Electronic Supplementary Material (ESI) for Analyst.

Supplementary data

Title: Combined use of quantitative ED-EPMA, Raman microspectrometry, and ATR-FTIR imaging techniques for the analysis of individual particles

Authors: Hae-Jin Jung[1], Hyo-Jin Eom[1], Hyun-Woo Kang[1], Myriam Moreau[2], Sophie Sobanska[2], and Chul-Un Ro[1,*]

[1] Department of Chemistry, Inha University, Yonghyun Dong, Nam Gu, 402-751, Incheon, South Korea

[2] Laboratoire de Spectrochimie Infrarouge et Raman, UMR CNRS 8516, Université de Lille 1, Bât. C5, 59655 Villeneuve d'Ascq Cedex, France

A summary of the supporting information:

Tables S1 and Figures S1-S13

Table S1. Raman and ATR-FTIR peaks of observed chemical species.

Chemical species	Raman and IR peaks (in cm^{-1})[ref.]	
Anhydrite	**Raman peaks [1]**	415, 497, 608, 626, 675, 1016, 1111, 1128, 1160
	ATR-FTIR peaks [2]	1133, 1096, 1016
Gypsum	**Raman peaks [3]**	415, 494, 620, 670, 1008, 1136
	ATR-FTIR peaks [2]	3505, 3400, 1682, 1618, 1104, 1004
Calcite	**Raman peaks [4]**	282, 713, 1087, 1437, 1748
	ATR-FTIR peaks [2]	1792, 1392, 866, 709
Quartz	**Raman peaks [5]**	128, 206, 264, 355, 394, 401, 464, 697, 807, 1161
	ATR-FTIR peaks [2]	1162, 1057, 796, 777
Sodium sulfate	**Raman peaks [6]**	450, 466, 620, 632, 647, 993, 1101, 1131, 1152
	ATR-FTIR peaks [7]	1102
Sodium nitrate	**Raman peaks [8]**	724, 1068, 1385
	IR peaks [9]	1789, 1349, 834
K-feldspar	**Raman peaks [10]**	256, 265, 286, 332, 373, 403, 452, 475, 513, 585, 651, 749, 813, 993, 1124, 1137
	ATR-FTIR peaks [2]	1133, 1048, 1006, 771, 727

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Figure S1. (A) Secondary electron image (SEI) from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1100 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 12 gypsum particles on Al foil.

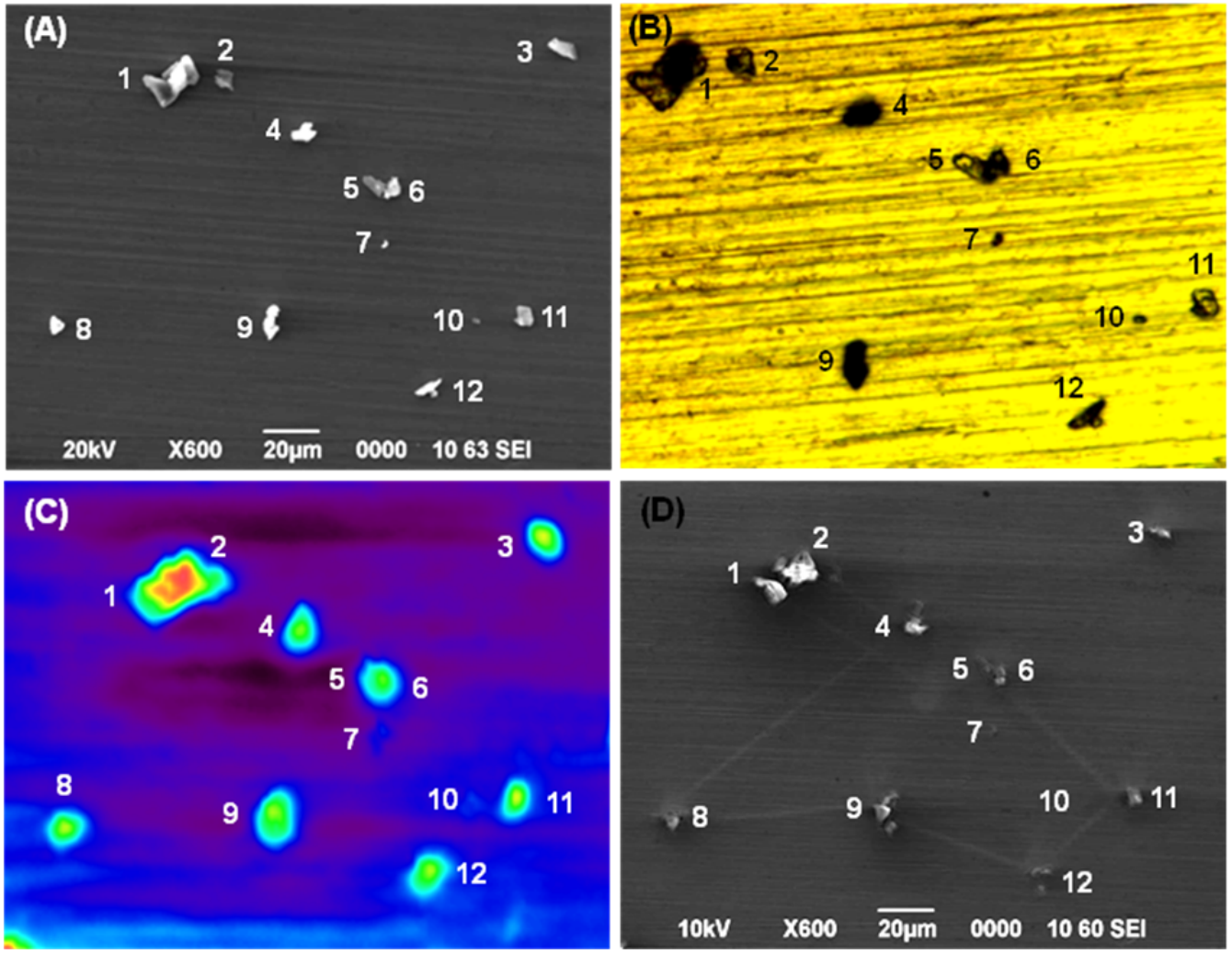

Figure S2. (A) SEI from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1390 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 15 calcite particles on Ag foil.

