Electronic Supplementary Material (ESI) for CrystEngComm.

The role of cavitation and gas bubbles in the non-photochemical laser-induced nucleation of sodium acetate

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SI1. Experimental details

Example images from activation of a handwarmer pouch containing sodium acetate solution are shown in Fig. S1. The experimental setup for NPLIN is shown in Fig. S2, with laser power densities given in Table S1. The glass vials used were cylindrical, with outer diameter 11.6 mm, holding an approximate volume of 1.5 mL, sealed with polypropylene screw caps with holes and silicone septa lined with poly(tetrafuoroethene) (PTFE).

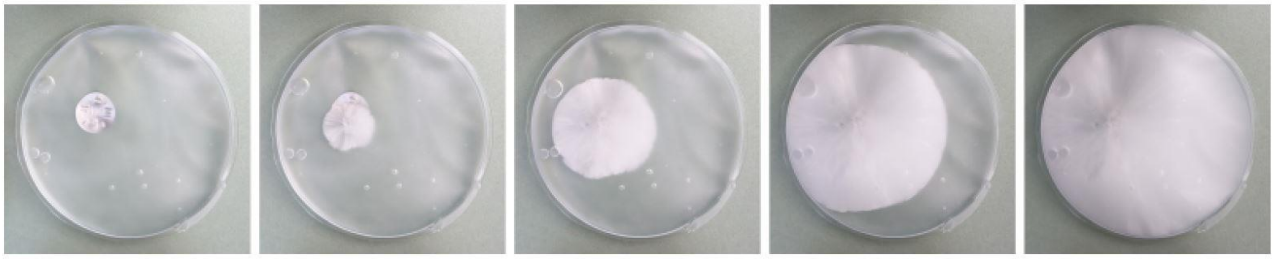

Fig. S1. Images of a reusable handwarmer, containing supersaturated aqueous sodium acetate solution, crystallising after the metal disk within is flexed. The formation of sodium acetate trihydrate crystals is rapid (approximately 10 s) and results in the release of heat.

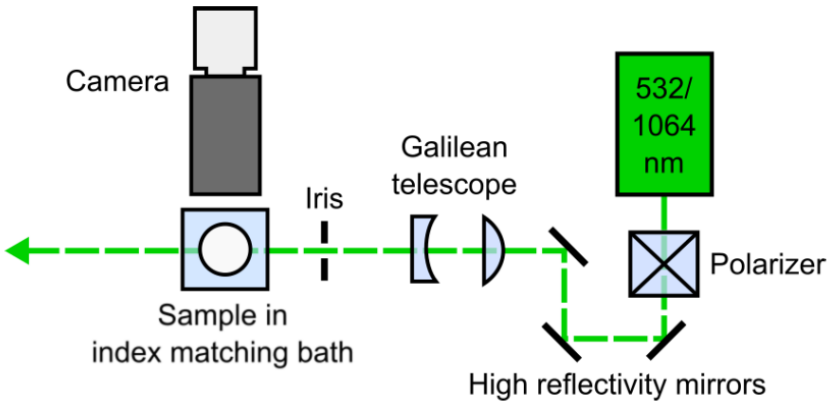

Fig. S2. A schematic diagram showing a typical optical setup for the irradiation of samples, including a polarizer (used for adjusting the laser power) and a Galilean telescope and iris (used for adjusting the beam diameter).

Pulse energy / mJ	Pulse energy density / mJ cm^{-2}	Peak power density / MW cm^{-2}
5	27.6	5.19
10	55.3	10.4
15	82.9	15.6
20	111	20.8
25	138	26.0
30	166	31.2
35	193	36.3
40	221	41.5
55	304	57.1
65	359	67.5

Table S1. Laser pulse energies, energy densities, and peak power densities used during NPLIN experiments on aqueous sodium acetate samples.

SI2. Experimental results

Laser pulse energy / mJ	Total samples tested	Samples nucleated	
		Crystals	Crystals and bubbles
5	10	3	7
10	1	1	0
15	13	13	0
40	1	1	0
55	5	5	0
65	9	9	0

Table S2. Observations following exposure, to a single laser pulse, of supersaturated sodium acetate solutions (C = 16.7 mol kg^{-1}, S = 2.72) containing no Na-PMAA polymer additive. The table shows the number of samples that nucleated to form crystals, or a combination of crystals and bubbles, for each solution at different laser pulse energies, alongside the total number of samples tested. This includes repeats of the same samples following regeneration.

