**Supplementary materials**

**Unlocking the Potential of Chemically Modified Carbon Gels in Gallic Acid Adsorption**

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**FTIR band assignation table**

**Table S1.** FT-IR spectra of the samples. Band assignment.

|  |  |  |
| --- | --- | --- |
| Wavenumber (cm-1) | Assignmenta | Atomic grouping |
| 3650-3200 | ν(O-H) | Hydroxy group, H-bonded OH stretch |
| ν(N-H) | Primary amine, NH stretch |
| 3000-2800 | ν(C-H) | Hydrocarbons (aliphatics, olefinic, and aromatic) |
| 1770-1650 | ν(C=O) | Carbonyl compounds |
| 1700-1500 | ν(C=C) | Olefinic and aromatic structures |
| 1480-1400 | δ(C-H) | Aliphatic structures |
| 1450-1200 | δ(C-H) | Olefinic and methyl groups |
| δ(O-H) | Primary or secondary alcohol and carboxylic acid |
| 1300-1200 | ν(C-O) | Ether structures and phenol |
| 1210-1100 | Tertiary alcohol |
| 1120-1070 | Secondary alcohol |
| 1075-1000 | Primary alcohol |
| 900-700 | γ(C-H) | Aromatic structure |

**Kinetic models**

The kinetic data were fitted to the pseudo-first-order (Lagergren), pseudo-second-order (Ho and McKay), and Weber and Morris kinetic models. The pseudo-first-order equation rearranged to a linear form is usually written as Equation (1):

(1)

Where qe and qt are the amounts of GA adsorbed at equilibrium and at time t (mg g-1), respectively, and K1 is the pseudo-first-order rate constant (h-1). The representation of log(qe - qt) versus t should be a straight line with slope log qe and intercept -K1/2.303.

Assuming that the adsorption capacity is proportional to the number of active sites occupied on the surface of the adsorbent, the linear form for the pseudo-second-order reaction is written as equation (2):

(2)

Where qe and qt have the same meaning as in the previous model, and K2 is the rate constant of pseudo-second-order adsorption (g mg-1 h-1). Here, the plot of t/qt versus t should generate a linear relationship, from which qe and K2 can be obtained from the slope and the intersection of the plot.

The model proposed by Weber and Morris allows us to know if the limiting step of the adsorption process is intraparticle diffusion. This model is not strictly kinetic but decides whether the adsorption rate depends on mass transfer within the adsorbent particle or on other factors. The equation of this model in linear form is written as equation (3):

(3)

Where Kid is the intraparticle diffusion rate constant (mg g-1 h-1/2), te is the equilibrium time (h-1), and C is the intercept with the vertical axis (mg g-1). This parameter gives an idea of the value of the boundary layer. The plot of qt versus t1/2 should provide a straight line in which Kid and C can be obtained from the slope and the intersection.

**Isotherm models**

The Langmuir and Freundlich isotherm models analyzed the adsorption of GA under equilibrium conditions. The isotherm model proposed by Langmuir admits that the solid has a limited adsorption capacity, where molecules are adsorbed on well-defined, energetically equivalent sites far enough away from each other not to allow interaction between molecules adsorbed on adjacent sites. Langmuir linear form is written as equation (4):

(4)

