

Supporting information for:

Elucidating the origin of superior electrochemical cycling performance: new insights on sodiation-desodation mechanism of SnSb from *operando* spectroscopy

Marcus Fehse,^{*,†,‡,¶} Moulay T. Sougrati,^{§,||} Ali Darwiche,[§] Vincent Gabaudan,[⊥]
Camille La Fontaine,[#] Laure Monconduit,^{§,||,¶} and Lorenzo Stievano^{*,§,||,¶}

[†]Dutch-Belgian (DUBBLE), ESRF-The European Synchrotron, CS 40220, 38043 Grenoble Cedex 9, France.

[‡]Faculty of Applied Sciences, Delft University of Technology, Delft, Netherlands.

[¶]Alistore European Research Institute, Université de Picardie Jules Verne, 33 rue Saint Leu, 80039 Amiens Cedex, France.

[§]Institut Charles Gerhardt - AIME (CNRS UMR 5253), Université de Montpellier, CC 1502, Pl. E. Bataillon, 34095 Montpellier Cedex 5, France.

^{||}Reseau sur le Stockage Electrochimique de l'Energie (RS2E), CNRS FR3459, 33 Rue Saint Leu, 80039 Amiens Cedex, France.

[⊥]Institut Charles Gerhardt - AIME (CNRS UMR 5253), Université de Montpellier, CC 1502, Pl. E. Bataillon, 34095 Montpellier Cedex 5, France.

[#]Synchrotron Soleil, L'Orme des Merisiers, Saint-Aubin, BP 48, 91192 Gif-sur-Yvette Cedex, France.