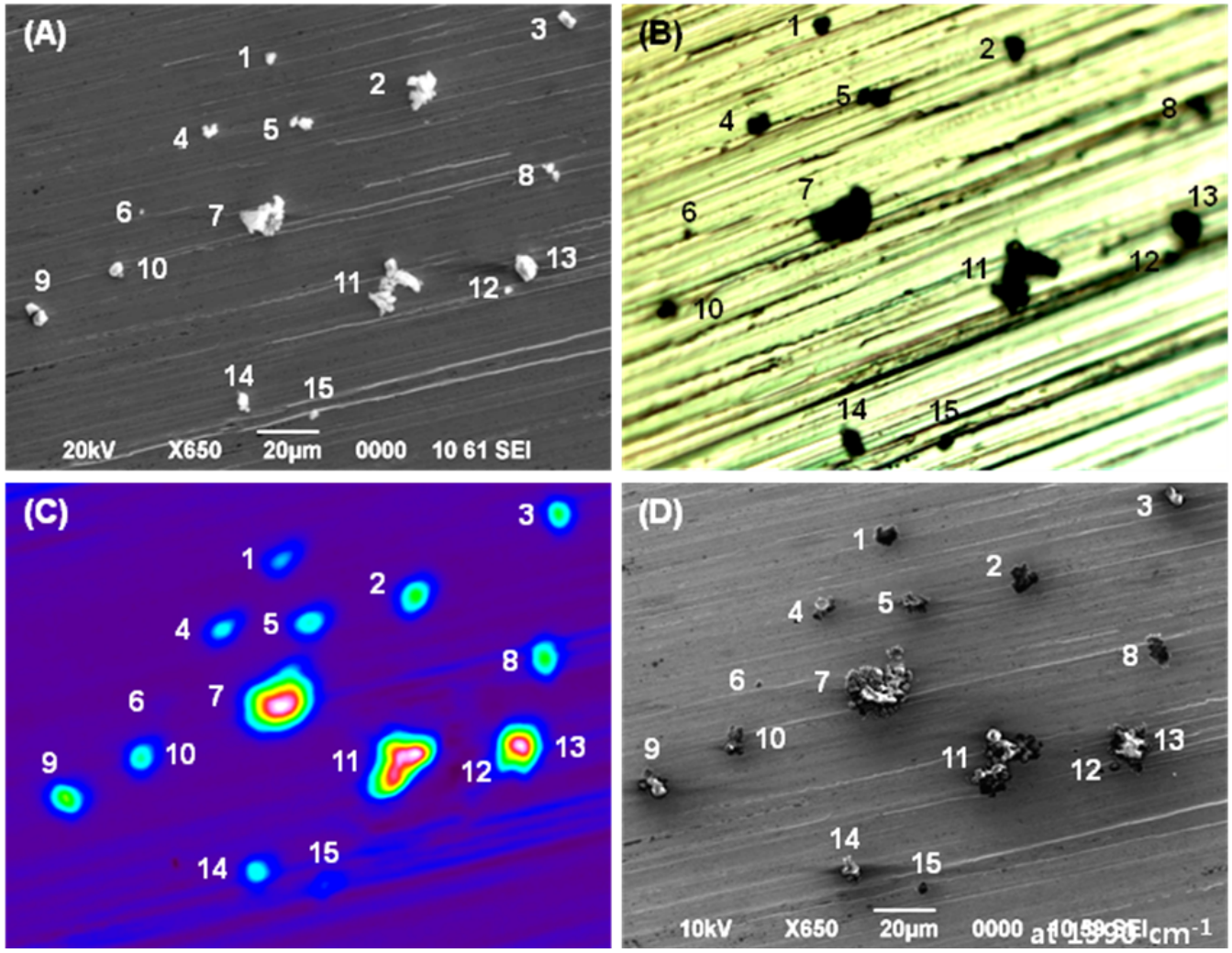

Figure S3. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of calcite particle #13, respectively, and (B) its X-ray spectrum, (C) Raman spectrum, and (D) ATR-FTIR spectrum.

