Photoinduced vitrification near the surfaces of single crystals of azobenzene-based molecular materials with glass-forming ability

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*** Electronic Supplementary Information ***

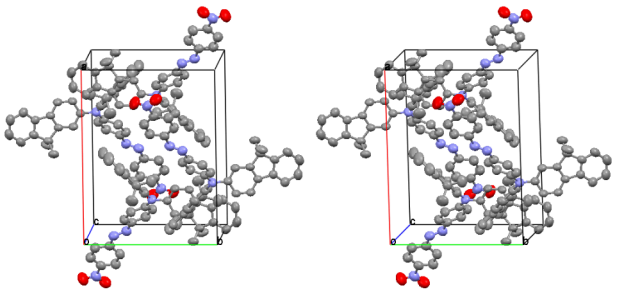

Fig. S1. Crystal Structure of NO_2-BFlAB (stereo view).

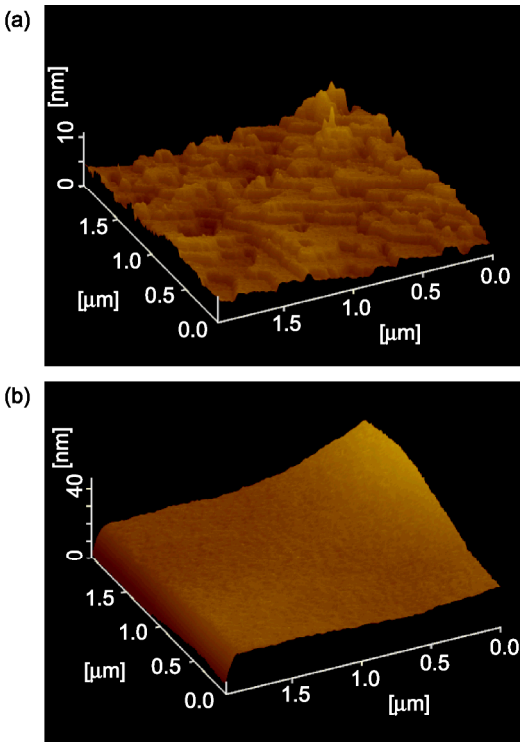

Fig. S2. 3D topography images of the (001) surface of NO_2-BFlAB crystal (a) before and (b) after photoirradiation.

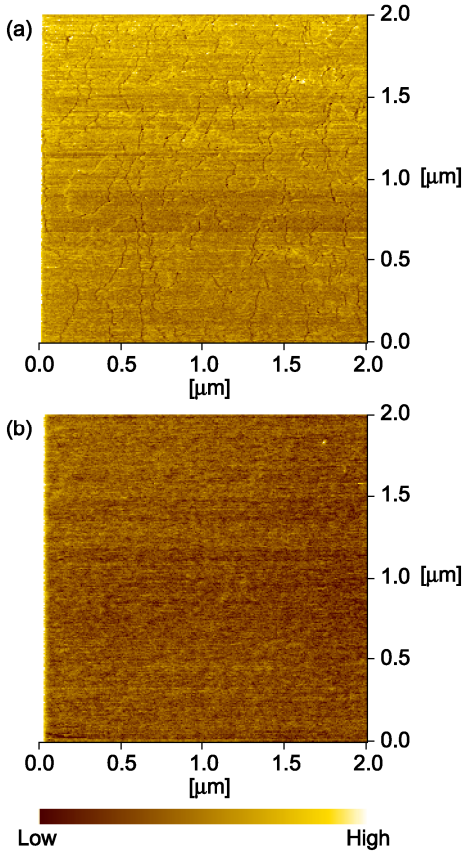

Fig. S3. 2D friction force images of the (001) surface of NO_2-BFlAB crystal (a) before and (b) after photoirradiation.

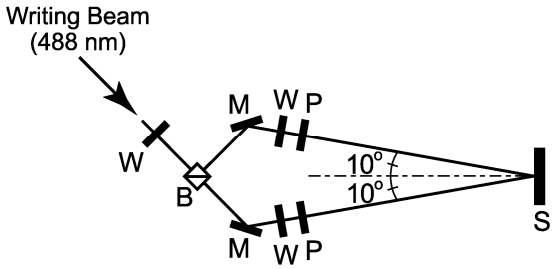

Fig. S4. Schematic experimental setup for photoinduced SRG formation. S: sample, P: polarizer, M: mirror, W: wave plate, B: beam splitter.

Experimentals

FFM was carried out by means of SPA-400 (Seiko Instruments, Inc.) with a cantilever (OMCL-TR400SPA-2, OLYMPUS). In order to measure the FFM images for the photoirradiated sample at the same area under the same conditions as those for the sample before photoirradiation, the sample crystal was irradiated in situ with the laser beam (488 nm: CYAN-488-100NH-W, Spectra Physics) in the FFM apparatus for ca. 1 min. Intensity of the laser beam at the surfaces of the sample crystals was unknown due to difficulty of intensity measurement at the quite small area in the apparatus. Photoinduced SRG formation was carried out by using the same laser (CYAN-488) as a source of writing beams and SRG formation was confirmed by AFM (JSTM-4200D, JEOL Ltd.) with a cantilever (OMCL-AC160T-C2, OLYMPUS).

X-Ray crystal structure analysis

X-Ray structure analyses for CN-BFlAB and NO_2-BFlAB were performed on a Rigaku RAXIS-RAPID Imaging Plate diffractometer with graphite-monochromated Cu-*K*α (1.54186 Å) radiation. Both structures were solved by direct methods and refined by full matrix least square method. The non-hydrogen atoms were refined anisotropically and the hydrogen atoms were fixed at their calculated positions. Experimental conditions and crystallographic parameters are summarized in Table S1. Crystallographic data (excluding structure factors) for CN-BFlAB and NO_2-BFlAB have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC-748894 and CCDC-748895, respectively. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: (internat.) +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk].

Table S1. Experimental conditions and crystallographic parameters of CN-BFlAB and NO_2-BFlAB

	CN-BFlAB	NO_2-BFlAB
Empirical Formula	$C_{43}H_{34}N_4$	$C_{42}H_{34}O_2N_4$
Formula Weight	606.77	626.76
Crystal Dimensions / mm^3	0.10 x 0.40 x 0.40	0.37 x 0.28 x 0.10
Crystal System	monoclinic	monoclinic
Number of Reflections Collected	65569	66349
Number of Unique Reflections	6586	6680
a / Å	16.5817(3)	16.5256(3)
b / Å	11.9938(2)	12.1737(2)
c / Å	17.3483(3)	17.4298(3)
β / °	100.1372(7)	100.7497(7)
V / $Å^3$	3396.3(1)	3444.9(1)
Space Group	$P2_1/a$	$P2_1/a$
Z value	4	4
D_{calc} / gcm^{-3}	1.187	1.208
F_{000}	1280.00	1320.00
μ(CuKα) / cm^{-1}	5.40	5.93
Temperature / °C	23.0	23.0
wR_2	0.162	0.163
$R_1[I>2\sigma(I)]$	0.049	0.050
Number of Reflections to calc R_1	5010	5149