Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

# Enhancement of Dissipated Energy by Large Bending of an Organic Single Crystal undergoing Twinning Deformation

Sajjad Husain Mir[a], Yuichi Takasaki[a,b], Emile R. Engel[a], Satoshi Takamizawa[a]*

[a]Department of Materials System Science, Graduate School of Nanobioscience, Yokohama City University, 22-2 Seto, Kanazawa-ku, Yokohama, Kanagawa 236-0027, Japan

[b]Kanagawa Institute of Industrial Science and Technology, Shimoimaizumi, 705-1 Ebina, Kanagawa, 243-0435, Japan

*E-mail: staka@yokohama-cu.ac.jp

## Table of contents



## Other supplementary material

Video file for bending action of **1** observed under a polarizing microscope:

(a) Stress-Strain test at 298 K: Takamizawa_movS1.qt

**Materials**

2-methyl-5-nitrobenzoic acid was purchased from Tokyo Chemical Industry, Japan. Solvents were purchased from Wako and used as received.

**Recrystallization**

Crystals of **1** were grown in acetone solution by slow evaporation. A mixture of small and long needle-shaped crystals was obtained.

## (a) Experimental information

i) Stress-strain test

Stress tests were carried out on a universal testing machine (Tensilon RTG-1210, A&D Co. Ltd.).

ii) Single-crystal X-ray diffraction experiment

Single-crystal X-ray analysis of **1** was performed at 298 K on a Bruker SMART APEX CCD area detector (graphite-monochromated Mo-K$\alpha$ radiation ($\lambda$ = 0.71073 Å)) with a nitrogen flow temperature controller. Empirical absorption corrections were applied using the SADABS program. The structure was solved by direct methods (SHELXS-97) and refined by full-matrix least squares calculations on $F^2$ (SHELXL-97) using the SHELX-TL program package. Non-hydrogen atoms were refined anisotropically; hydrogen atoms were refined in a riding model. The crystal face indexing was carried out using SMART in a SHELXTL Ver.6.12 program package with a twin resolution program. Crystallographic data of the structure is summarized in Tab. S1.

(b) Crystallographic data

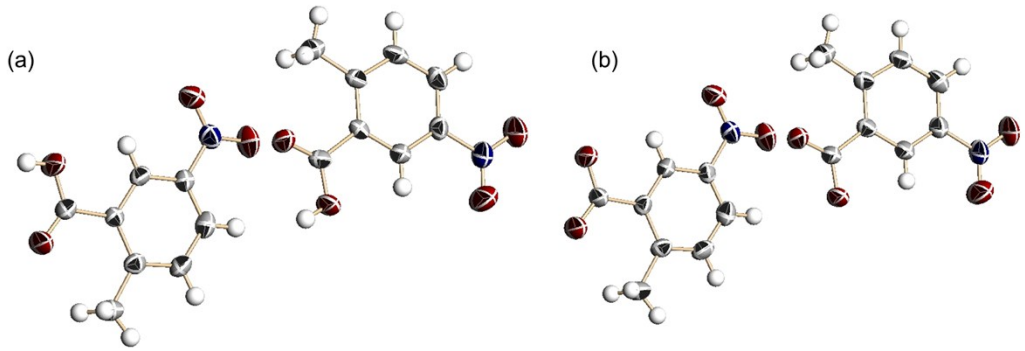


**Figure S1**. Molecular structures of **1** in (a) mother domain and (b) twinned domain as ORTEP representations drawn at 50% probability level for the ellipsoid obtained from single crystal X-ray diffraction measurement at 298 K.

**Table S1**. Crystallographic data of **1** in bent shape.

| Domain | mother ($\alpha_0$) | daughter ($\alpha_1$) |
|---|---|---|
| T /K | 298 | 298 |
| Empirical formula | $C_8H_7NO_4$ | $C_8H_7NO_4$ |
| M | 181.15 | 181.15 |
| Crystal system | Triclinic | Triclinic |
| Space group | *P*-1 | *P*-1 |
| a /Å | 7.611 (15) | 7.636 (13) |
| b /Å | 10.47 (2) | 10.426 (19) |
| c /Å | 10.55 (2) | 10.520 (18) |
| α /° | 89.45 (3) | 89.28 (3) |
| β /° | 81.45 (3) | 81.80 (3) |
| γ /° | 76.75 (3) | 76.32 (3) |
| V /Å$^3$ | 810 (3) | 805 (2) |
| Z | 4 | 4 |
| $D_{calc}$/Mg m$^{-3}$ | 1.485 | 1.495 |
| μ(Mo Kα) mm$^{-1}$ | 0.121 | 0.122 |
| Reflections collected | 2759 | 2769 |
| Independent reflections ($R_{int}$) | 1674 | 1554 |
| Goodness of fit | 1.071 | 1.161 |
| $R_1(I > 2\sigma$ (all data)) | 0.0601 | 0.1016 |
| $_wR_2(I > 2\sigma$ (all data)) | 0.1786 | 0.3546 |
| Leastdiff.peak (hole) /eÅ$^3$ | 0.233(-0.243) | 0.466(-0.431) |

(c) Crystal phase indexing

The crystal face indexing showed deformation twinning of **1**. Shear stress formed daughter domain $\alpha_1$ from $\alpha_0$ in rotational twinning. The twinning interfaces are $(-21-1)_{\alpha 0}//(-21-1)_{\alpha 1}$ (or $(-21-1_{\alpha 0}//(-21-1)_{\alpha 1}$).