E-mail: marcus.fehse@esrf.fr; lorenzo.stievano@umontpellier.fr

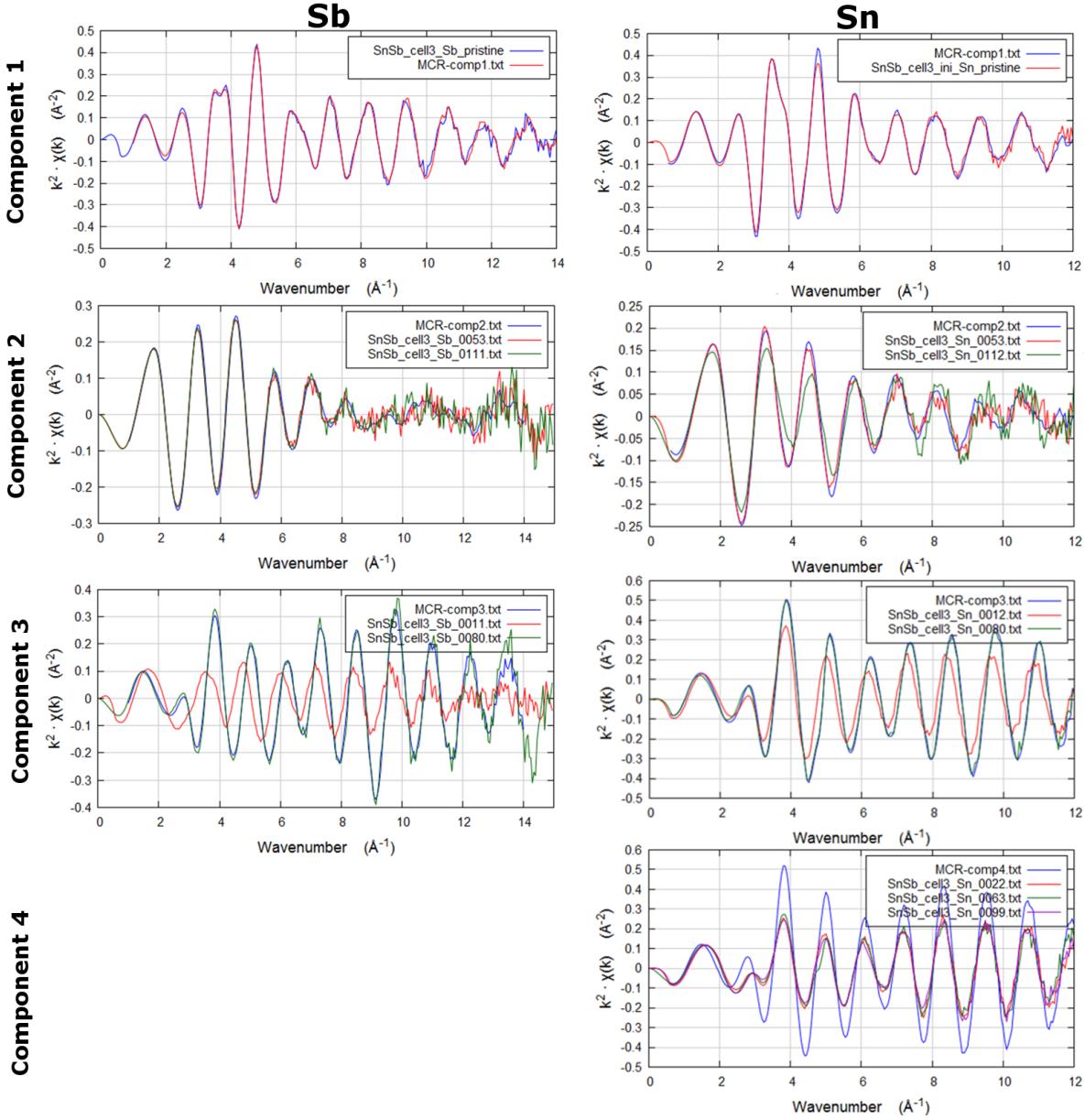


Figure S1: EXAFS signal of components obtained via MCR-ALS compared to specific experimental spectra,

