

Non-Destructive Reflection-Mode Terahertz Characterization of Dye-Contaminated Aqueous Samples Using a Custom PTFE Liquid Cell

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INTRODUCTION & AIM

Dye-contaminated water is a relevant environmental problem in industrial and urban watersheds. In the Aburrá-Medellín River basin, recurrent color-discharge events have highlighted the need for rapid and non-destructive screening strategies. In this work, methylene blue is used as a representative cationic blue dye and model pollutant to evaluate the response of contaminated aqueous samples. Since water strongly attenuates THz radiation, a reflection-mode THz-TDS configuration with a custom PTFE liquid cell is proposed to assess measurable changes in the reflected waveform and spectrum.

METHODS

Experimental setup

THz-TDS measurements were performed using a BATOP TDS-1008 spectrometer operated in reflection mode with an SHR reflection mount. The incident THz beam was focused and redirected toward the lower surface of the PTFE liquid cell placed on the sample plane. Deionized water and methylene-blue aqueous solutions were measured under identical acquisition conditions, using a time step of 0.055 ps, a temporal acquisition window from 260 to 360 ps, and an integration time of 0.5 s.

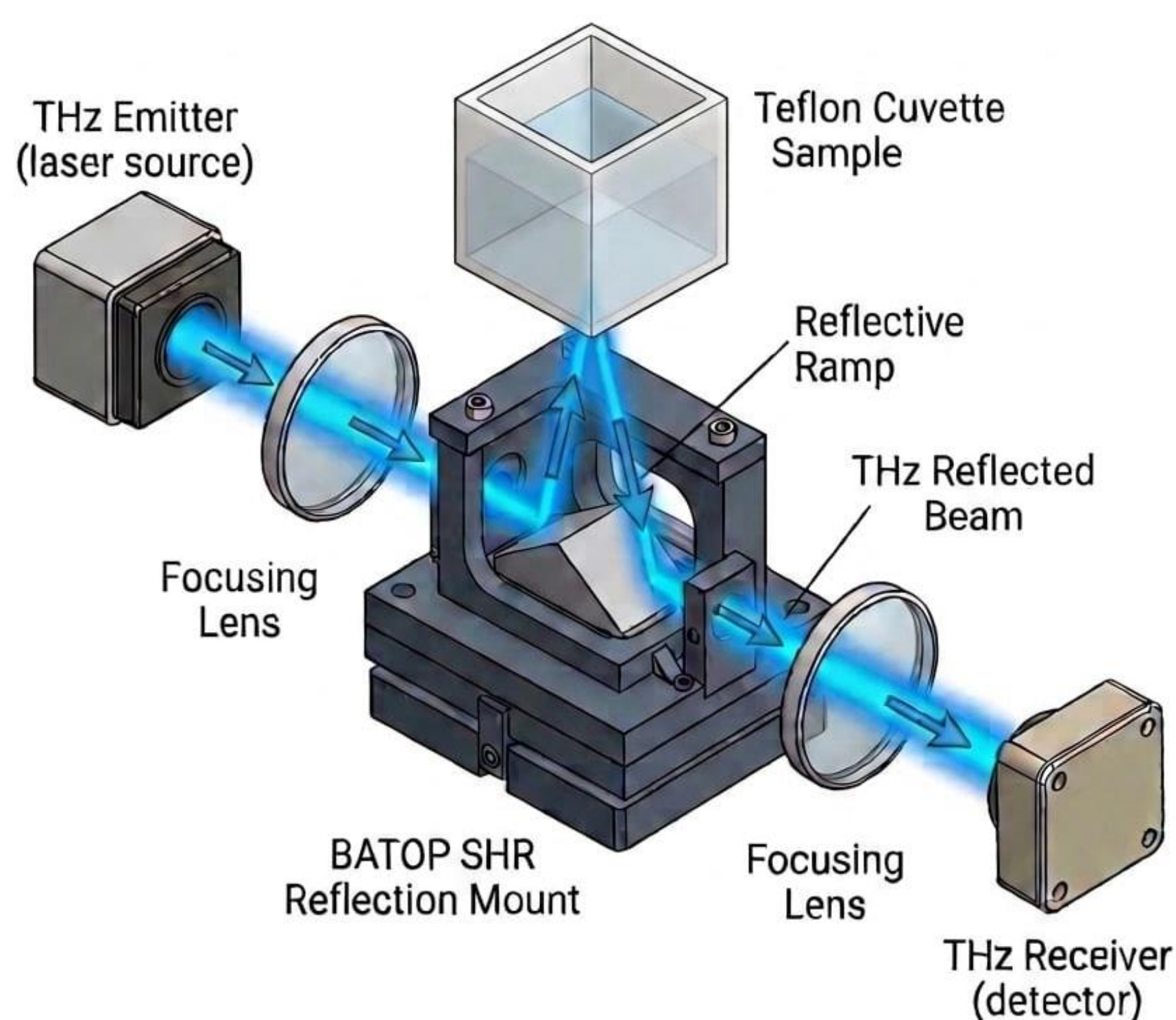


Figure 1. Experimental THz reflection spectroscopy setup used for water measurements.

