Supporting information for "The persistence of a proxy for cooking emissions in megacities: a kinetic study of the ozonolysis of self-assembled thin films by simultaneous Small & Wide Angle X-ray Scattering (SAXS/WAXS) and Raman microscopy."

Faraday Discussions

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S1 Kinetic Data

Cap	*d / μm*	*d (uncert.) / μm*	*kobs / x 10^{-2} min^{-1}*	*kobs (uncert.) / x 10^{-2} min^{-1}*	*e-folding time / min*	*Fraction remaining*
1	8.8	0.3	3.45	0.09	28.95	0.02
1	10.4	0.4	4.16	0.08	24.06	0.01
1	15.5	0.5	2.46	0.04	40.58	0.06
1	16.8	0.6	1.14	0.05	87.78	0.23
1	17.1	0.6	0.84	0.05	119.30	0.29
1	20.7	0.7	1.32	0.04	75.82	0.10
1	21.1	0.7	2.63	0.08	38.09	0.06
1	21.4	0.7	2.05	0.04	48.77	0.09
1	29	1	1.38	0.03	72.72	0.22
1	42	1	1.63	0.02	61.33	0.21
1	45	2	1.45	0.02	68.87	0.23
2	5.5	0.2	5.0	0.2	19.91	N/A
2	6.8	0.2	5.2	0.1	19.28	N/A
2	8.5	0.3	4.7	0.1	21.40	N/A
2	11.0	0.4	4.28	0.09	23.34	N/A
2	12.6	0.4	2.89	0.08	34.58	N/A
2	14.0	0.5	3.91	0.07	25.56	N/A
2	14.2	0.5	2.92	0.07	34.28	N/A
2	15.0	0.5	2.88	0.08	34.69	N/A
2	15.4	0.5	3.42	0.07	29.23	N/A
3	0.59	0.02	7	5	13.64	0.00
3	0.91	0.03	7	2	14.65	0.00
3	0.98	0.03	4.5	0.6	22.08	0.00
3	1.66	0.06	3.3	0.5	30.63	0.00
3	4.9	0.2	2.4	0.2	40.99	0.05
3	25.0	0.9	0.89	0.04	112.74	0.31
3	38	1	1.24	0.02	80.68	0.31
3	40	1	0.97	0.02	103.12	0.31
3	46	2	1.07	0.02	93.53	0.37
3	61	2	0.71	0.01	141.73	0.50
3	73	2	0.64	0.01	155.57	0.53
4	1.76	0.06	8.5	0.4	11.82	N/A
4	1.81	0.06	5.9	0.5	17.04	N/A
4	1.89	0.06	5.5	0.7	18.07	N/A
4	1.96	0.07	6.8	0.5	14.72	N/A
4	1.99	0.07	4.2	0.5	23.91	N/A
4	2.05	0.07	7.5	0.5	13.30	N/A
4	2.15	0.07	6.2	0.2	16.10	N/A
4	2.19	0.07	4.5	0.4	22.47	N/A
4	2.23	0.08	6.4	0.3	15.62	N/A
4	2.39	0.08	6.5	0.4	15.28	N/A
4	2.41	0.08	6.0	0.4	16.70	N/A
5	7.1	0.2	3.9	0.2	25.53	N/A
5	8.6	0.3	3.85	0.07	25.99	N/A
5	9.2	0.3	2.8	0.1	35.66	N/A

5	9.3	0.3	3.3	0.1	30.07	N/A
5	9.6	0.3	3.4	0.2	29.26	N/A
5	10.1	0.3	4.7	0.1	21.32	N/A
5	10.9	0.4	2.32	0.04	43.16	N/A
5	12.5	0.4	4.0	0.2	24.64	N/A
5	13.0	0.4	2.4	0.2	41.35	N/A
5	13.5	0.5	3.1	0.1	31.96	N/A
5	13.8	0.5	2.82	0.06	35.47	N/A

Table S1. Collection of measured first order decay constants (k_{obs}) for differing film thicknesses (d) observed along coated capillaries. Sorted by capillary number (Cap) and d. Uncertainties in d and k_{obs} (d(uncert.) & k_{obs}(uncert.)) are quoted in their respective adjacent columns. *Measurement of the fastest stage of reactive decay (explanation in the main text sect. 3.1). **Fraction remaining after ~ 175 min when the reaction was deemed to have stagnated significantly for the thickest films and when the experiments were stopped – only values from experiments which were allowed to continue to 175 min are presented. Note that this is ~ 175 min experiment time, not the corrected reaction time explained in the main text.

