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How to get Raman spectra harmonization from twinned devices

Raman spectroscopy is increasingly widespread in different industrial applications as it allows characterizing advanced materials in different industrial stages: from design and manufacturing, to performance, end of life and recycling, improving the quality of products and processes. Unlike the calibration protocols, the intercompatibility among different Raman devices in terms of comparability, reproducibility and reliability of the data, it is an aspect not sufficiently explored in this characterization technique [1,2]. For this reason, in this work, a harmonization protocol has been developed for the first time, that allows defining a correction factor (CF) to twin two different Raman spectrometers. This CF is a constant that includes all the differences that exist between both spectrometers such us spot size, density power, optical path, detector. From it, harmonized spectra measured from different Raman spectrometers have been obtained.
For the development of this protocol, a homogeneous reference sample with a high compositional control has been manufactured with a composite material of epoxy and 0.5% by wt. of anatase TiO_2 particles. The protocol consists of different steps for each Raman twinning, that allow obtain the CF calculating the slope of the regression line of the intensity of the main TiO_2 band at different laser powers in each Raman device.
The study was performed in two different devices with different optical paths and wavelengths. Figure 1 shows an example of $K_{0.5}Na_{0.5}O_3$ (KNN) spectra harmonization. In Figure 1a it can be seen the reference spectra (A) and the spectra to be harmonized (B) at different laser powers measured with a 785 nm laser showing different intensities. After multiplying the spectra B by CF, both spectra are harmonized in terms of intensities (Figure 1b). The similarity between reference and harmonized spectra is greater than 95% for all laser powers, proving that high quality of harmonization can be obtained with this new protocol.
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References

[1] A. Ntziouni, J. Thomson, I. Xiarchos, X. Li, M.A. Bañares, C. Charitidis, R. Portela, E. Lozano Diz, Appl. Spectrosc., 76 (2022) 747–772.
[2] B. Barton, J. Thomson, E. Lozano Diz, R. Portela, Appl. Spectrosc. 76 (2022) 1021–1041.

Figures

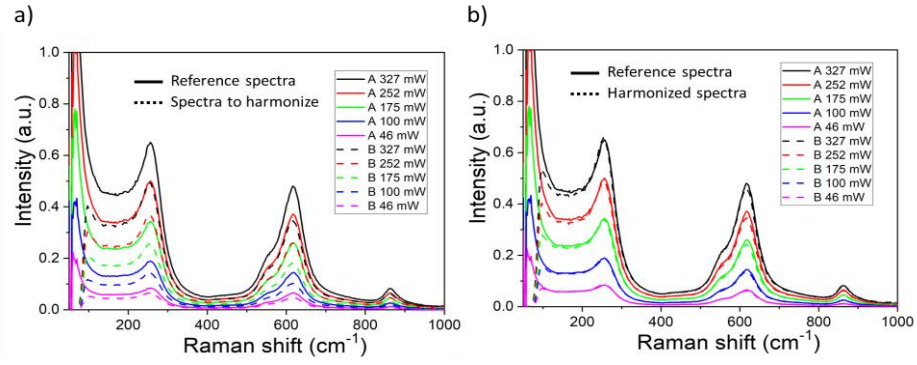

Figure 1: KNN spectra of spectrometer A and spectrometer B before (a) and after (b) Raman harmonization.