Supporting Information

Effect of particle properties of powders on the generation and transmission of Raman scattering

Nichola Townshend,[1] Alison Nordon,*[1] David Littlejohn,*[1] John Andrews[2] and Paul Dallin[2]

[1] WestCHEM, Department of Pure and Applied Chemistry and CPACT, University of Strathclyde, 295 Cathedral Street, Glasgow, G1 1XL, UK

[2] Clairet Scientific Ltd., 17/18 Scirocco Close, Moulton Park Industrial Estate, Northampton, NN3 6AP, UK

* denotes authors to whom correspondence should be sent

(Email: d.littlejohn@strath.ac.uk and alison.nordon@strath.ac.uk)

Table of contents

Raman spectra of materials

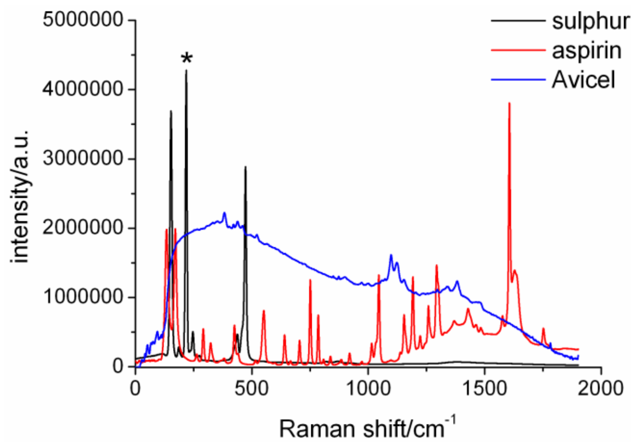

Figure S-1. Transmission Raman spectra of Avicel (signal multiplied by 100), aspirin (signal multiplied by 12) powder and a compressed flowers of sulphur disc. * indicates the peak at 218 cm^{-1} in the sulphur spectrum.

Calculation of the 2nd derivative removed the background fluorescence signal in the Avicel spectrum, which meant that the sulphur peak at 218 cm^{-1} was free from overlap with any other peaks.

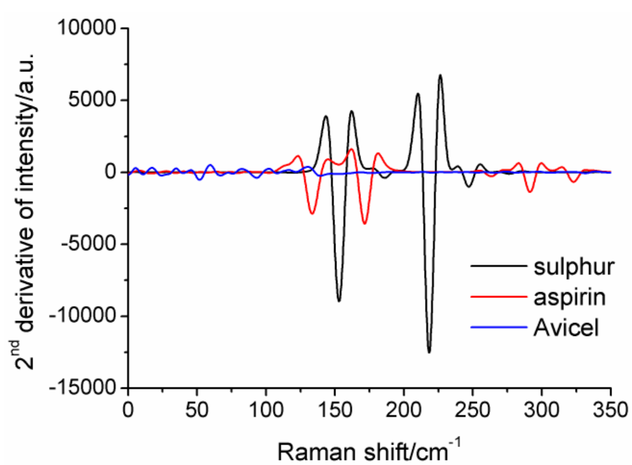

Figure S-2. Part of the 2nd derivative transmission Raman spectra of Avicel (signal multiplied by 100), aspirin (signal multiplied by 12) powder and a compressed flowers of sulphur disc.

Calculation of the estimated sulphur intensity for the propagation of laser photons through different depths of powder

The sulphur Raman signal for sample configurations P1 to P5 (see Figure 1a) arises from the combined effect of the influence of the different powders on the propagation of the laser and Raman photons. In comparison, the sulphur Raman signal for configurations A to E (see Figure 1b) arises from the effect of the different powders on the attenuation of the Raman signal generated by the sulphur disc. The Kaiser Raman Workstation, which illuminated the sample from below, was used for the two sets of experiments. From a comparison of Figures 1a and 1b, it is apparent that configurations P1 and A, P2 and B, P3 and C, P4 and D and P5 and E are related in the sense that for each pair there is the same amount of powder on top of the Raman active disc; only the depth of powder before the sulphur disc is different, which will provide information on the attenuation of the exciting laser intensity. Consequently, each powder's effect on the propagation of the laser and the Raman photons in the transmission measurements can be decoupled by comparing the two sets of measurements.

