SUPPORTING INFORMATION

Cytosine Monohydrate Crystals Under Mechanical Stress

Megan E. Fleming[a], Daniel E. Hooks[b,c], Michael McBride[c], Nan Li[c] and Jennifer A. Swift[a*]

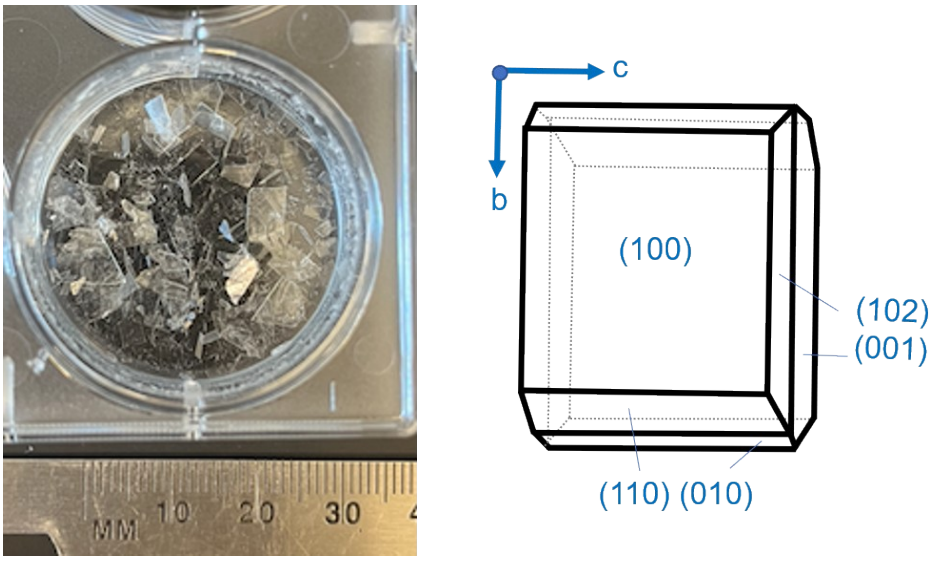


Fig. S1 Micrograph of CM crystals grown from aqueous solution and a schematic of the typical morphology.

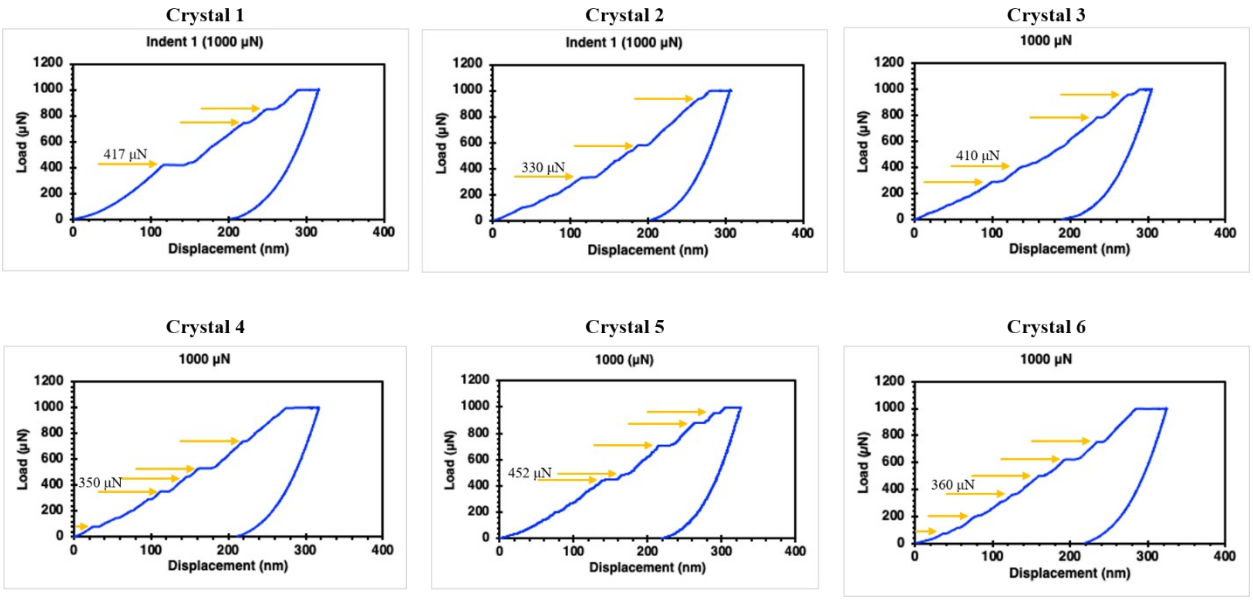


Fig. S2 Representative load-displacement curves from 6 different crystals, all with max load of 1000 µN. The pop-in frequency and displacement depth varied from crystal to crystal.