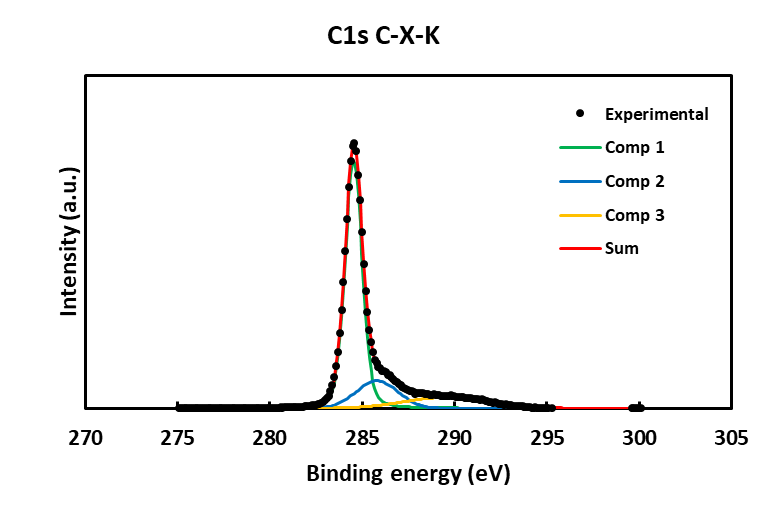
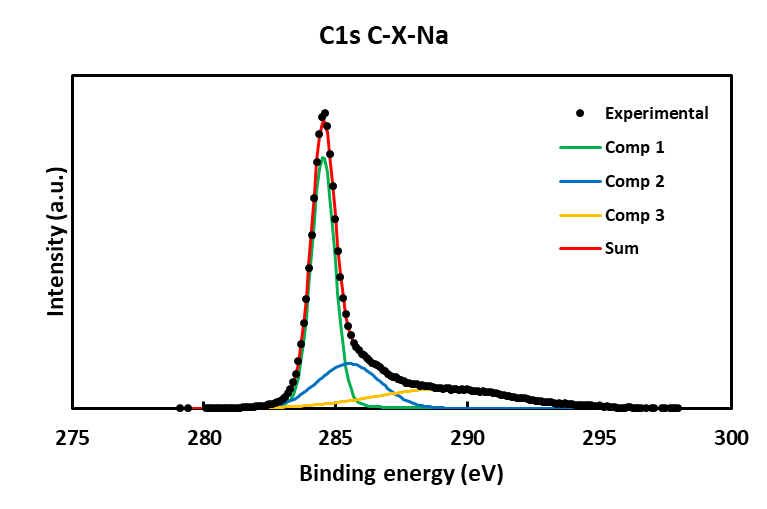
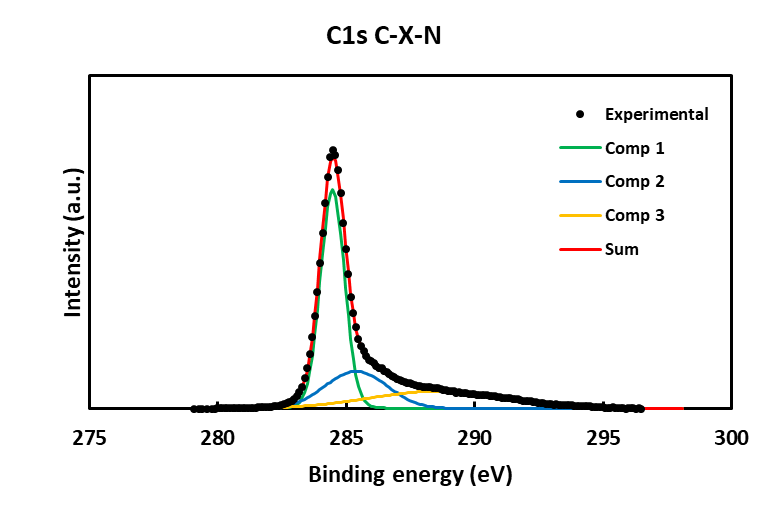
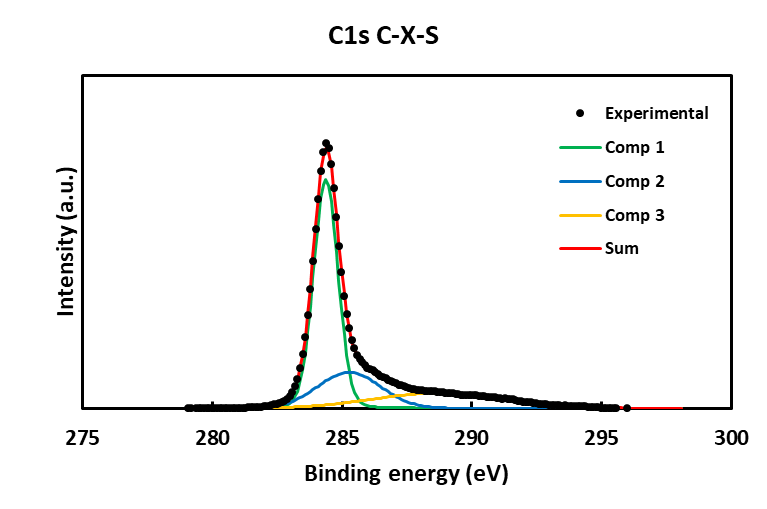
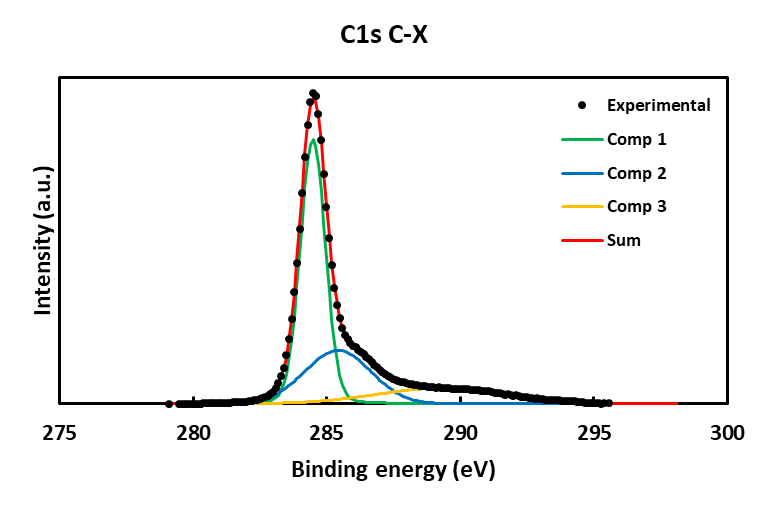
Where Ce is the equilibrium concentration in the liquid phase (mg L-1), qe is the amount adsorbed per unit of adsorbent mass (mg g-1), Sm is the constant related to the maximum adsorption capacity (mg g-1), and KL is the Langmuir constant associated with the intensity of adsorption (L mg-1). The representation of Ce/qe against Ce generates a straight line; thus, from the slope and the intersection of the graph, 1/Sm and 1/SmKL can be obtained.

The Freundlich isotherm arises to explain adsorption in multilayers with interaction between adsorbed molecules. The application of this model suggests that the adsorption energy decreases exponentially once the adsorption active sites are complete. This model applies to adsorption on heterogeneous surfaces with a uniform energy distribution and reversible adsorption. The equation describing the isotherm is given in equation (5):