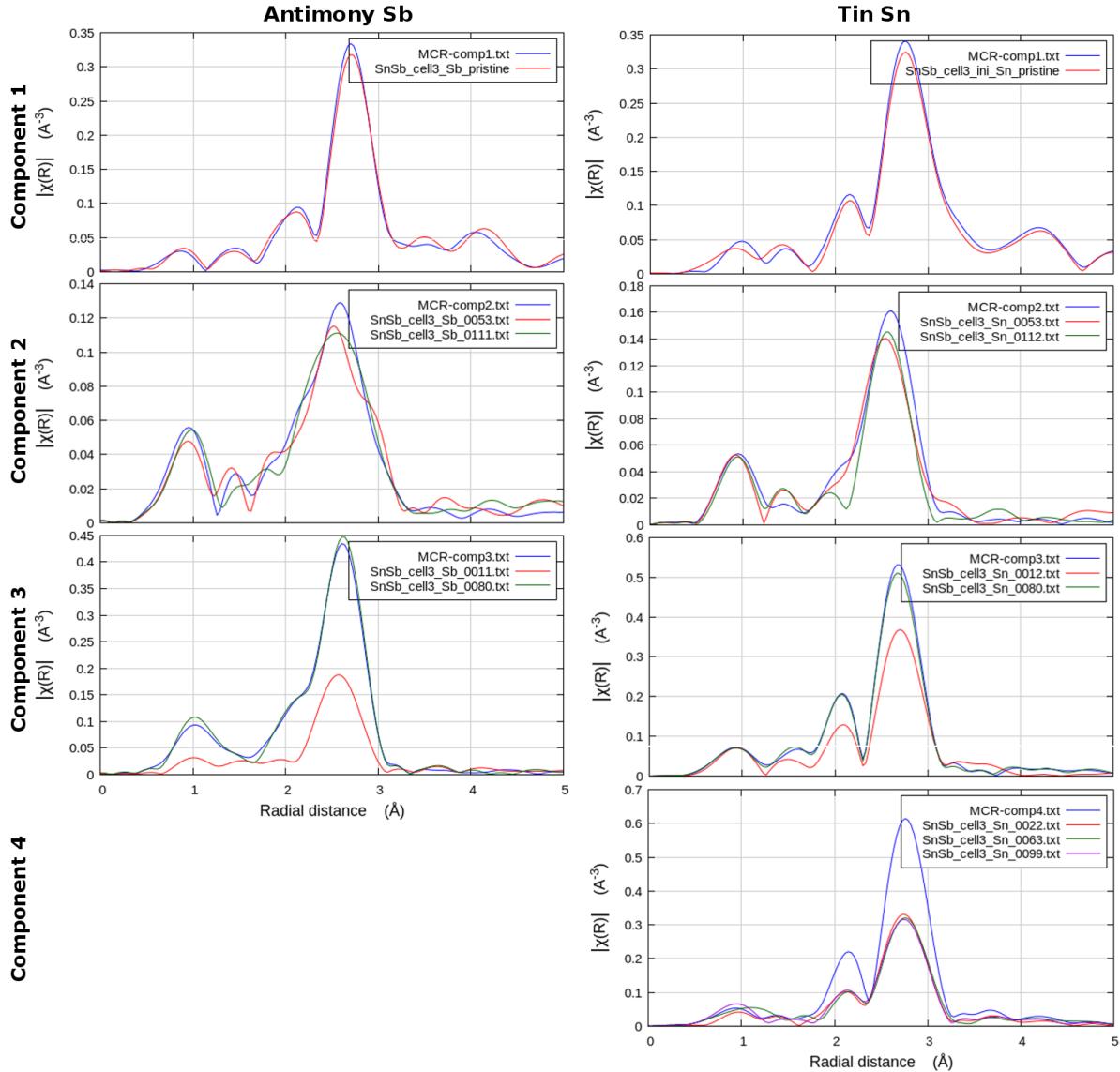


Figure S2: EXAFS real space components obtained via MCR-ALS compared to specific experimental spectra, i.e #53 = End of first discharge (EOD), #80 = end of first cycle (EOC), for Sb (*left*) and Sn (*right*).