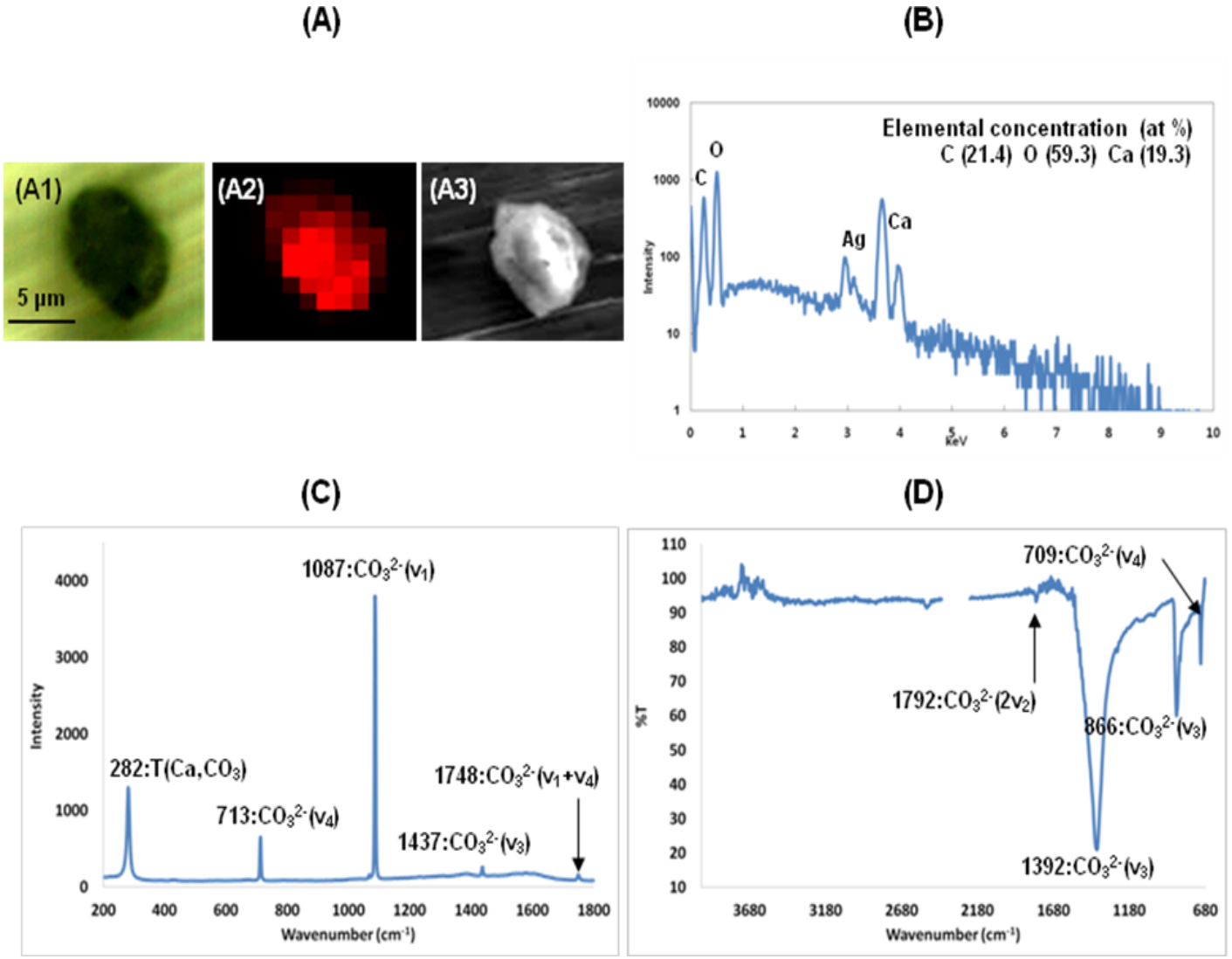

Figure S4. (A) SEI from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1060 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 25 quartz particles on Ag foil.

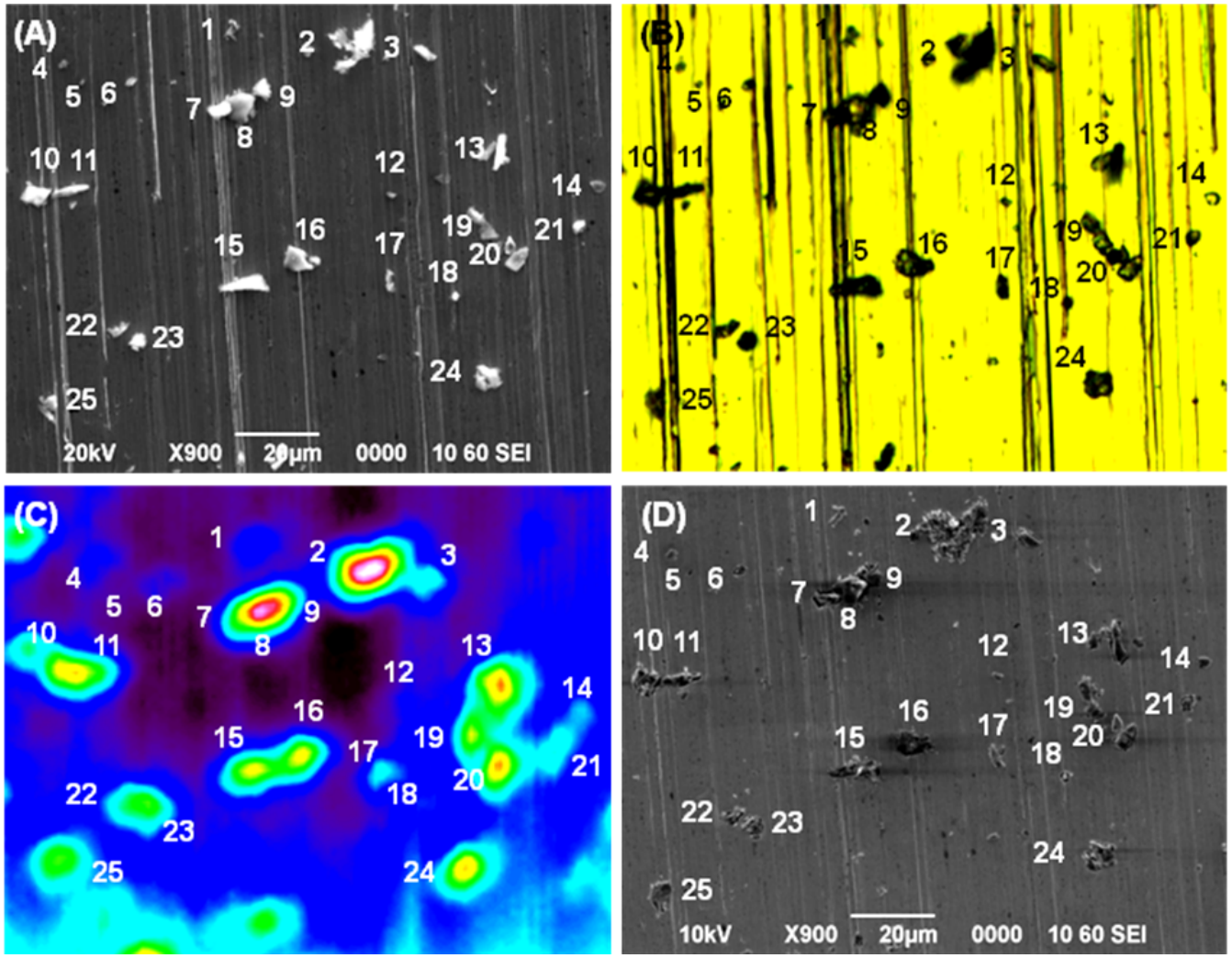

Figure S5. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of quartz particle #15, respectively, and (B) its X-ray spectrum, (C) Raman spectrum, and (D) ATR-FTIR spectrum.