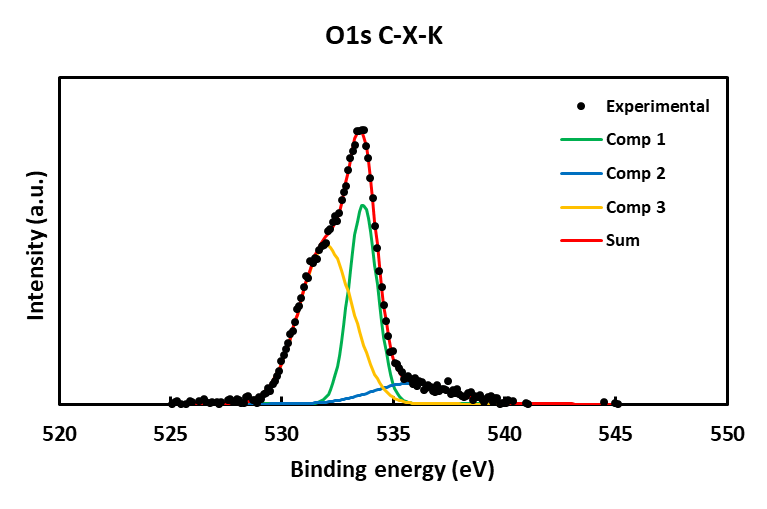
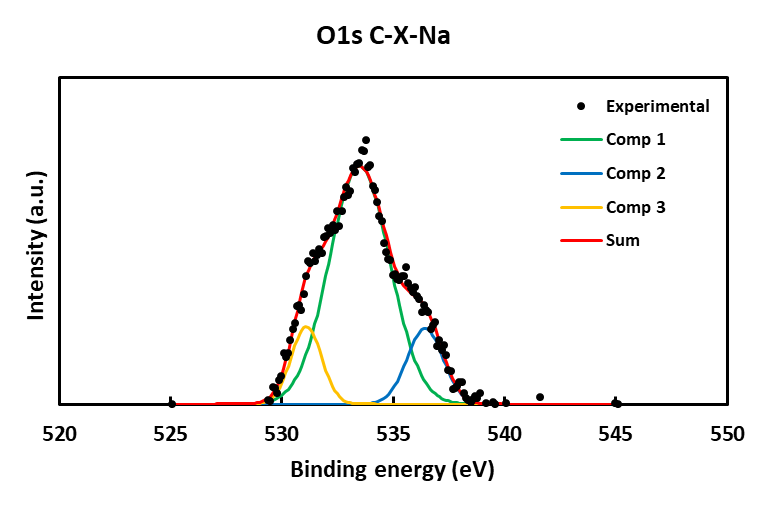
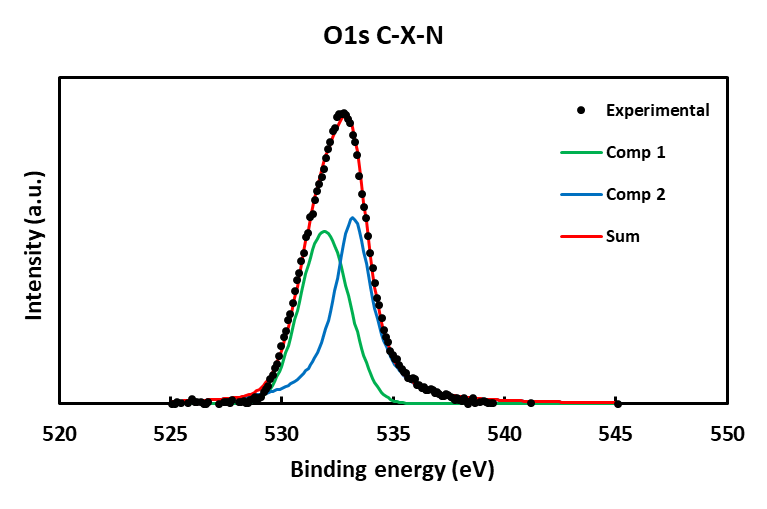
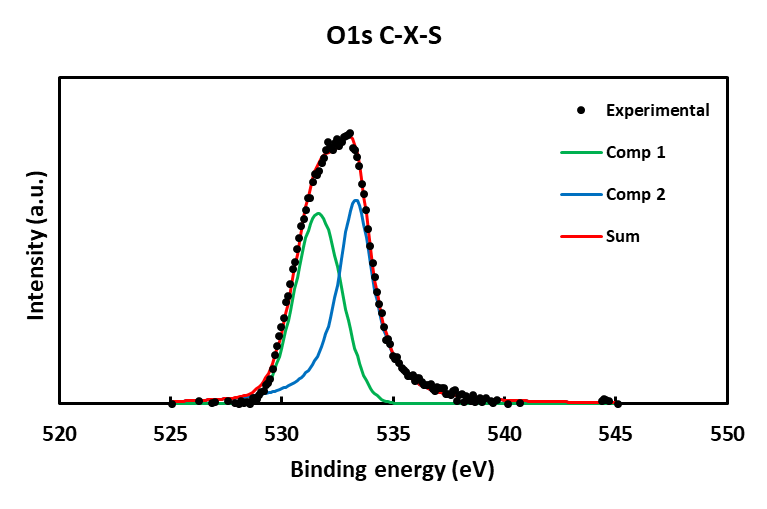
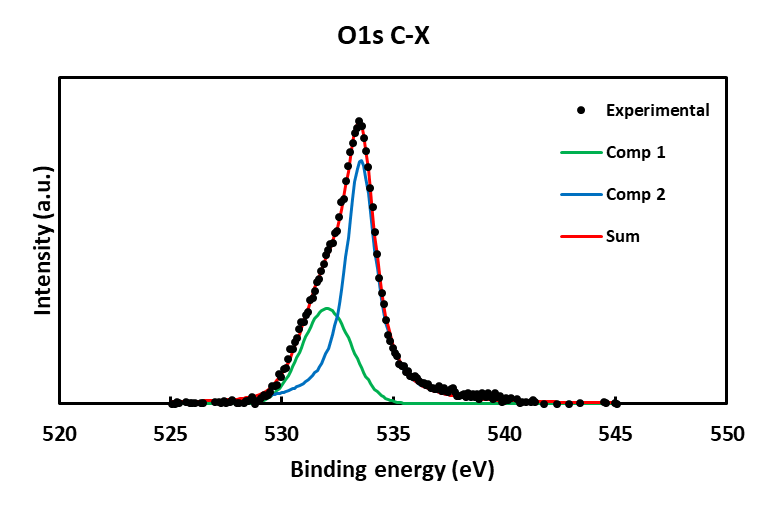
(5)

Where qe and Ce have the same meaning as in the previous model, KF (mg g-1) and 1/n are the Freundlich constants, with 1/n and KF being computed from the slope and intercept of the Freundlich plot of log qe against log Ce.

