Light scattering geometry for Raman spectroscopy measurements. The case of lithium iron phosphate microparticles

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Raman microspectroscopy is a great tool to study particulate lithium battery materials of micron and submicron sizes. It allows to observe lithium ions deintercalation, to judge the heterogeneity of the sample, etc. But for a proper interpretation of experimental results, it is important to understand the geometry of laser radiation propagation in the object under study as accurately as possible.

Previously, we studied the locality of Raman spectra measurements and revealed a significant optical inhomogeneity for individual particles of lithium iron phosphate $LiFePO_4$ (LFP), a popular cathode material for lithium-ion batteries. The measurements revealed not only the dispersion of the radiation penetration depth for the transparent LFP, but also the enhancement of the signal of the Raman-active silicon substrate under the particle and the blocking of the response at its edges [1, 2].

In the current study, to more accurately interpret the results obtained, we performed modeling in the COMSOL Multiphysics software package and additional vertical Raman mapping of single LFP particles on a silicon substrate.

Although the amplitude of the main characteristic band of silicon substrate (at 521 cm^{-1}) was expected to reach the maximum value aside a particle, the performed measurements have demonstrated mainly the opposite results. Si band amplitude was about 1.5 to 2 times greater being focused on the substate with particle comparing with substrate without one (Figure 1). Response from Si substrate was blocked, but mainly at the particle edges, and this effect varied from particle to particle.

The present study provides insights into the light scattering in LFP single particles underlying the importance of their geometry, which helps to explain heterogeneity of the Raman signal of Si substrate. Also, while there are better techniques for amplifying the Raman signal, the study is relevant for interpreting measurements and understanding the region of signal generation.

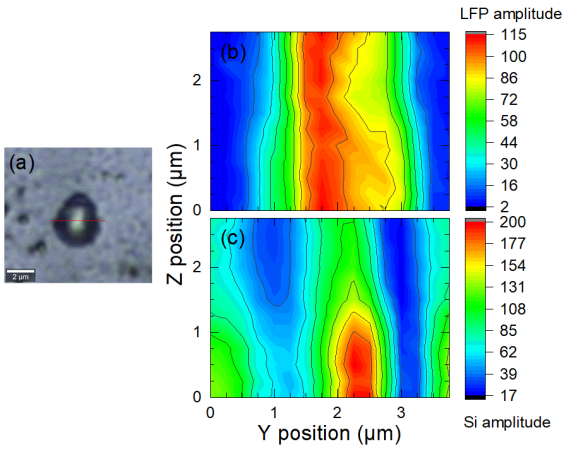

Figure 1. The optical image of LFP particle (a) with corresponding Raman mapping of amplitude of LFP band at 951 cm^{-1} (b) and Si band at 521 cm^{-1} (c) along red line.

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References

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