S2 SAXS patterns before and after ozonolysis

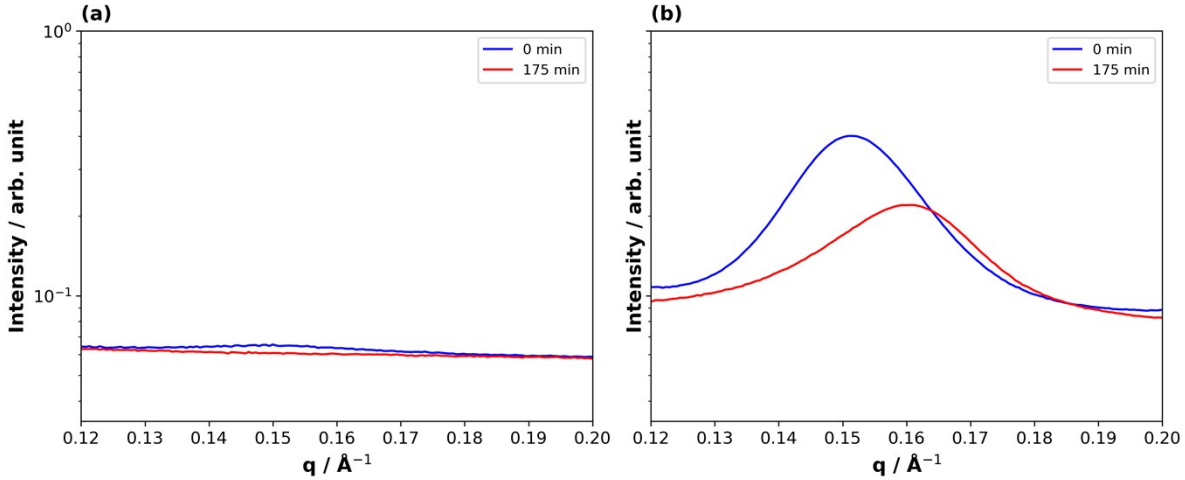
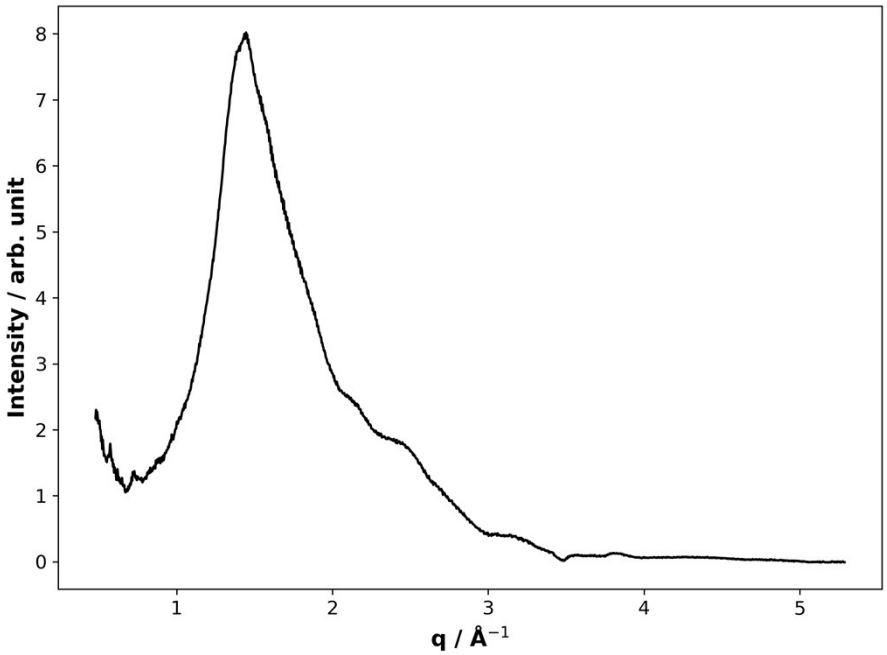


Figure S1. SAXS patterns showing the lamellar peak (~ 0.15 Å^{-1}) at the start and after 175 min of ozonolysis: (a) d = 0.59 ± 0.02 µm, (b) d = 73 ± 2 µm; [O_3] = 77 ± 5 ppm.

