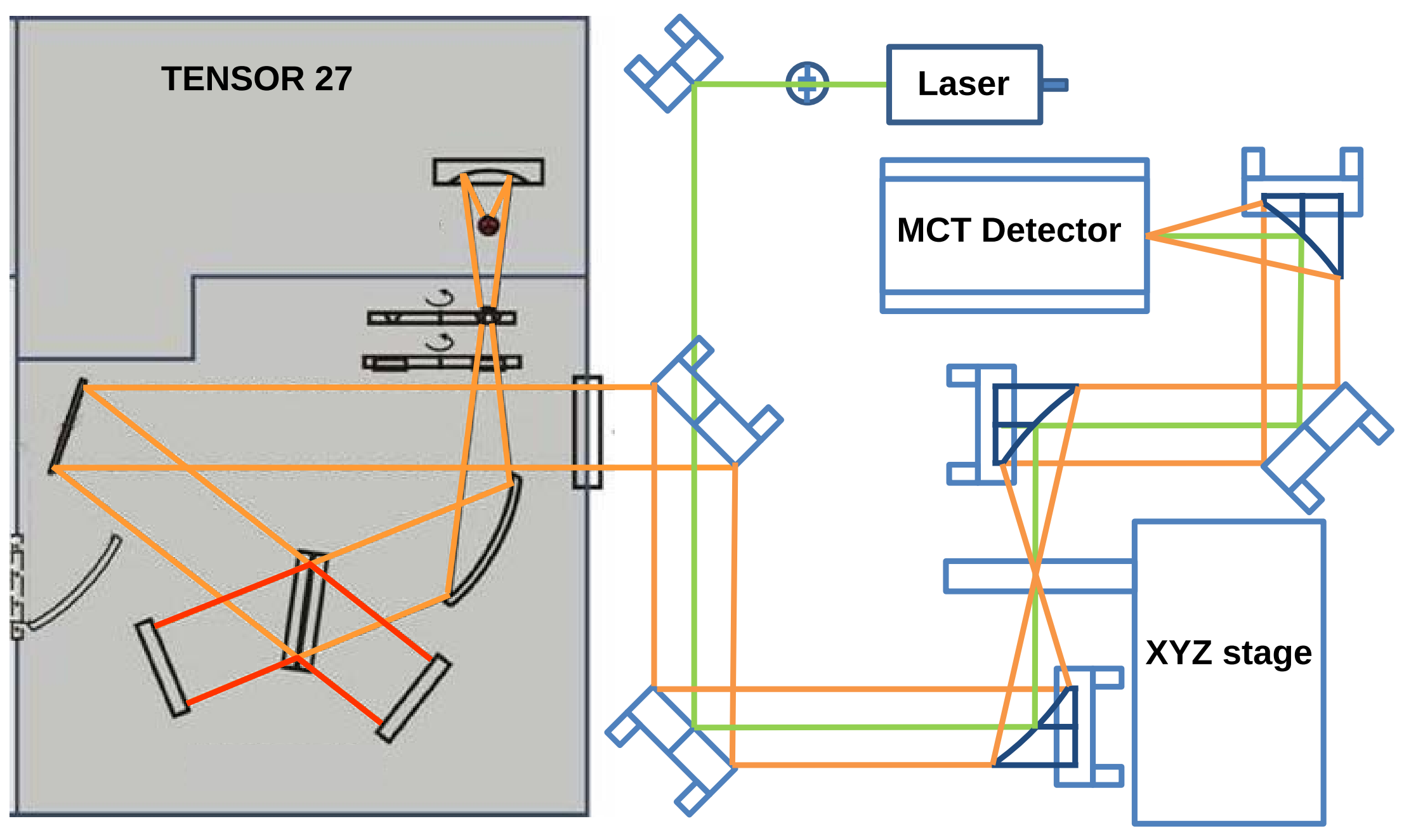

Figure 1 The Micro-FTIR system was constructed based on Tensor 27 FTIR spectrometer. The system is equipped with a XYZ stage, MCT (Mercury-Cadmium-Telluride) detector, and F/2 optics.