Sample preparation

Methylene-blue aqueous samples were prepared from a 1000 ppm stock solution obtained by dissolving 1 g of methylene blue in 1 L of deionized water. Working solutions of 10, 25, 50, and 100 ppm were prepared by controlled dilution to a final volume of 100 mL. For each measurement, 1 mL of sample was transferred to the PTFE liquid cell and analyzed using the BATOP TDS-1008 spectrometer under unchanged acquisition conditions. Each concentration was measured three times.

RESULTS & DISCUSSION

Figure 2 shows the time-domain waveforms obtained for the empty PTFE, deionized water, and methylene-blue solutions at different concentrations. To isolate the effect of the dye, the deionized-water response was subtracted from each methylene-blue measurement. This analysis revealed two temporal windows with clear residual features at 281.3–284.0 ps and 293.3–295.3 ps, as shown in Figure 3(left).

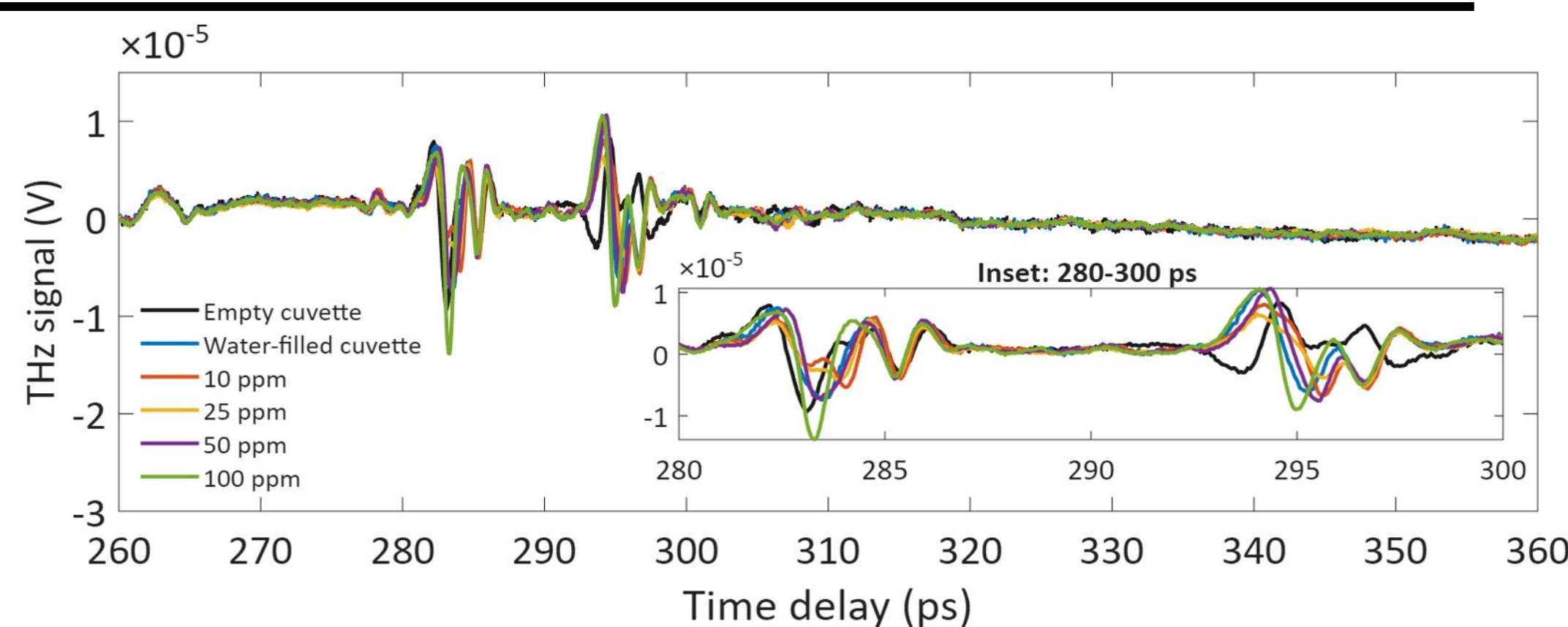


Figure 2. Time-domain THz waveforms measured in reflection mode for the empty PTFE, deionized water, and methylene-blue aqueous solutions at different concentrations.

The calibration curves shown in Figure 3(right) revealed a near-linear concentration-dependent temporal shift in both selected windows. The first exhibited the highest sensitivity, with -0.02113 ps/ppm and $R^2 = 0.969$, compared with -0.01806 ps/ppm and $R^2 = 0.960$ for Window 2. This indicates that the first temporal region is more sensitive to dye-induced changes in the effective PTFE–liquid interaction. Temporal positions are reported as mean $\pm$ standard deviation from three measurements, with a maximum standard deviation of 0.0317 ps.