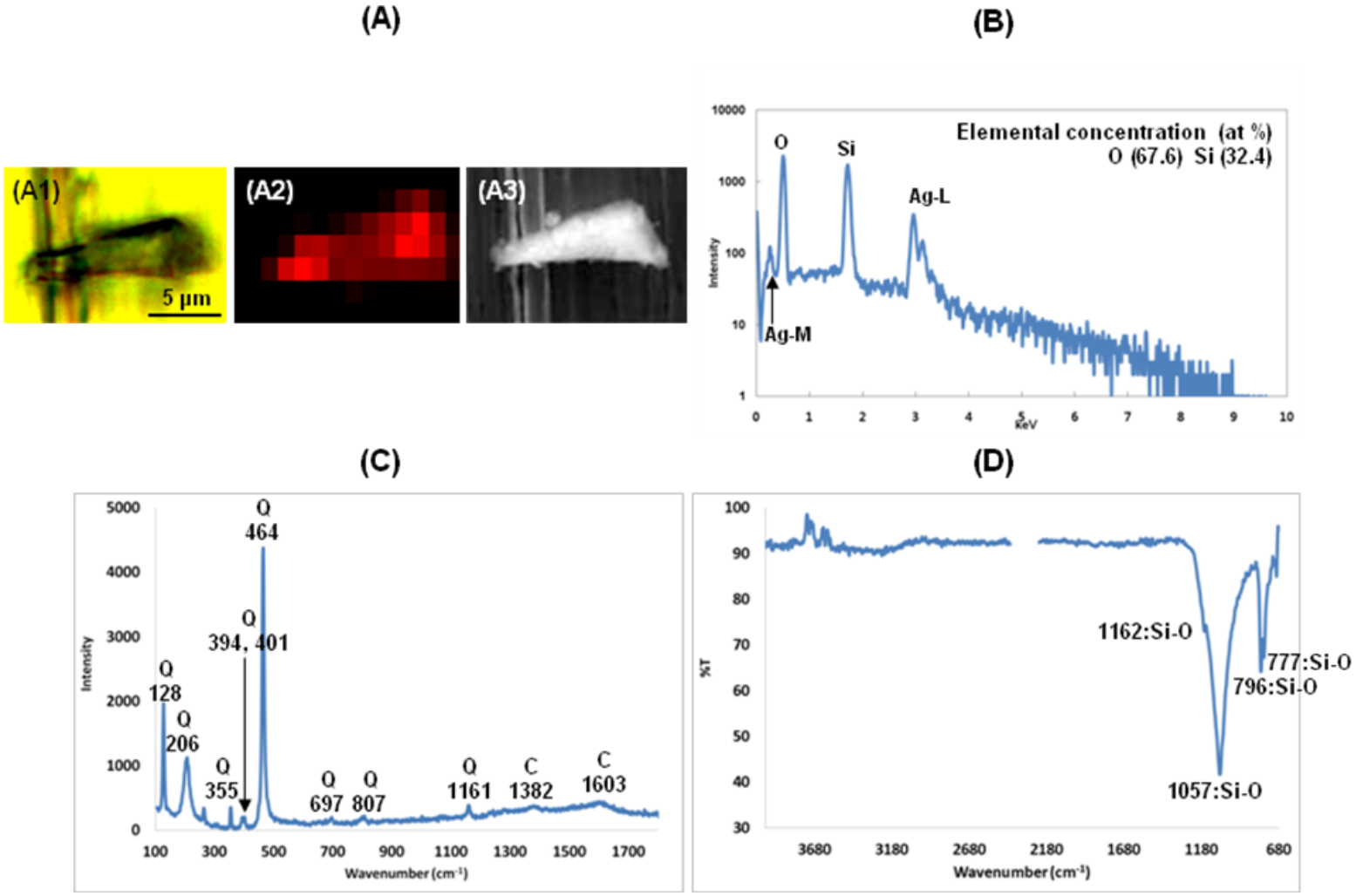

Figure S6. (A) SEI from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1100 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 10 sodium sulfate particles on Al foil.

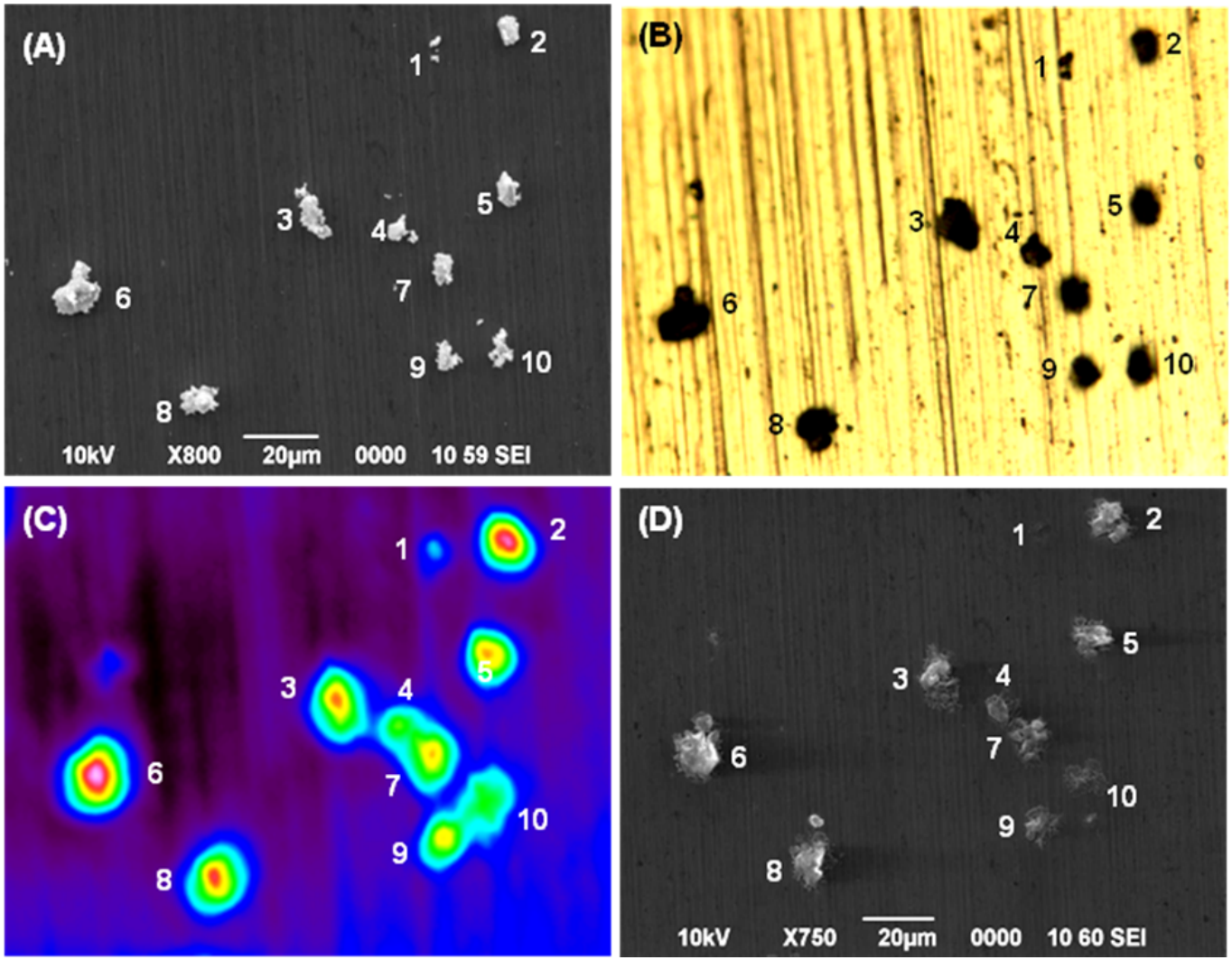

Figure S7. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of sodium sulfate particle #2, respectively, and (B) its X-ray spectrum, (C) Raman spectrum, and (D) ATR-FTIR spectrum.