Beam profile of Micro-FTIR

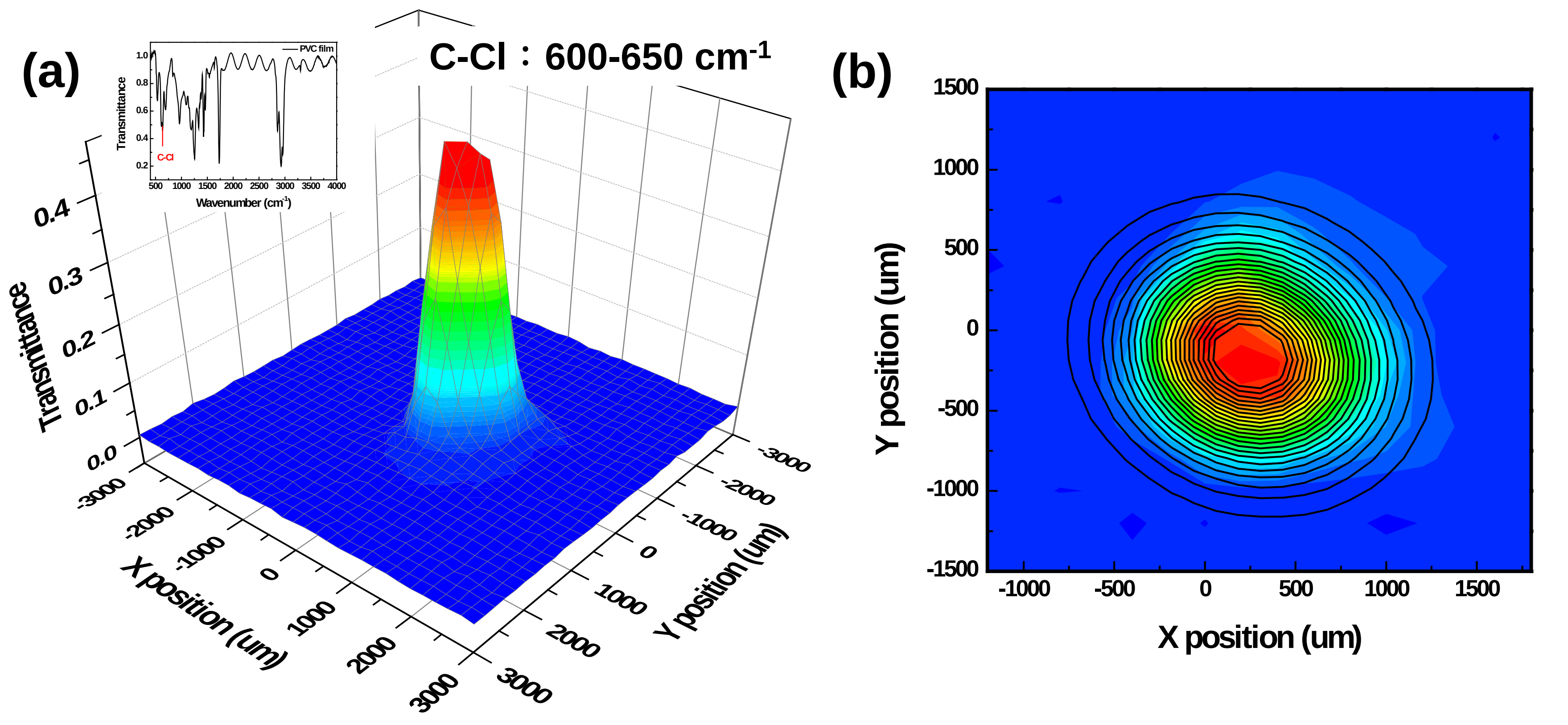

Figure 2 (a): FTIR 2D mapping of 200 μm pinhole covered with one layer of PVC film. The peaks in the range of 600-650 cm^{-1} correspond to C-Cl gauche bond of PVC. The scan area is 6 x 6 mm^2 with 200 μm/point scan step. The parameter of FTIR spectra: 4 cm^{-1} resolution, 16 scans, and range from 400-4000 cm^{-1}. (b): Gaussian2D fitting of (a). The FWHM of x-axis and y-axis are 960 μm and 860 μm. The spatial resolution of the system is about 900 μm.