Finally, the limit of detection (LoD) was estimated using the maximum standard deviation as a conservative noise estimate and the sensitivity. This resulted in LoD values of 4.50 ppm for Window 1 and 5.27 ppm for Window 2.

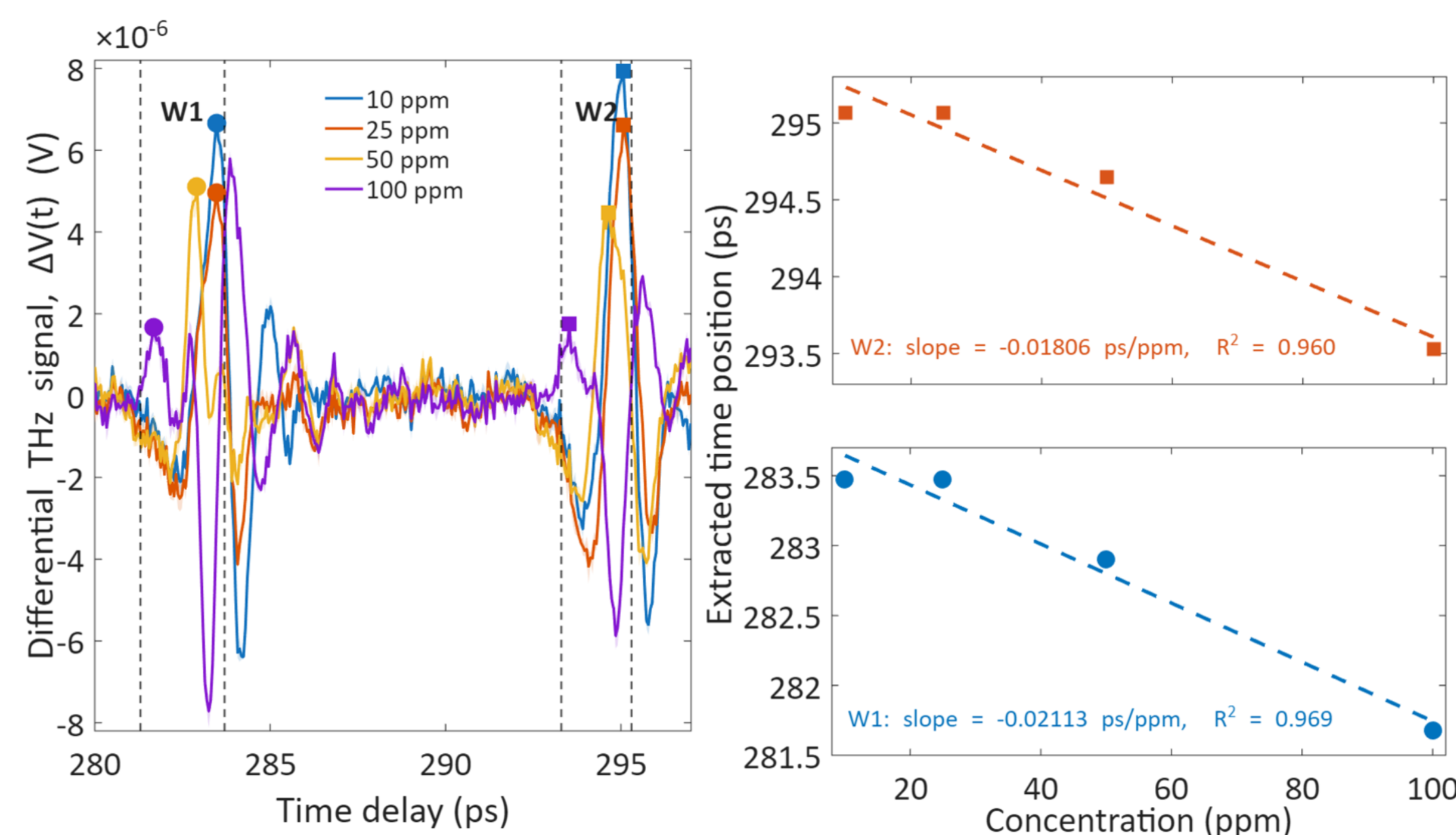


Figure 3. Residual time-domain signals obtained after subtracting the deionized-water response from each methylene-blue measurement, and calibration curves for the two selected temporal windows.

CONCLUSION

The proposed reflection-mode THz-TDS strategy proved to be suitable for analyzing highly absorbing aqueous samples. This approach shows potential as a rapid and non-destructive screening tool for dye-contaminated water and motivates further validation with lower concentrations and real environmental samples.

REFERENCES

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