ML-driven Thermal Sensing Using FTIR Spectroscopy

Emigdio Chavez Angel[1], Martin Kreuzer[2] Jianying He[3], and Aitor Mugarza[1, 4]
[1] Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain
[2] CELLS-ALBA, Synchrotron Light Source, 08290 Barcelona, Spain
[3] NTNU Nanomechanical Lab, Department of Structural Engineering, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway
[4] Institución Catalana de Investigación y Estudios Avanzados (ICREA), 08010 Barcelona, Spain

emigdio.chavez@icn2.cat

Abstract

Thermal imaging at the microscale remains a challenging and time-intensive process. It is crucial for applications in engineering, microelectronics, optics, and biochemistry. In electronic circuits, it offers valuable insights into hot spots, power densities, and heat distribution in CMOS platforms. This study introduces a non-invasive, contactless thermal mapping technique using synchrotron radiation-based FTIR microspectroscopy, achieving spatial resolution below 10 µm over areas of 12,000 µm^2 on PMMA films on CaF_2 substrates. Infrared spectra from films heated with a wire were analysed using linear regression and machine learning algorithms, including random forest and k-nearest neighbours, enabling rapid signal analysis and the creation of hyperspectral temperature maps. This method demonstrates the potential of infrared absorbance for precise heat distribution and thermal property measurements, with applications in CMOS technologies and other electronic devices.

Sample preparation

A 1 µm poly(methyl methacrylate) (PMMA) solution was spin-coated onto CaF_2 substrates and cured at 50 C for 4 h in a vacuum oven. Later, a titanium-gold wire was evaporated onto the film to serve as a heating element, creating a controlled temperature gradient through applied currents.

Experiment

The experiment consisted of two steps: first, calibrating the FTIR signal of the polymer as a function of temperature using a cryostat, and second, generating a temperature distribution with the heater. Once calibrated, the FTIR signal was mapped across the surface to monitor local temperature distributions, translating the FTIR map into precise temperature measurements.

The calibration of the temperature-dependent infrared absorbance was performed using synchrotron radiation-based FTIR microspectroscopy. The measurements were carried out over a temperature range of T = 283 K to 373 K. Then, FTIR spectra were analysed to identify temperature-sensitive peaks, which were used as indicators for thermal imaging. Data were collected through line scans and hyperspectral imaging across the polymer surface, achieving spatial resolutions of 10 µm. The captured data were processed using linear regression for peak-based temperature predictions and machine learning models (see Figure 1), including random forest (RF) and k-nearest neighbour (kNN) algorithms, to analyse the full spectral range and generate high-resolution thermal maps.

Figure 1. Insert caption to place caption below figure

Results

Figure 2 shows the optical (a) and thermal image generated by metal wire heated at 376 K (b and c). For each measurement point, the temperature was predicted using the RF (Figure 2a) and the k-NN (Figure 2b) algorithms. This technique allows us to have a very fast estimation of the thermal mapping using the raw signal directly. Avoiding the individual fitting of 540 spectra and using the whole frequency windows instead of a single peak. [1]

Figure 2. (a) Optical image with the metallic gold coating (black) on a PMMA thin film (blue) and the sampled area of the hyperspectral imaging in white. Hyperspectral images showing the temperatures predicted by the (b) random forest and (c) kNN machine learning algorithms. The regions of the metallic gold wire are masked in black.

References

[1] Emigdio Chavez-Angel, Ryan C. Ng, Susanne Sandell, Jianying He, Alejandro Castro-Alvarez, Clivia Sotomayor Torres and Martin Kreuzer, Polymers, 15 (2023) 536.