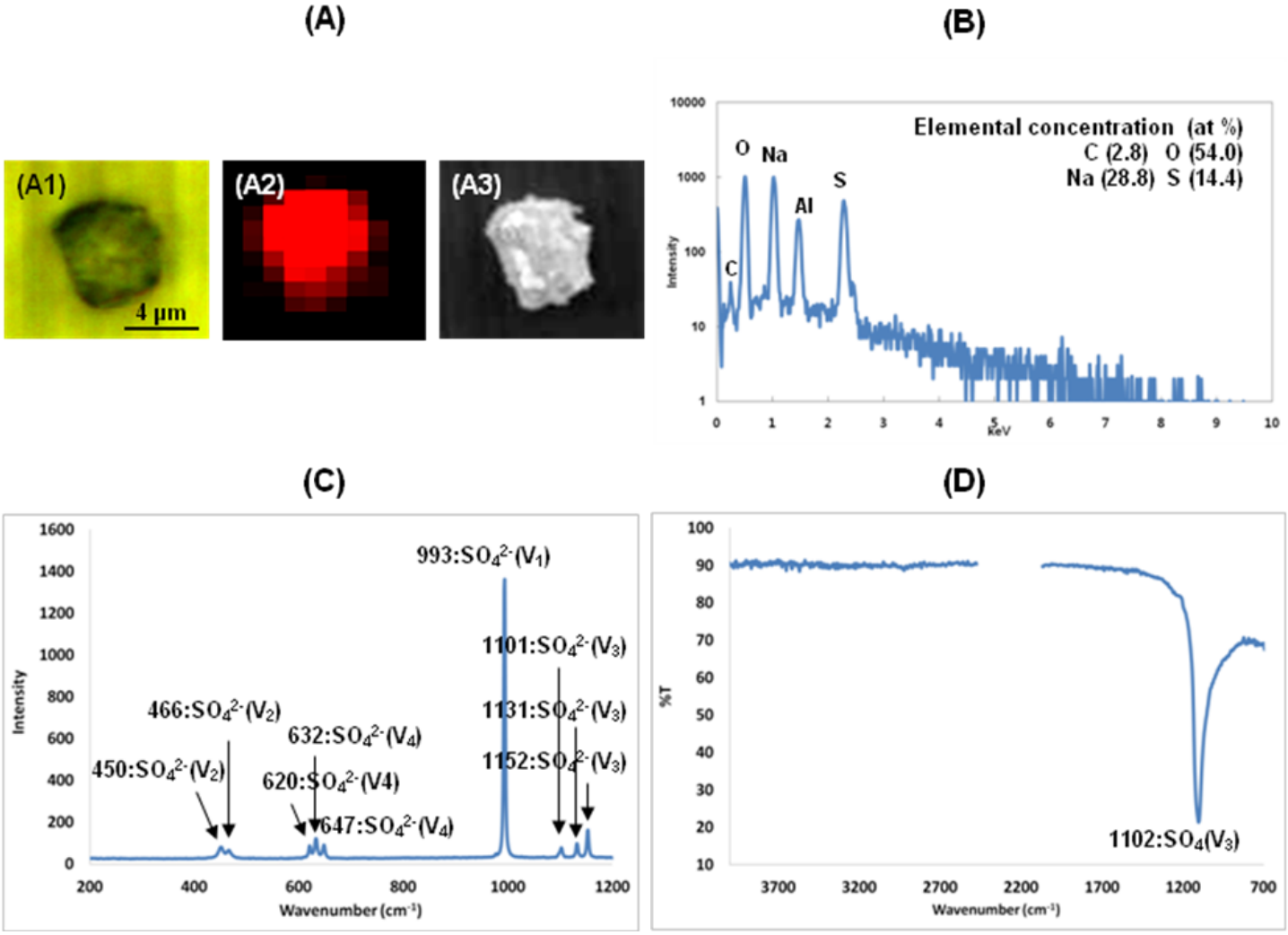

Figure S8. (A) SEI from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1350 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 16 sodium nitrate particles on Al foil.