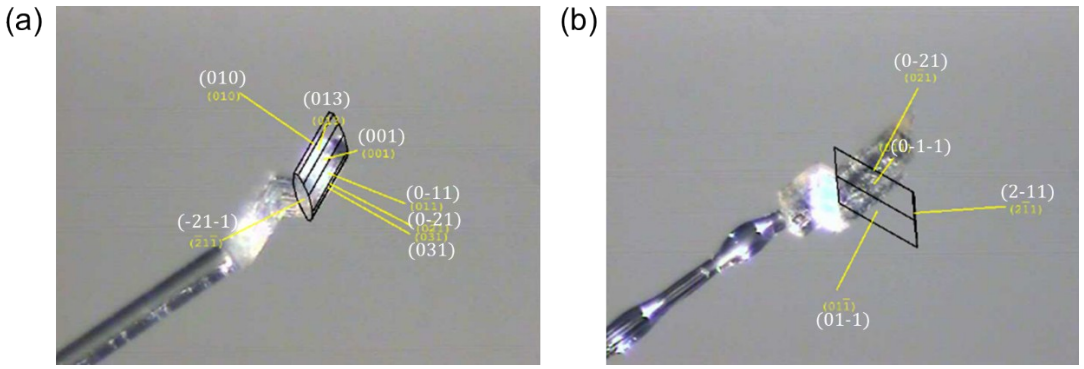


**Figure S2**. a) Crystal face indices of $\alpha_0$ domain (a) and $\alpha_1$ domain (b).

(d) Detail information for observation of stress-strain test

**Table S2:** Conditions of cyclic shear test on crystal **1**, shown in Fig. 3b

| Temperature / °C | Loading surface | Crystal dimension | | Displacement Velocity / μm $min^{-1}$ |
|---|---|---|---|---|
| | | width / μm | Thickness / μm | |
| 25 | -1-10 | 32.48 | 286.96 | 30 |

(e) Enlarged color figures described in the main text

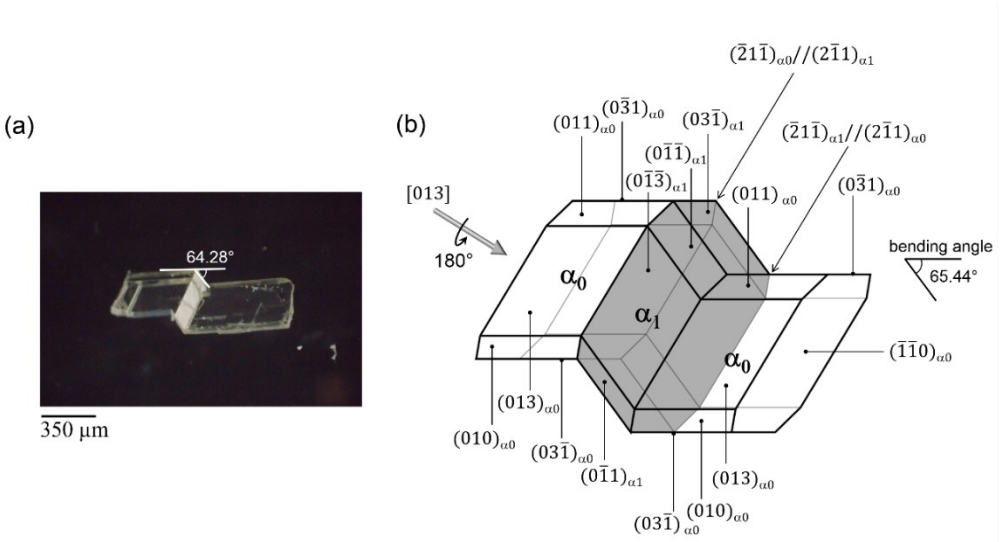


**Figure S3**. a) Optical image of the twinned crystal by compression on crystal surface (110)$\alpha_0$, [013] and b) crystal face indices of the mechanically twinned crystal.