Interstitial oxygen in silicon wafer

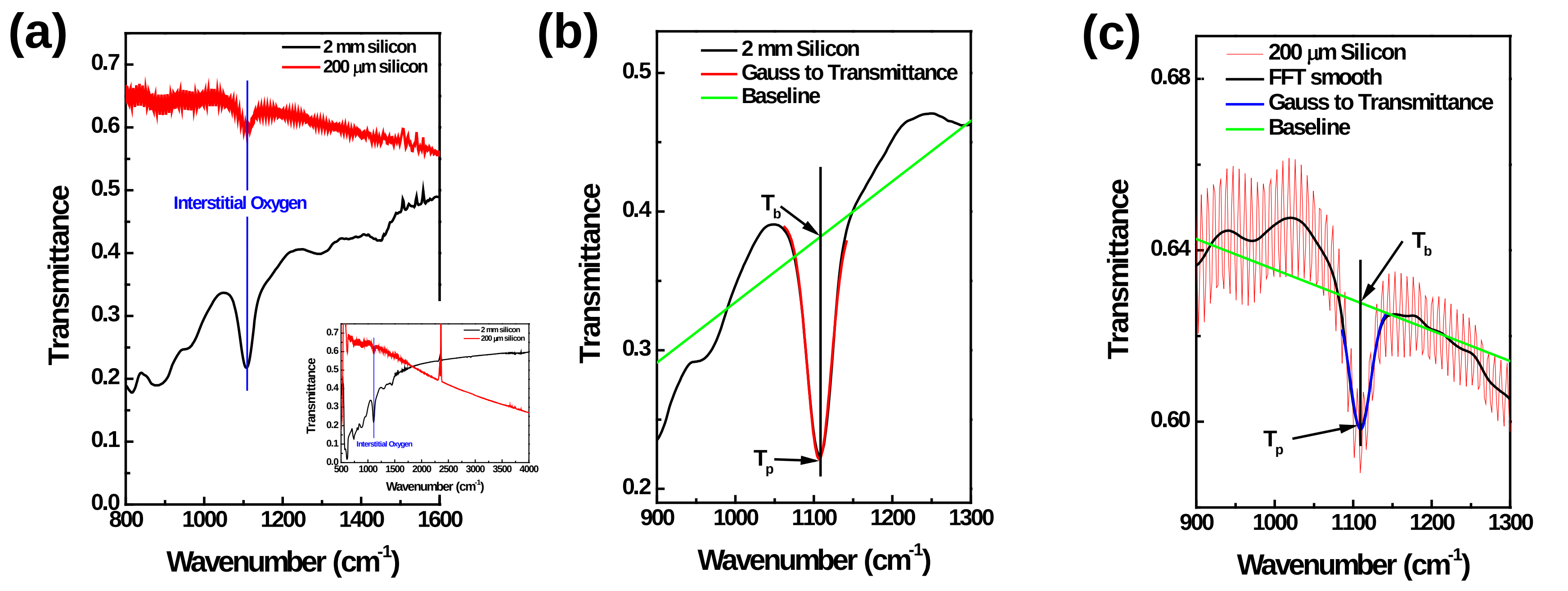

Figure 3 (a): FTIR spectra of 2 mm and 200 μm silicon wafers which are from the same silicon ingot. The band at 1107 cm^{-1} is from interstitial oxygen (Oi) in silicon wafer. (b) (c): Fitting the Si-O band by Gaussian function and drawing a baseline from 900 to 1300 cm^{-1} to define T_p and T_b. The endpoints of the baseline is defined by using the average transmittance in the regions from 900 to 1000 cm^{-1}, and 1200 to 1300 cm^{-1}.

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Calculation of Interstitial oxygen

Standard Test Method ASTM F1188-00:

$$\alpha_p = -\frac{1}{x} ln\left[\frac{\left(0.09 - e^{1.70x}\right) + \sqrt{(0.09 - e^{1.70x})^2 + 0.36T_p^2 e^{1.70x}}}{0.18T_p}\right]$$

$$\alpha_b = -\frac{1}{x} ln\left[\frac{\left(0.09 - e^{1.70x}\right) + \sqrt{(0.09 - e^{1.70x})^2 + 0.36T_b^2 e^{1.70x}}}{0.18T_b}\right]$$

$$\alpha_o = \alpha_p - \alpha_b$$

α_p = peak absorption coefficient
α_b = baseline absorption coefficient
α_o = interstitial oxygen absorption coefficient
T_p = peak transmittance
T_b = baseline transmittance
x = thickness (cm)

Interstitial oxygen concentration(N_{Oi})

$$N_{Oi} = 6.28 \times \alpha_o \ (ppm\ atomic)$$
$$= 3.14 \times 10^{17} \times \alpha_o \ (atoms/cm^3)$$

By using the method from Standard ASTM F1188-00, the Oi concentration of 2 mm silicon wafers from two different silicon ingots (Si A and Si B) are:

Sample	α_p	α_b	α_o	Reference* N_{Oi} (ppma)	N_{Oi} (ppma)	Error (%)
2 mm (Si A)	2.77	0.60	2.17	13.80	13.66	-1.03%
2 mm (Si B)	2.71	0.62	2.09	13.42	13.13	-2.14%

* Reference concentration measured by commercial FTIR system from Thermo Fisher Scientific.