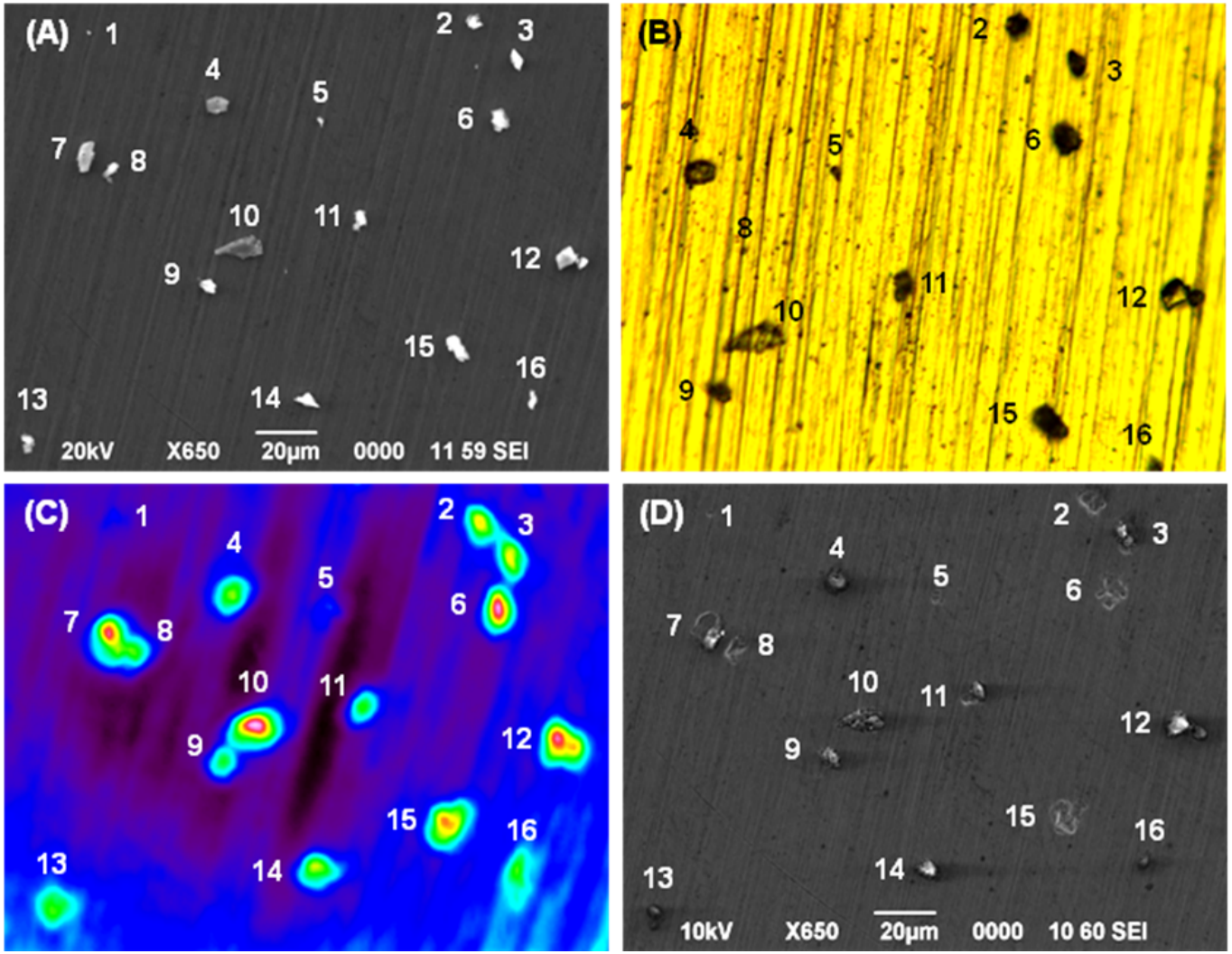

Figure S9. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of sodium nitrate particle #12, respectively, and (B) its X-ray spectrum, (C) Raman spectrum, and (D) ATR-FTIR spectrum.

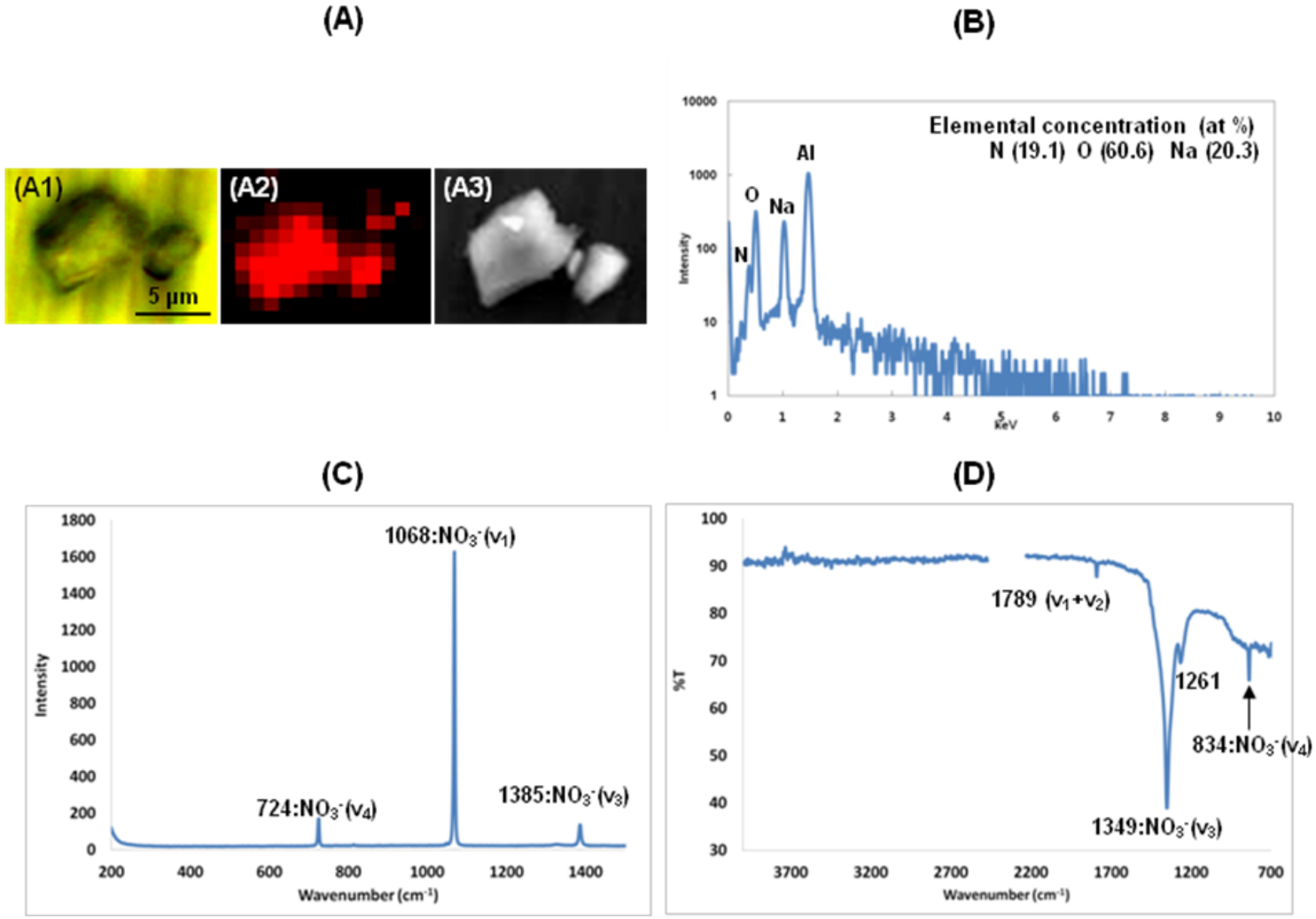

Figure S10. (A) SEI from SEM before ATR-FTIR measurement, (B) optical image from Raman spectrometer, (C) ATR-FTIR image at 1010 cm^{-1}, and (D) SEI after ATR-FTIR measurement of the same 19 K-feldspar particles on Al foil.