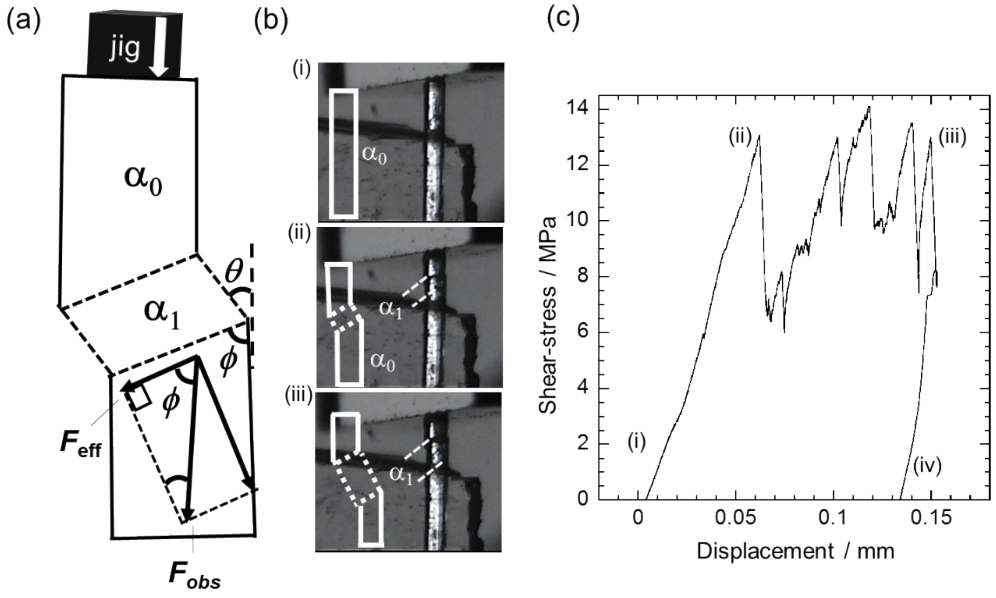


**Figure S4**. Measurement of stress-strain curve, a) Cartoon illustration of crystal deformation pattern and force components, b) snapshots of the twinning deformation of shear-stress (i-iii) (Movie S1) with inset sketches of the deformation pattern, and c) stress-strain curve at 298 K

Effective stress: $\sigma_{eff}$

$F_{eff} = F_{obs} \cos\phi \qquad (\phi = 57.28°)$

$\sigma_{eff} = F_{eff}$ / cross-sectional area

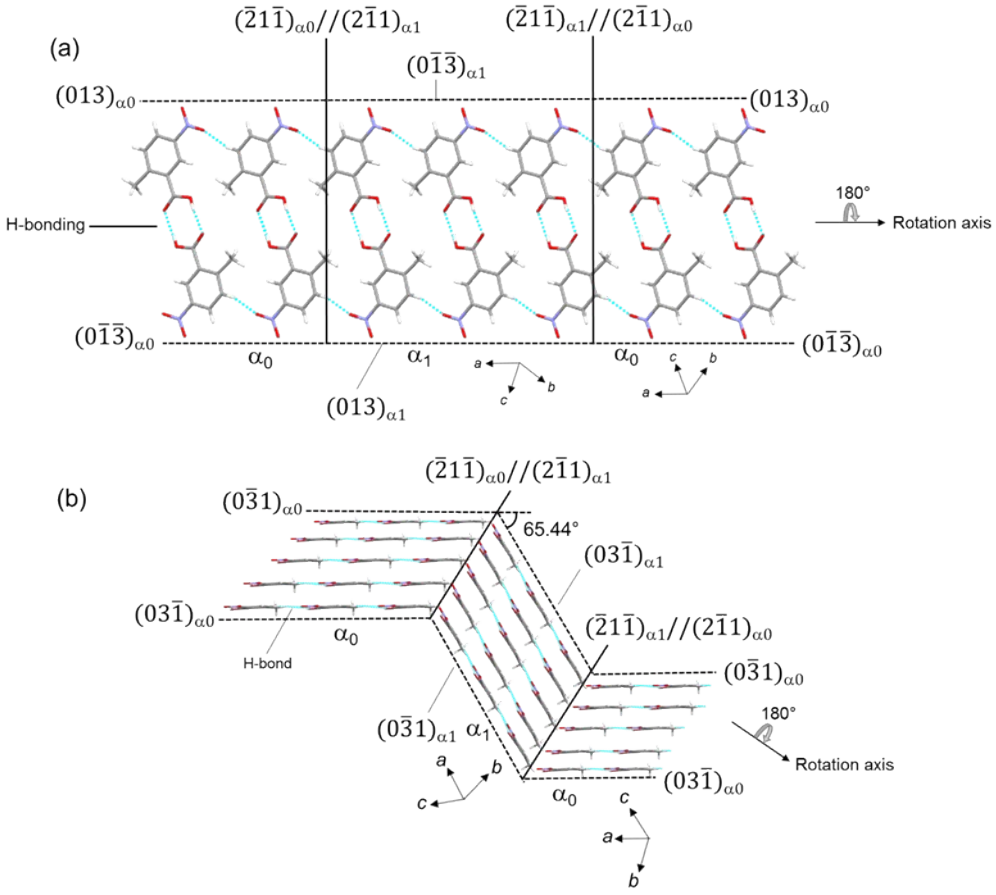


**Figure S5.** Partial packing diagrams of overlapping mother ($\alpha_0$) and daughter domain ($\alpha_1$) of **1** viewed (a) along $[013]_{\alpha0}$ and (b) along $[0\bar{3}1]_{\alpha0}$. Molecules form 2D molecular chains by hydrogen bonding (indicated as dotted lines).