The initial SAXS patterns collected for the thinnest and thickest films (Fig. S1) probed in this study show a large difference in peak intensity. The main source of error in kinetic values measured in this study arises when, for the thinnest films, the lamellar peak approached the background signal making peak integration less accurate. This is reflected in the errors associated with k_{obs} (see Table S1) and peak area measurements in the decay plots presented in the main text (Fig. 3(b) – main text). Note the change in lamellar peak position and peak broadening as a result of the disordering of the lamellar structure during ozonolysis (Fig. S1(b)).



S3 WAXS pattern of the self-assembled proxy

Figure S2. The WAXS pattern of the lamellar phase oleic acid:sodium oleate (1:1 wt) proxy which exhibits a clear peak at ~ 1.43 Å^{-1} which corresponds to a 4.41 Å spacing between alkyl chains in the lamellar structure.

S4 Grazing-Incidence (GI)-SAXS image of the self-assembled proxy

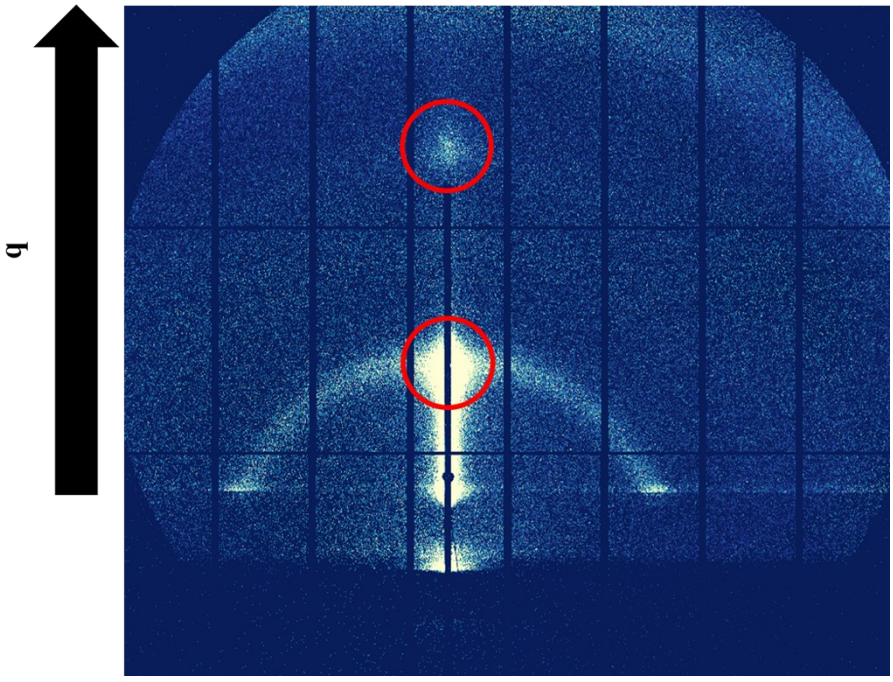


Figure S3. 2D GI-SAXS pattern of the lamellar phase oleic acid:sodium oleate (1:1 wt) proxy coated on a silicon wafer. Direction of *q* is indicated and aligned lamellar peaks are highlighted by red circles.

The proxy was deposited onto a silicon wafer by spin coating of the solution prepared as described in the main text. The sample was then exposed to X-rays at a 0.4 ^{o} angle of incidence (grazing incidence) in order to determine the alignment of the lamellar sheets in the proxy. Note that in GI-SAXS experiments only “half” of the scattering pattern is observed due to only the X-rays scattered from the sample side of the silicon wafer being detected. Areas of increased intensity aligned with the reflected X-ray signal (the bright streak starting from the beamstop to the first lamellar ring) indicate that there is a degree of alignment of the lamellar sheets parallel to the silicon surface, meaning that the alkyl chains in the lamellar structure are perpendicular to the surface. There is, however, a broad ring most prominent for the first lamellar reflection, suggesting that there is also a degree of random orientation.