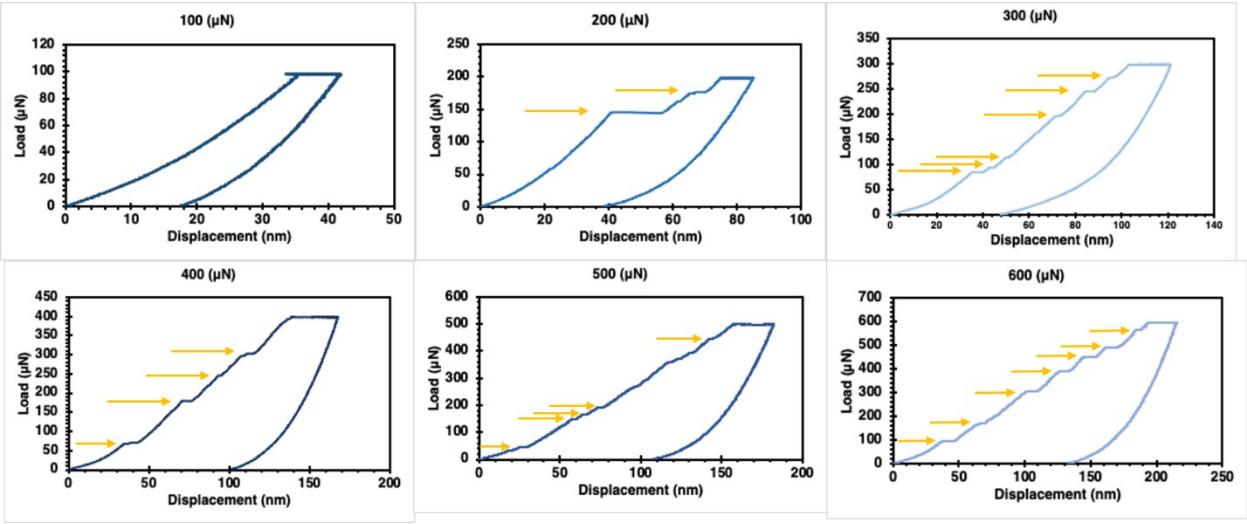


Fig. S3 Representative load-displacement curves from 6 different spots within the same CM crystal, with varying loads. Pop-ins are observed at minimum load of 150 μN but otherwise vary in frequency and displacement depth.