**XPS spectra**

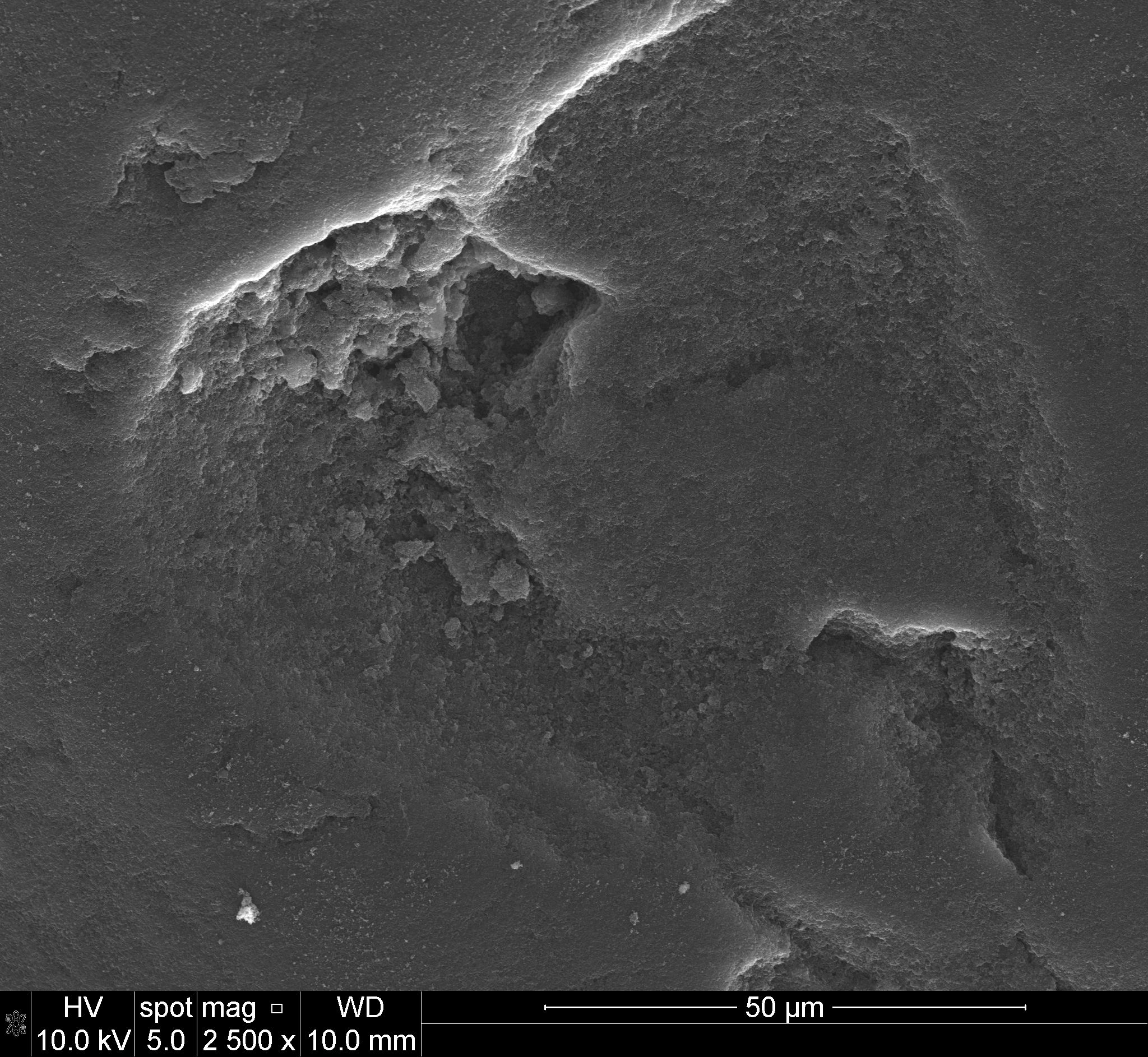
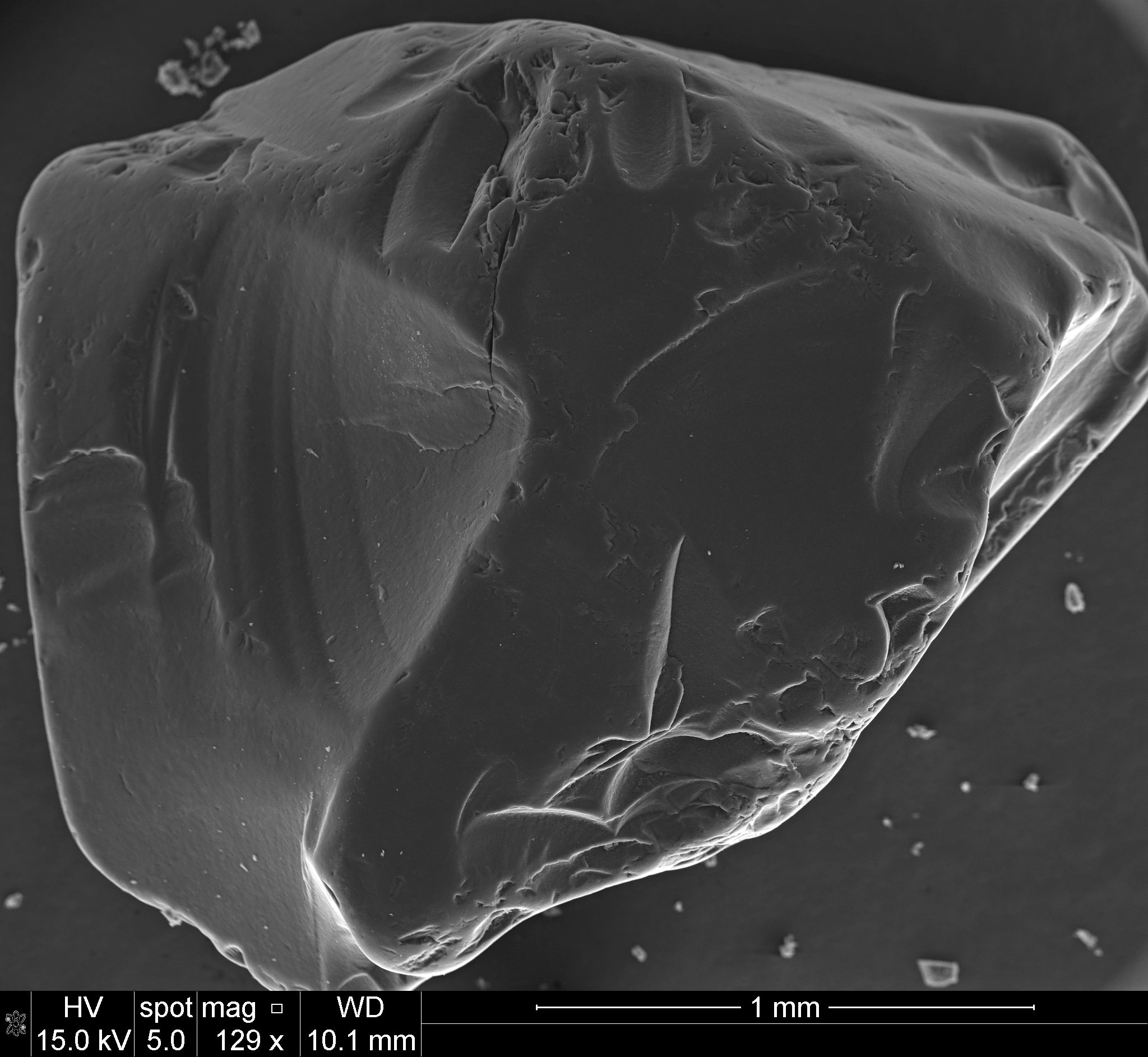