Stack of 200 μm silicon wafers

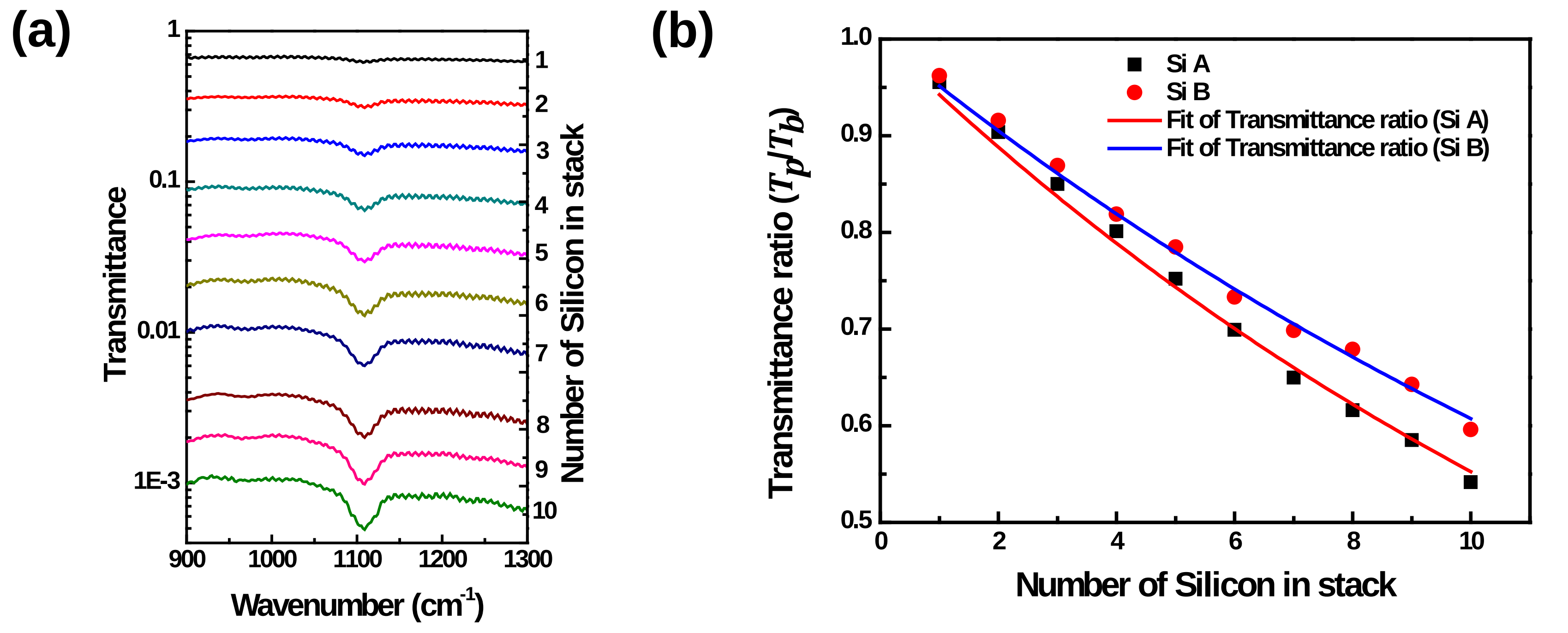

Figure 4 (a) FTIR spectra from stacking of different number of 200 μm silicon wafer in stack (1 to 10). (b) Fitting the transmittance ratio to calculate the interstitial oxygen coefficient of Oi for 200 μm silicon wafer (Si A and Si B).

Absorption Equation :

$$T_p = [(1-R)e^{-(a+b)x}]^n \qquad T_p/T_b = e^{-bxn}$$
$$T_b = [(1-R)e^{-ax}]^n$$

R = Reflectance of silicon surface
a = background absorption coefficient
b = Interstitial oxygen absorption coefficient
x = thickness (cm)
n = number of silicon in stack

Sample	x (cm)	b	Reference N_{Oi} (ppma)	Calibration factor (N_{Oi}/b)	N_{Oi} (ppma)	Error (%)
Si A	0.02	3.22	13.80	4.29		
Si B	0.02	2.81	13.42	4.29	12.06	-10.12%

Conclusion **Our home-built Micro-FTIR system provides 900 μm spatial resolution with 2D mapping capability. A new method is developed to measure the interstitial oxygen concentration (N_{Oi}) of silicon wafer with 200 μm thickness. The derived N_{Oi} value is compared with that of the reference sample and shows reasonable agreement but with 10% fluctuation. We suggest that the fluctuation may be due to the baseline determination. This Micro-FTIR system is proposed to explore 2D emergent materials in the near future.**