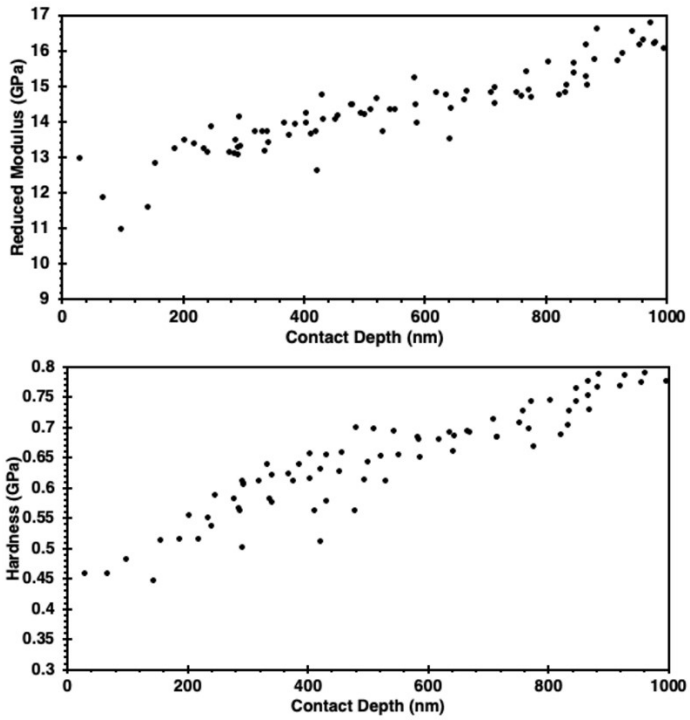
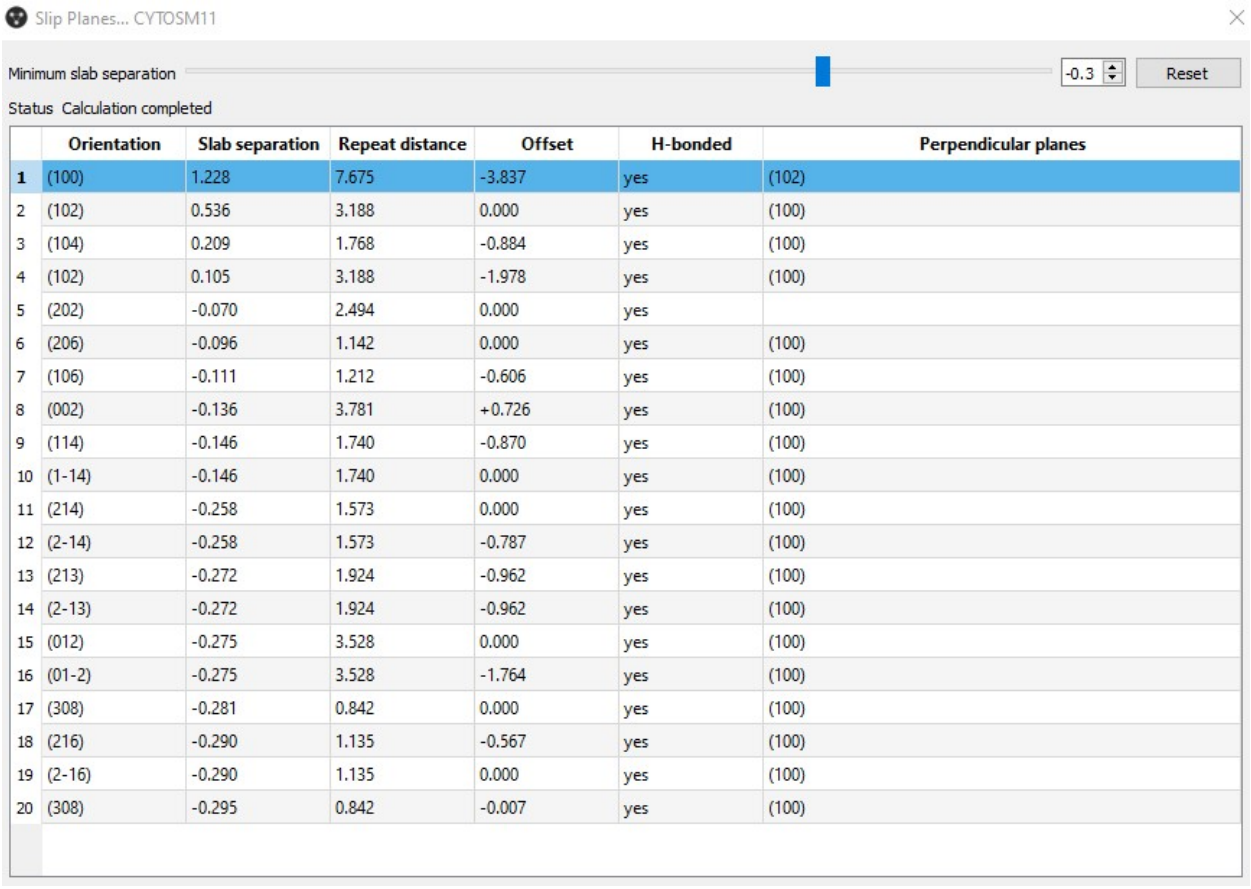


Fig. S4 Reduced modulus (top) and hardness (bottom) values derived from load-displacement curves from indents 100 - 8000 μN show a scaling effect with increased loads. Values at contact depths < 110 nm and above 900 nm may have large associated errors owing to limitations of the contact geometry model.



	Orientation	Slab separation	Repeat distance	Offset	H-bonded	Perpendicular planes
1	(100)	1.228	7.675	-3.837	yes	(102)
2	(102)	0.536	3.188	0.000	yes	(100)
3	(104)	0.209	1.768	-0.884	yes	(100)
4	(102)	0.105	3.188	-1.978	yes	(100)
5	(202)	-0.070	2.494	0.000	yes	
6	(206)	-0.096	1.142	0.000	yes	(100)
7	(106)	-0.111	1.212	-0.606	yes	(100)
8	(002)	-0.136	3.781	+0.726	yes	(100)
9	(114)	-0.146	1.740	-0.870	yes	(100)
10	(1-14)	-0.146	1.740	0.000	yes	(100)
11	(214)	-0.258	1.573	0.000	yes	(100)
12	(2-14)	-0.258	1.573	-0.787	yes	(100)
13	(213)	-0.272	1.924	-0.962	yes	(100)
14	(2-13)	-0.272	1.924	-0.962	yes	(100)
15	(012)	-0.275	3.528	0.000	yes	(100)
16	(01-2)	-0.275	3.528	-1.764	yes	(100)
17	(308)	-0.281	0.842	0.000	yes	(100)
18	(216)	-0.290	1.135	-0.567	yes	(100)
19	(2-16)	-0.290	1.135	0.000	yes	(100)
20	(308)	-0.295	0.842	-0.007	yes	(100)

Fig. S5 Slip planes calculated using the CSD-Particle module in Mercury.