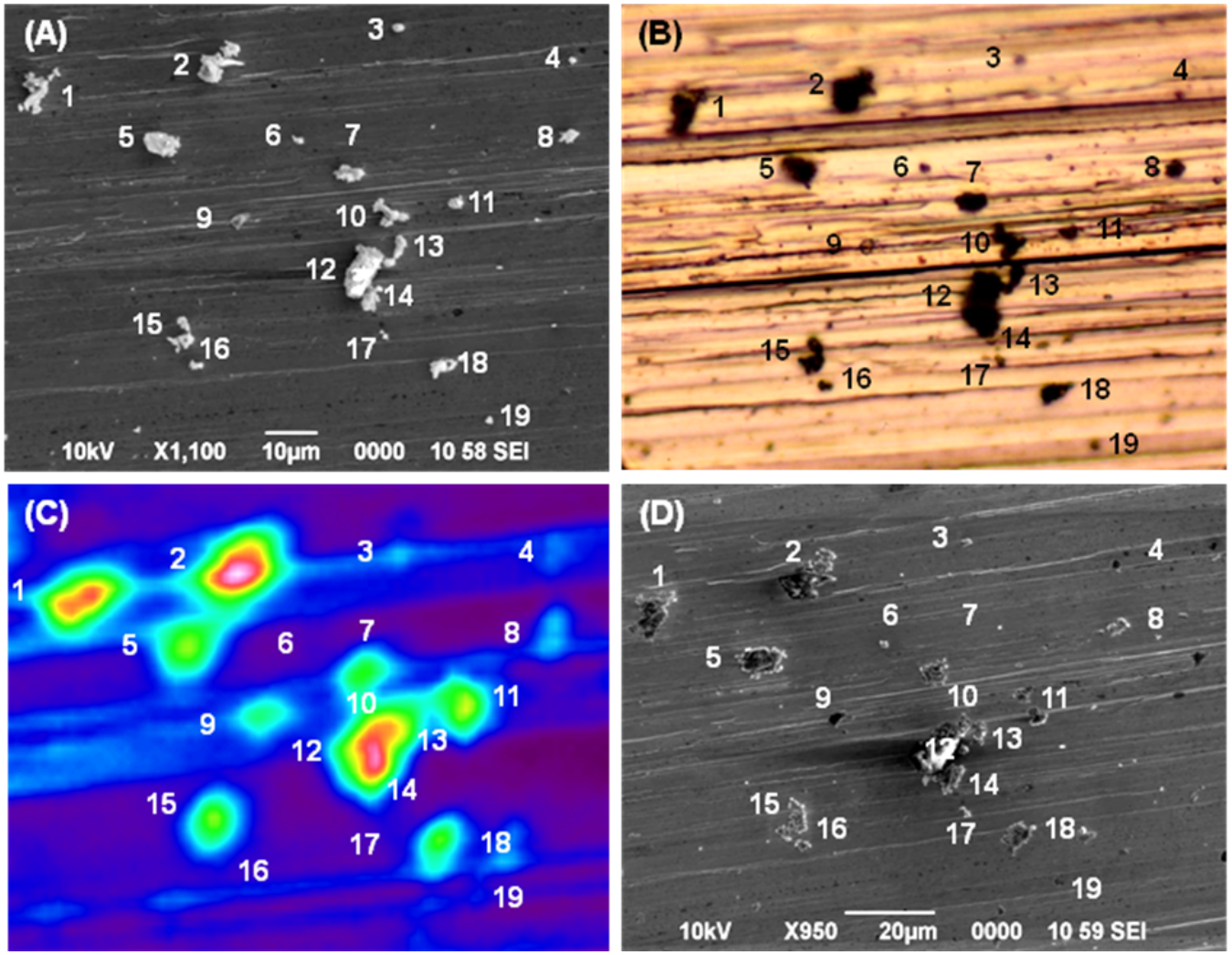

Figure S11. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of K-feldspar particle #15, respectively, and (B) its X-ray spectrum, (C) Raman spectrum, and (D) ATR-FTIR spectrum.