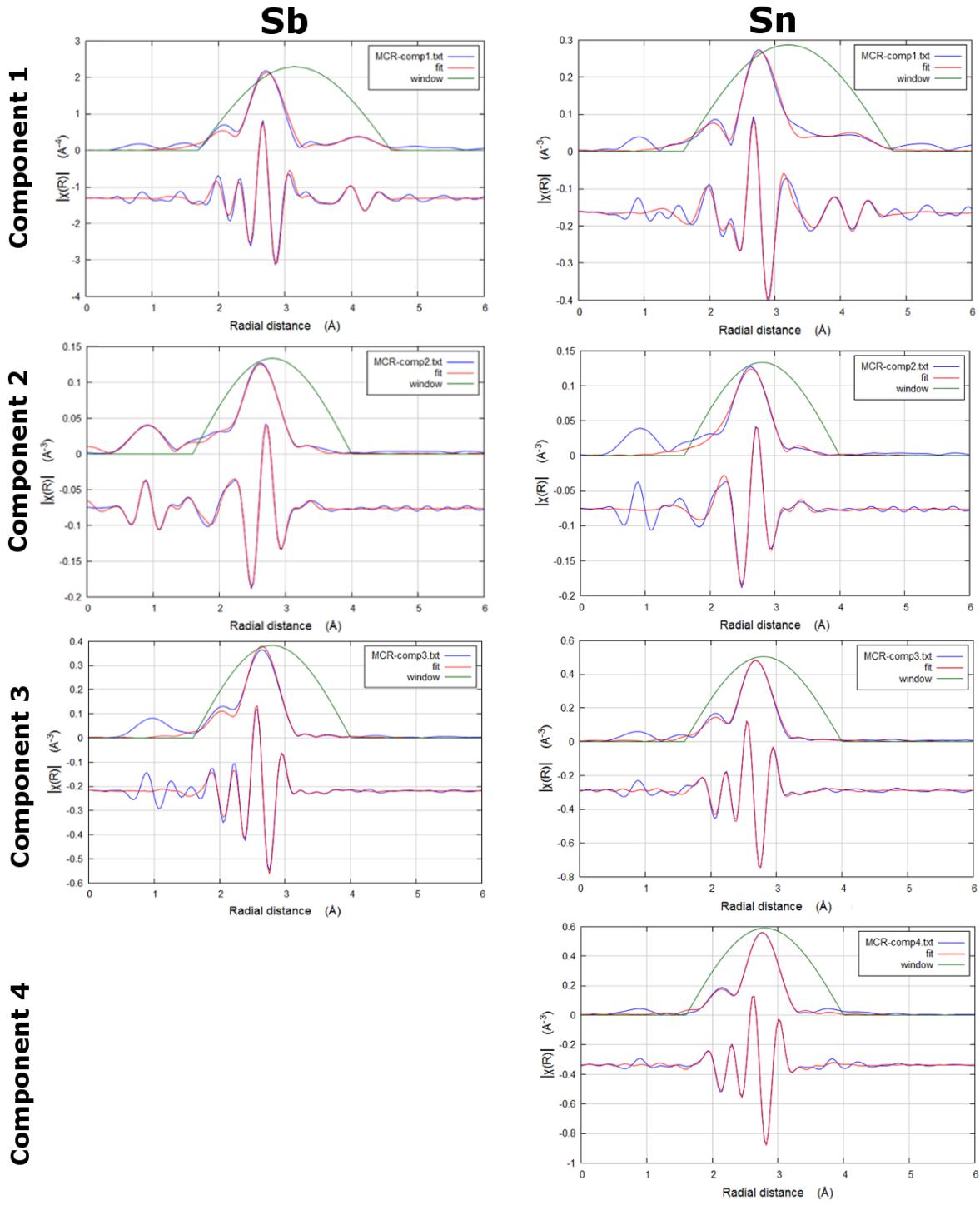


Figure S3: EXAFS signal of components obtained via MCR-ALS and fit in R-space

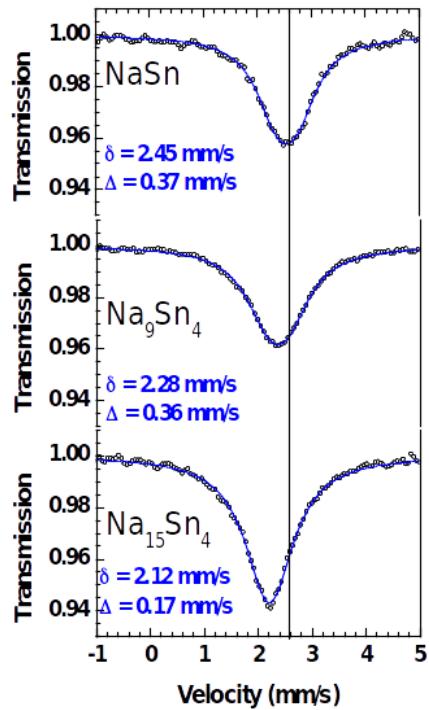


Figure S4: Mössbauer spectra and fit of sodiated tin reference samples NaSn, Na₉Sn₄, and Na₁₅Sn₄ prepared via ball milling.

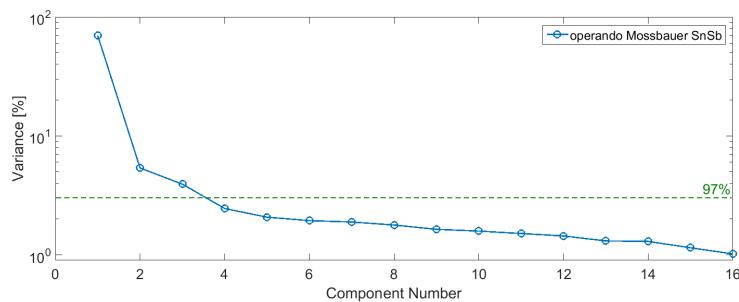


Figure S5: Variance plot obtained through PCA analysis of the ¹¹⁹Sn Mössbauer spectra during sodiation of SnSb. Components below 3% are considered to originate from instrumental noise.

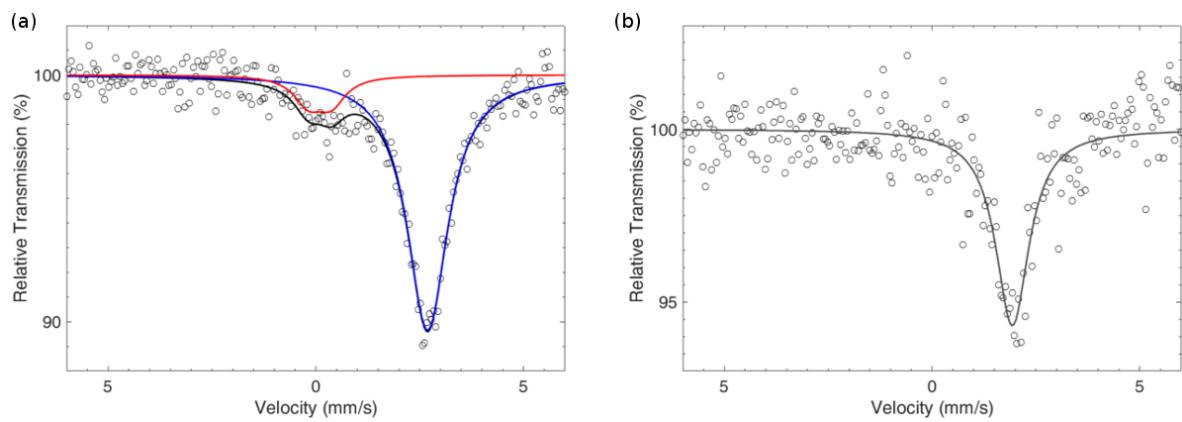


Figure S6: Pure component Mössbauer spectra 1 and 2 obtained via MCR and fit depicted in (a) and (b), respectively.