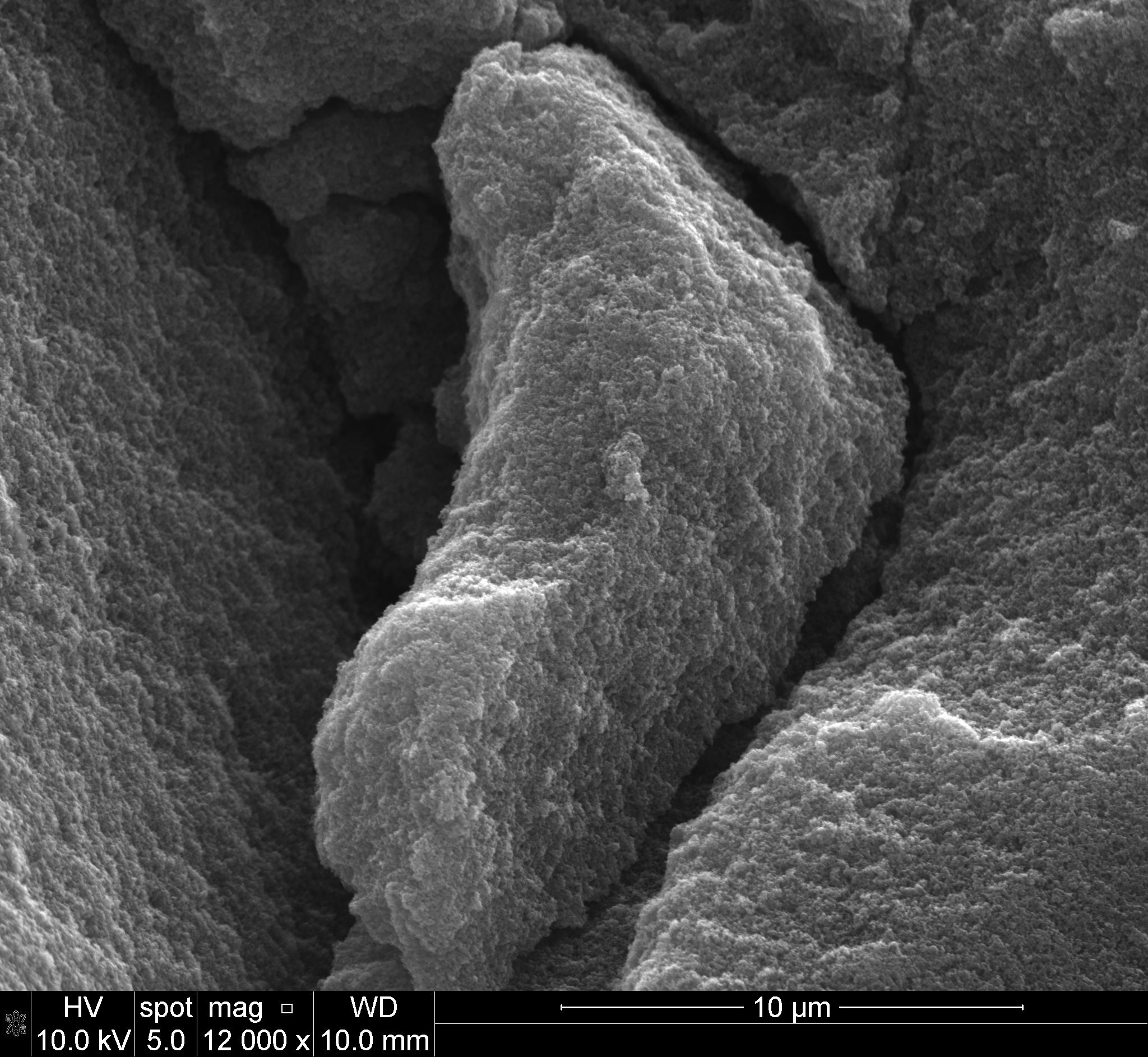
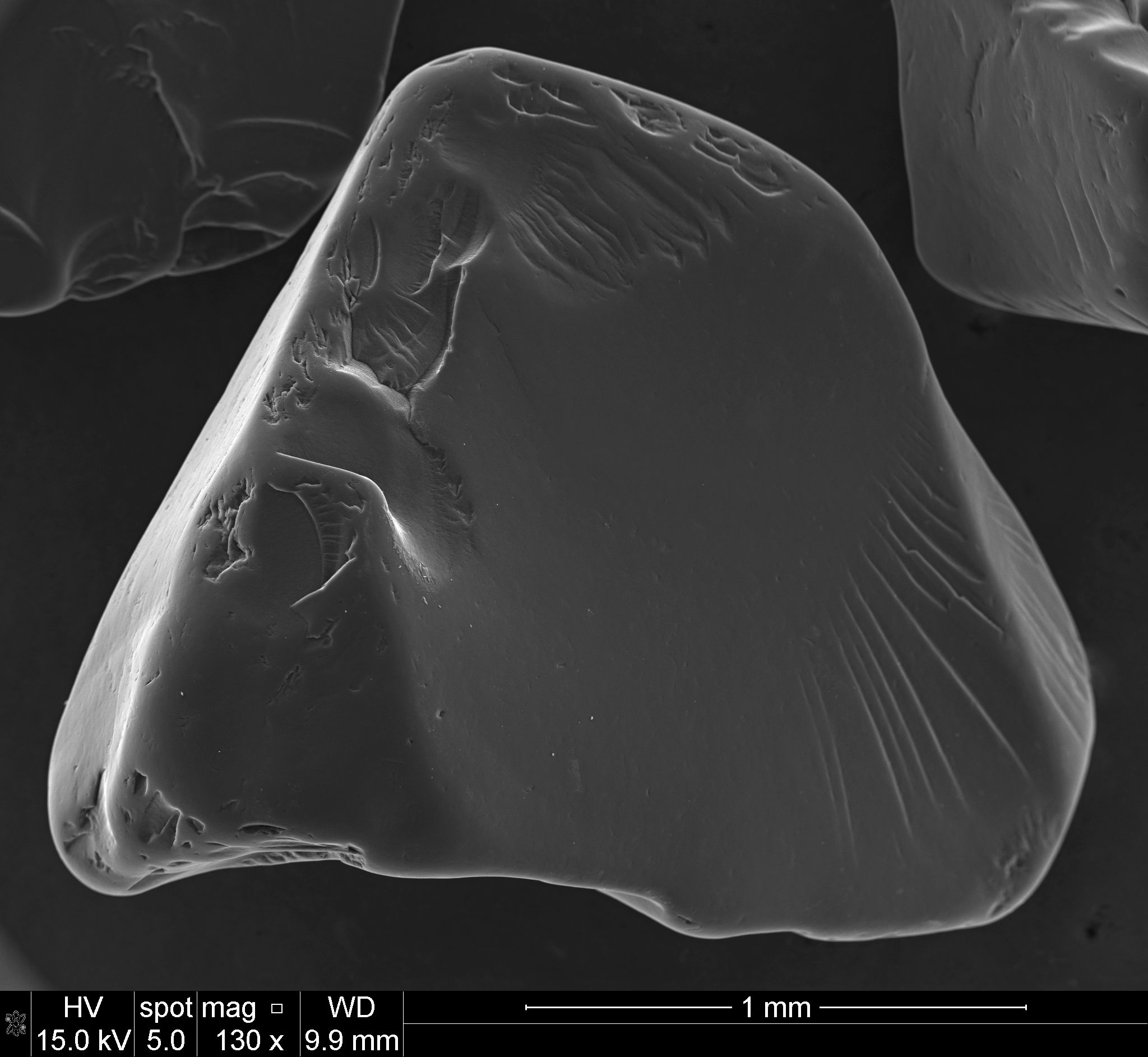