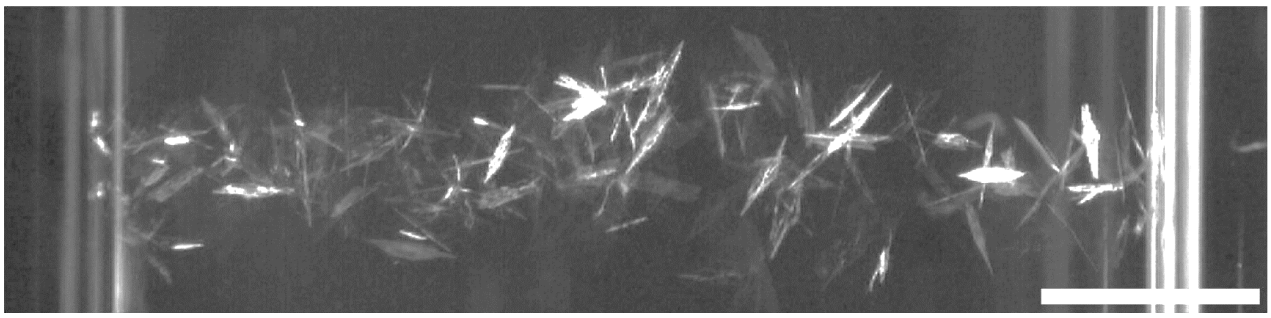

Fig. S3. Close-up of plate-like sodium acetate crystals following NPLIN with a single laser pulse growing in a supersaturated aqueous solution (C = 16.7 mol kg^{-1}, S = 2.72) with no Na-PMAA polymer additive. The incident laser pulse had an energy density of 27.6 mJ cm^{-2}. The image was taken 87 s after exposure to the laser pulse, before the emergence of cloud-like crystals. Scale bar represents 2 mm.

Na-PMMA concentration / (% w/w)	Laser pulse energy / mJ	Number of samples tested	Number of samples nucleated		
			Crystals	Crystals and bubbles	Bubbles
0.25 (low)	15	10	4	3	3
0.73 (high)	5	9	0	0	9
	15	31	0	4	26
	20	13	0	3	10
	25	15	0	1	14
	30	13	0	0	13
	35	11	0	0	11
	40	15	0	0	15

Table S3. Observations following exposure of supersaturated sodium acetate solutions (C = 16.7 mol kg^{-1}, S = 2.72) containing different amounts of Na-PMAA polymer additive, to a single laser pulse (532 nm, 5.0 ns). The table shows the total number of samples tested, and the resulting number of samples that nucleated to form crystals, bubbles, or a combination of the two for each solution, at different laser pulse energies. These results include repeats of the same samples following regeneration.

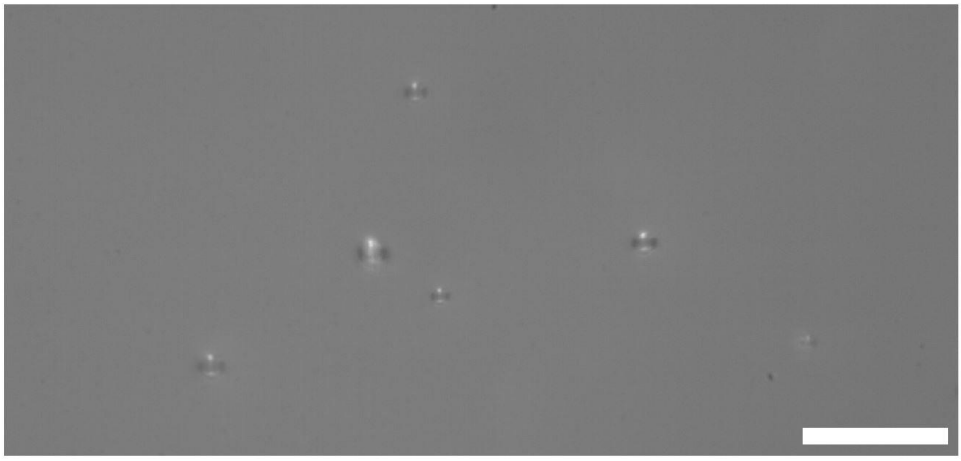

Fig. S4. Image of bubbles in a supersaturated aqueous solution of sodium acetate (C = 16.7 mol kg^{-1}, S = 2.72) containing high Na-PMAA (0.73% w/w), following exposure to a single laser pulse. The incident pulse had an energy density of 221 mJ cm^{-2}. The image was taken approximately 13 minutes after the laser pulse. Bubbles are clearly identifiable, and a range of bubble sizes is observed. Scale bar represents 100 µm.

SI3. Power dependence and image analysis

There was a large amount of variation between samples, especially for bubbles: the count depended strongly on the individual sample solution used. We attribute this to variations in the populations of impurity nanoparticles between individual samples. As a result of this, comparisons of the bubble count at different power densities were carried out only within sets of the same samples, which were regenerated and reused for every power density. Images selected for analysis were taken between 10 s and 5 minutes after the laser pulse, depending on the speed of particle growth and image quality. The background was subtracted from each image, where the background was a frame taken from before each laser pulse, and the number of particles was counted using the “find maxima” tool. The noise tolerance was adjusted manually so that all visible particles were counted. When counting crystals, because we have a stack of images, it was possible to select an image where the crystals were small and clearly separated.