An example of the results obtained with the configurations in Figure 1a is shown in Table S-1 for Avicel particles in the range 150 – 212 μm. Equivalent data obtained with the configurations in Figure 1b are given in Table S-2. In both cases, the results have been normalised to the common configuration, P1 and A, respectively.

Table S-1. Data corresponding to the change in the sulphur Raman signal as the sulphur disc is moved through the 4 mm depth of Avicel 150-212 µm (n=3).

Depth of Avicel 150 – 212 µm below the sulphur disc/mm	Sample configuration identity (see Figure 1a)	Magnitude of average 2nd derivative sulphur Raman intensity at 218 cm^{-1}/a.u.	Normalised average 2nd derivative sulphur Raman intensity*
0	P1	188	1
1	P2	516	2.7
2	P3	561	3.0
3	P4	473	2.5
4	P5	190	1.0

*Data normalised to configuration P1.

Table S-2. Data corresponding to the change in the sulphur Raman signal as the depth of Avicel 150 – 212 µm on the disc is increased (n=3).

Depth of Avicel 150 – 212 µm on the sulphur disc/mm	Sample configuration identity (see Figure 1b)	Magnitude of average 2nd derivative sulphur Raman intensity at 218 cm^{-1}/a.u.	Normalised average 2nd derivative sulphur Raman intensity*
0	E	12743	84.8
1	D	3494	23.3
2	C	1056	7.0
3	B	395	2.6
4	A	150	1

*Data normalised to configuration A.

To estimate the attenuation of the exciting laser intensity by, for example 3 mm of 150 – 212 μm Avicel, the normalised intensities given in Tables S-1 and S-2 for configurations E, D and P4 in Figures 1a and 1b were used. The relationship between these configurations and the one for which the information is required is illustrated pictorially in Figure S-3.

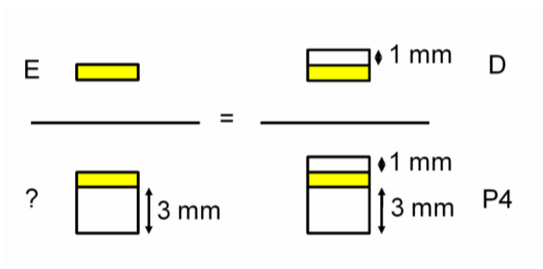

Figure S-3. Relationship between sample configurations E, D, P4 and the 'unknown' with a depth of 3 mm of powder before the sulphur disc.

When considering the general case, Figure S-3 can be rewritten in equation form as:

$$\frac{\text{Intensity(E)}}{\text{Intensity(x)}_{\text{calc}}} = \frac{\text{Intensity(Z)}}{\text{Intensity(P)}} \qquad \text{Equation 1}$$

where Intensity(P) is the measured sulphur signal intensity for configuration P1, P2, P3, P4 or P5, Intensity(Z) is the measured sulphur signal intensity for configuration A, B, C, D or E, Intensity(E) is the measured sulphur signal intensity for configuration E and $\text{Intensity(x)}_{\text{calc}}$ gives the calculated sulphur signal intensity when there is a depth of x mm of powder before the sulphur disc.

When Equation 1 was used to estimate the sulphur signal intensities obtained for propagation of laser photons through different depths of 150 – 212 μm Avicel powder prior to reaching the sulphur disc (i.e. $\text{Intensity(x)}_{\text{calc}}$), corresponding to the sample configurations in Figure 1d (for x = 0 to 4), the values in Table S-3 were obtained.

Table S-3. Calculated 2nd derivative Raman sulphur intensities at 218 cm^{-1} for different depths of Avicel 150 – 212 μm before the sulphur-containing disc as depicted in Figure 1d (illumination from below the sample).

Sample configurations being compared (see Figures 1a and 1b)	Depth of Avicel 150 – 212 μm below the sulphur disc/mm	Calculated 2nd derivative Raman sulphur intensity/a.u.
P1 and A	0	84.8
P2 and B	1	88.1
P3 and C	2	36.0
P4 and D	3	9.2
P5 and E	4	1.0