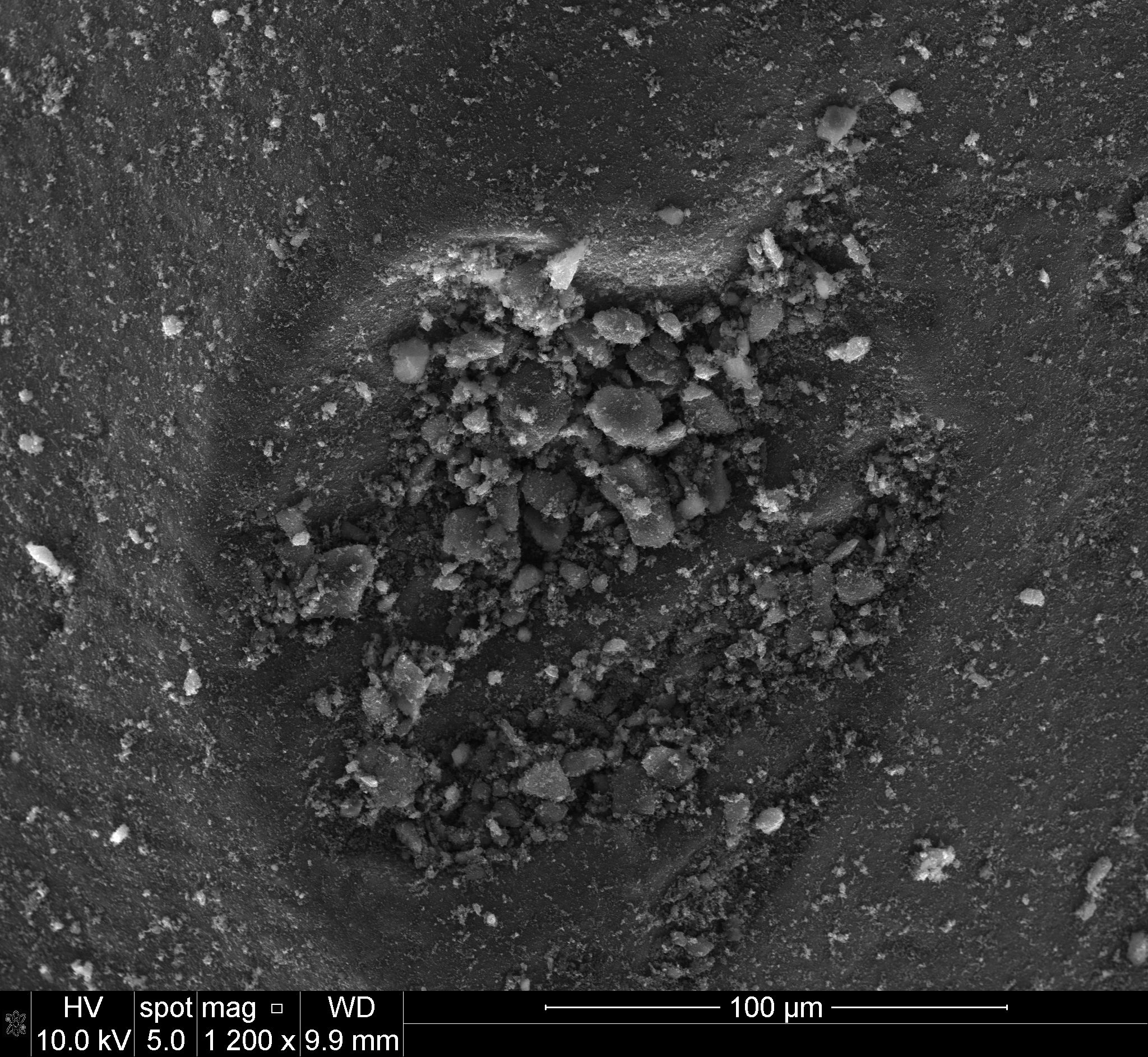
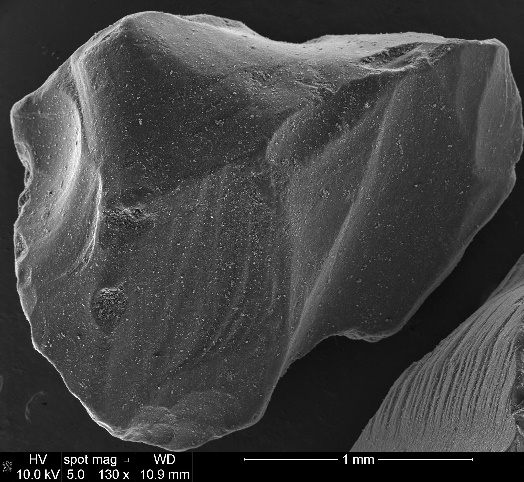


