Solvent-Mediated Elasticity in Flexible Single Crystals

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Single crystals have demonstrated remarkable flexibility in response to various stimuli such as mechanical stress [1], electromagnetic radiation [2] and variations in temperature [3]. The flexibility of a crystal is influenced by its structure – i.e. composition, packing and intermolecular interactions. Hence it should be possible to tailor the flexibility of a crystal by applying the principles of supramolecular chemistry and crystal engineering, e.g. if crystals are to be incorporated into mechanical devices such as actuators. This approach requires a system that is amenable to modification while yielding predictable structures and morphologies. Our group has reported a system that satisfies these criteria: an organic molecular host (**1**) with a needle-shaped morphology that forms an isoskeletal series of inclusion compounds with itself as well as with a range of small guest molecules [4]. Given the predictably invariant host packing arrangements for a range of different guests, the inclusion compound crystals of **1** are ideally suited for a systematic study aimed at influencing the mechanical properties of crystals by means of guest substitution.

Quantification of flexibility is a well-developed field in mechanical and civil engineering, and the strategies employed by these disciplines can be extended to measure flexibility in crystals. However, because of considerations that are peculiar to crystals (e.g. anisotropy, size, brittleness, etc.), these methods may need to be adapted. The relative flexibility of a crystal is given by the Young's modulus (E) and is commonly determined by means of nanoindentation [5] and atomic force microscopy [6]. However, neither of these methods require the crystal to undergo flexion during the measurement. To effectively measure elastic flexibility for actuation applications, an instrument needs to satisfy the following criteria: 1) the value of E should be measured by bending the crystal, 2) the measurement should be repeatable and should therefore not damage the crystal and 3) the direction of bending should be known (and preferably selectable). In order to satisfy all of these criteria, we constructed an instrument based on the single-point bending approach (Fig. 1).

In this work the value of E was determined for five inclusion compounds using our in-house developed instrument: the *Flexometer*. Our results suggest that the relative flexibility of the inclusion compounds of **1** can be tuned by selective guest inclusion, however, the overall flexibility of each crystal is predominantly affected by the host packing. Additionally, the durability of each crystal was tested by comparing the X-ray diffraction reflection images before and after the bending experiments to confirm that the single crystallinity was retained.

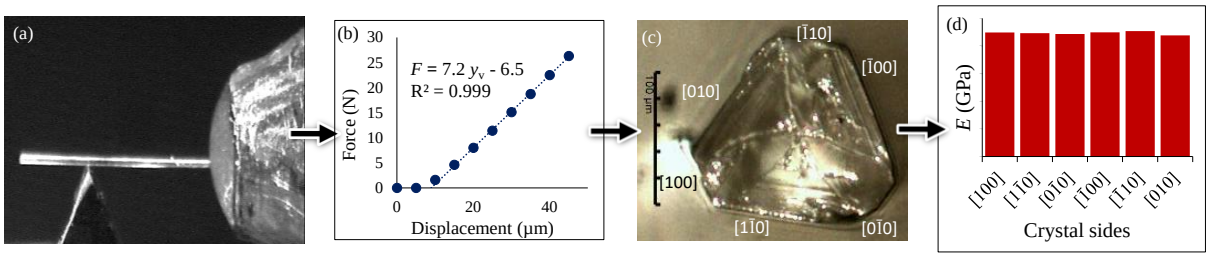

Fig. 1 Experimental method to determine the value of E for a single crystal of **1**. (a) Bending experiment carried out on a single crystal. (b) Force *vs* displacement measurements performed on the *Flexometer*. (c) Crystal indexing and normalisation processing. (d) Calculation of the value of E for each face of the crystal.

References

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