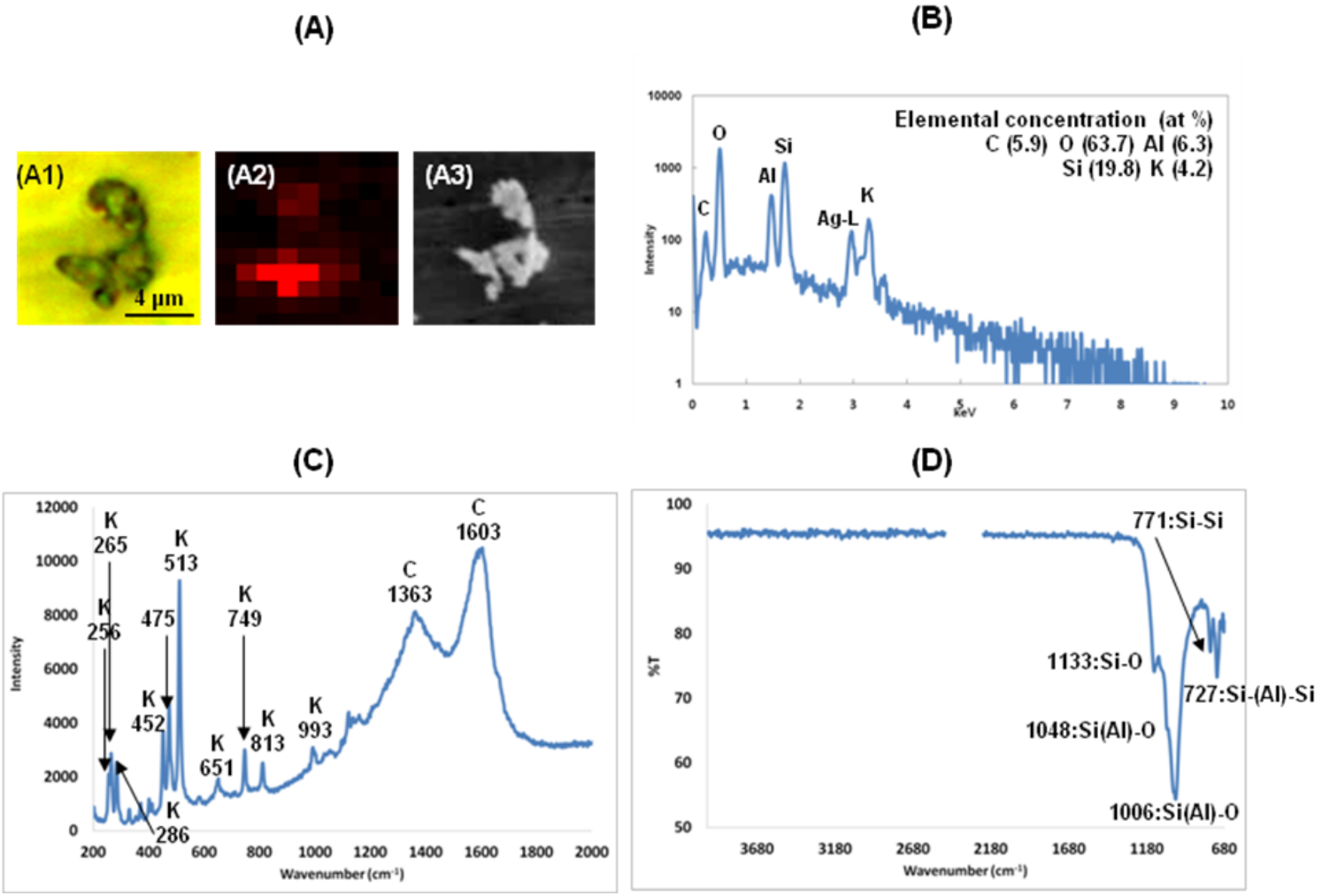

Figure S12. (A) Optical images from Raman spectrometer (A1), corresponding Raman images ((A2), (A3), and (A4)) of standard anhydrite particles #3 and #4, (B) ATR-FT-IR images ((B1) at 1090 cm^{-1} and (B2) at 1400cm^{-1}) of the anhydrite particles and (C) X-ray spectrum, (D) Raman spectra, and (E) ATR-FT-IR spectra of particle #4, respectively.

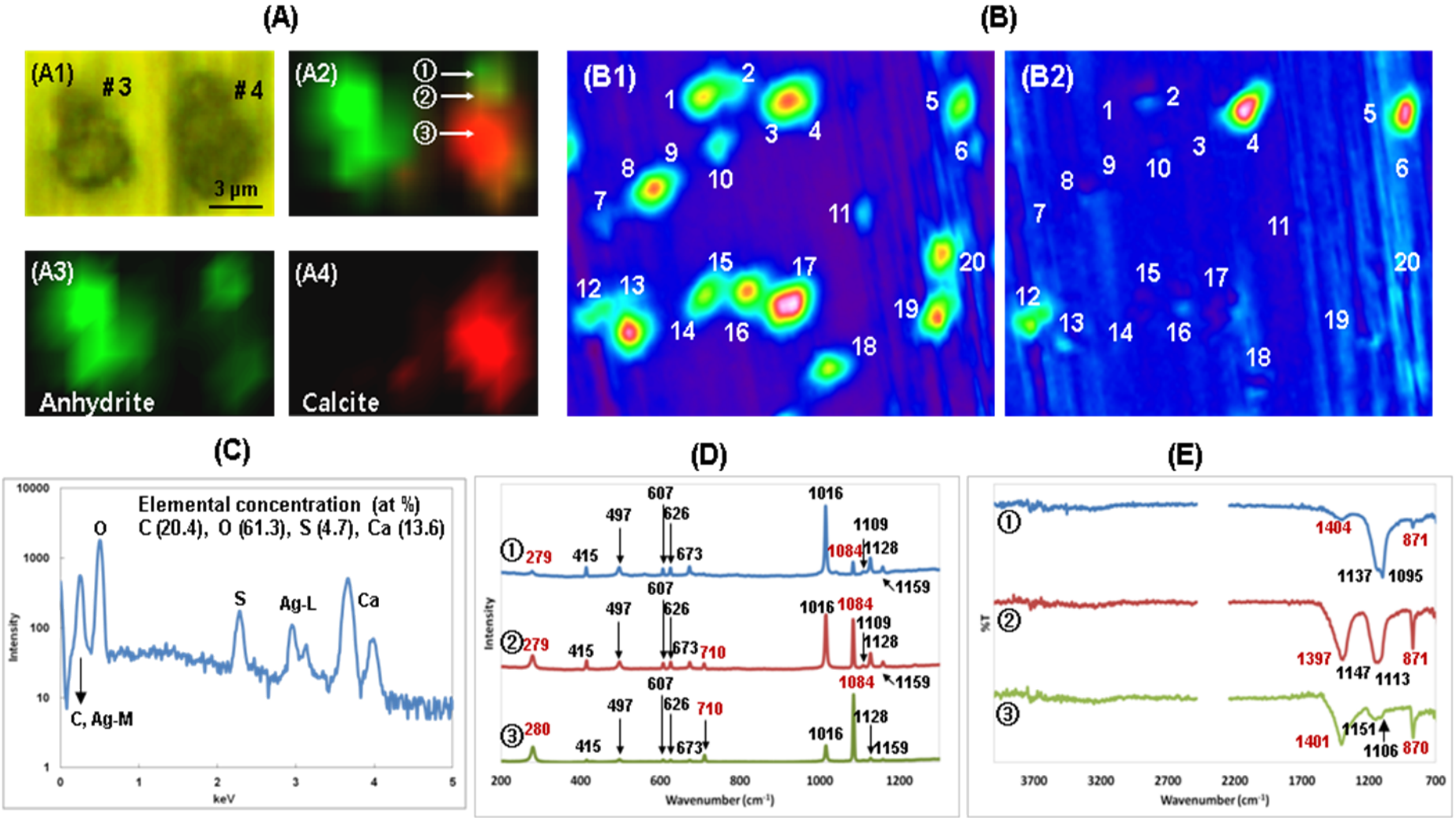

Figure S13. (A1) Optical image from Raman spectrometer, (A2) corresponding Raman image, and (A3) SEI of a gypsum particle (particle #9 in Figure S1) mixed with anhydrite, and (B) its X-ray spectrum, (C) Raman spectra, and (D) ATR-FTIR spectra.