**Figure S1**. XPS spectra of C 1s



**Figure S2**. XPS spectra of O 1s

**SEM images**



a

b

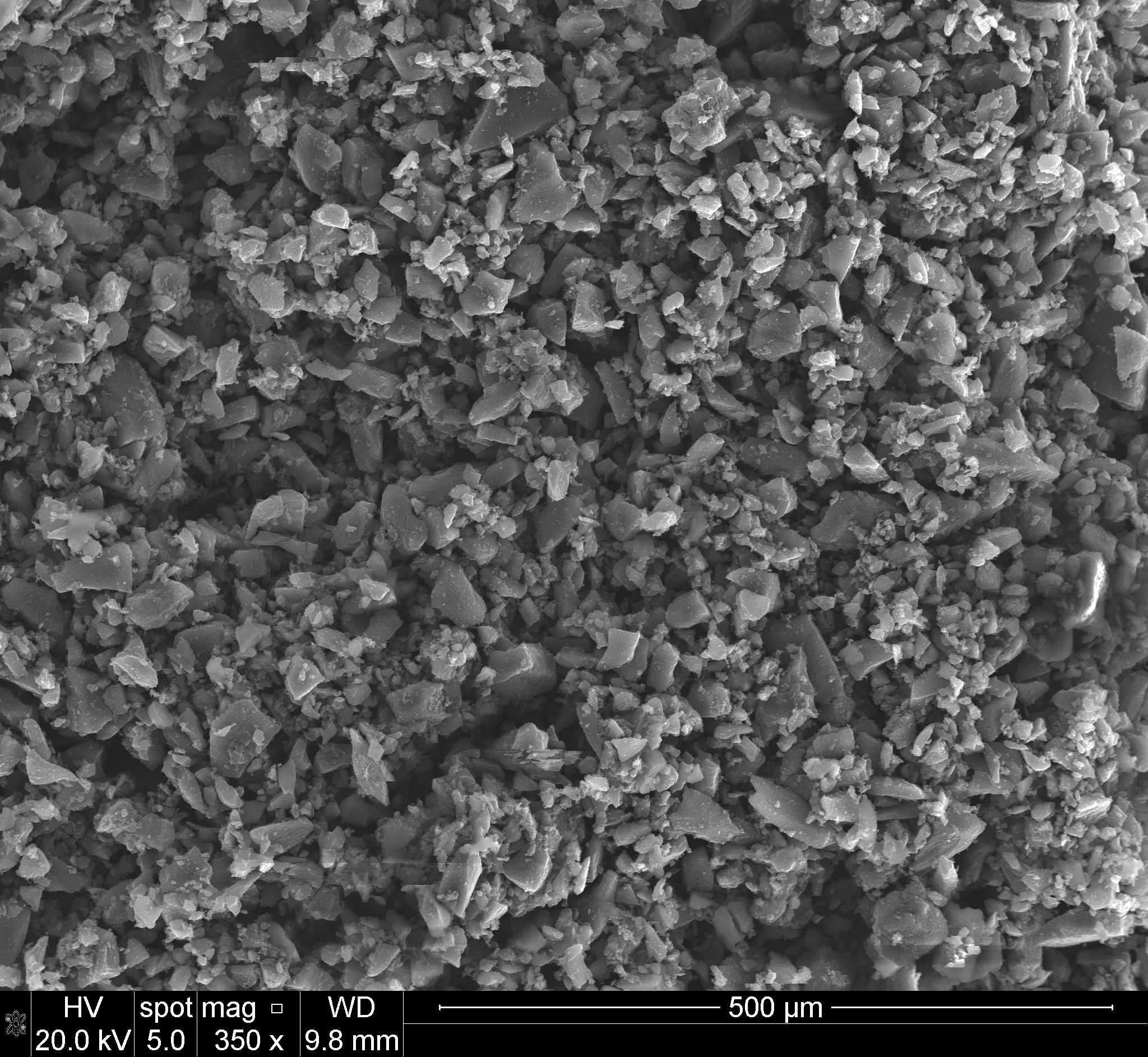
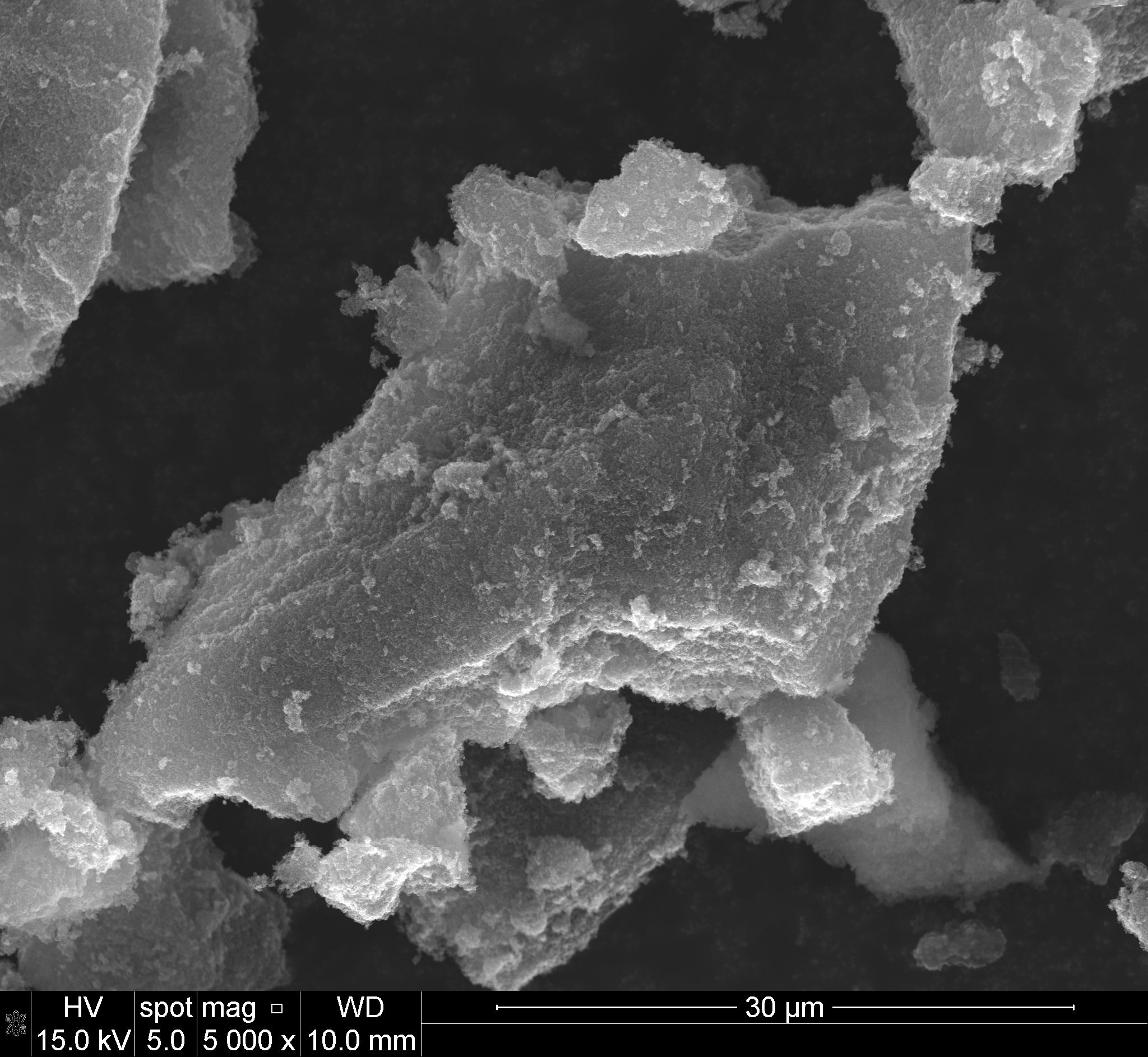
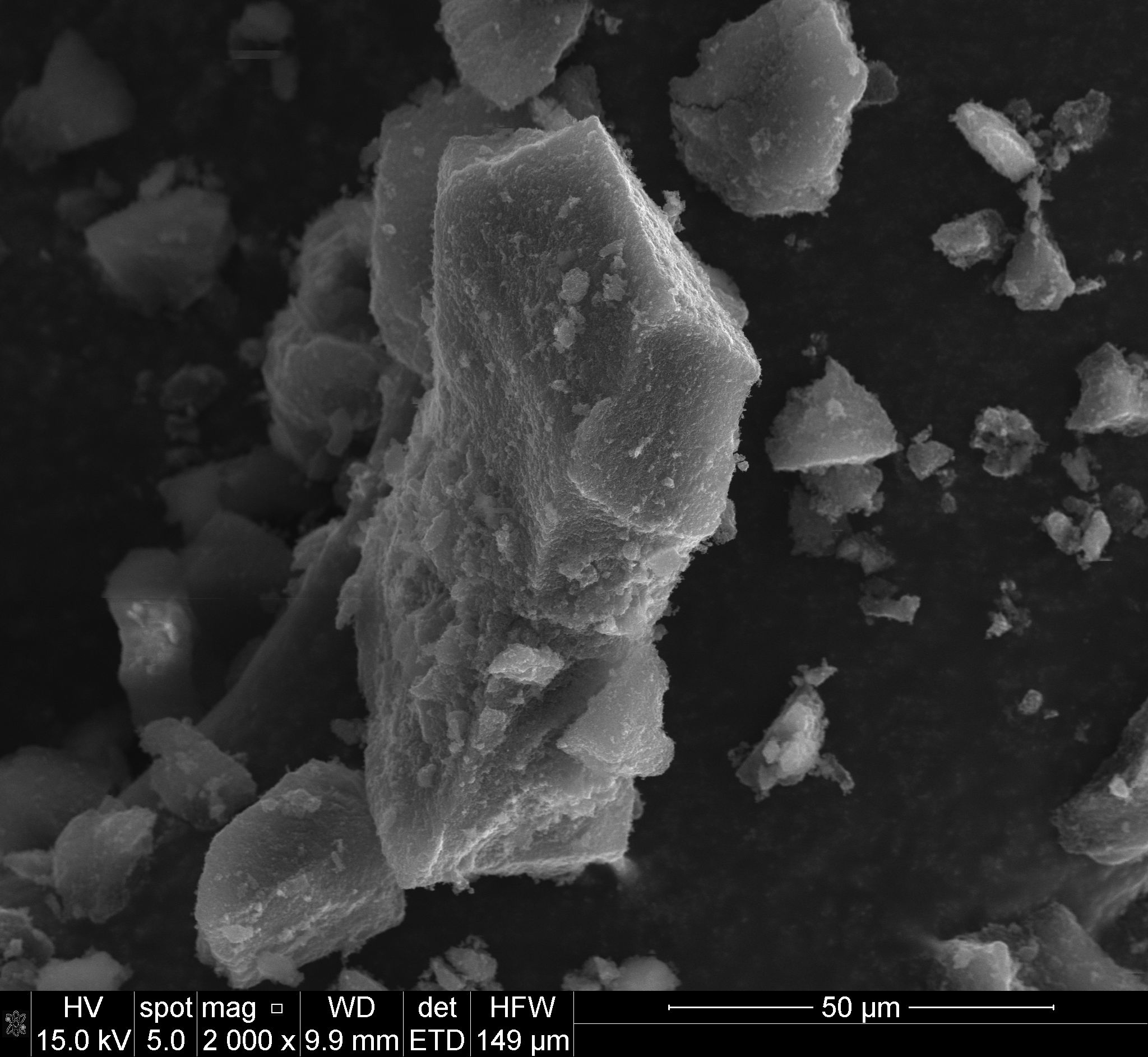
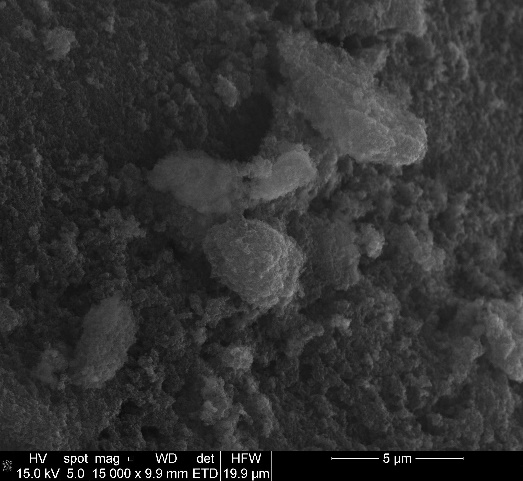
c

d

e

f

**Figure S3**. SEM images of C-X (a, b), C-X-N (c, d), C-X-S (e, f).



a

b

c

d

**Figure S4**. SEM images of C-X-Na (a, b), C-X-K (c, d).