# Exploring the mechanism of elastically flexible crystals by automatic analysis

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A recent surge in reports of crystals exhibiting elastic flexibility has changed the way we view these materials. With potential applications in flexible electronics, in depth research is required to understand why some crystals can be tied into knots, while others shatter under an applied force. Different rationales for elastic flexibility have been proposed: many crystals have been engineered to impart flexibility through isotropic interactions, although other elastic crystals have anisotropic interactions [1]. Clearly, the different interactions present result in diverse bending mechanisms. The mechanism of flexibility in elastic crystals can be resolved on an atomic-scale by use of micro-focused synchrotron radiation [2]. By examining the localised crystal structure at multiple positions across a bent crystal, the deformations of the cell parameters can be quantified (Fig. 1). Isotropic and anisotropic crystals have been analysed using this technique to determine their respective mechanisms.

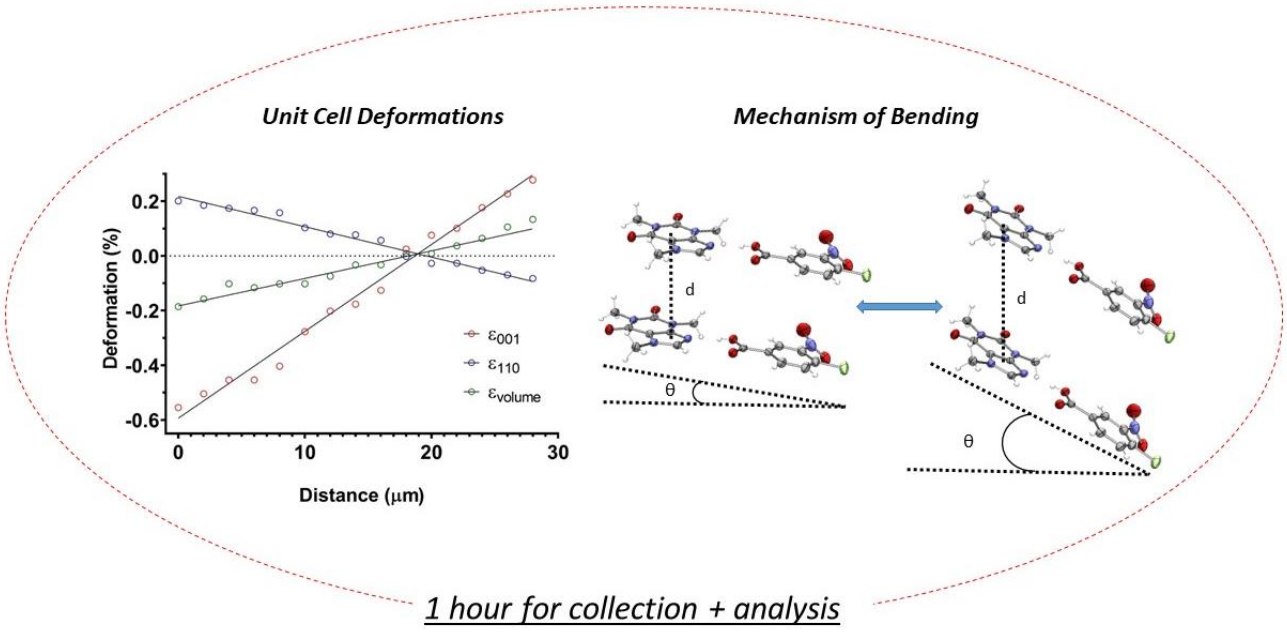


**Figure 1**. Unit cell deformations of a bent crystal analysed via the auto-processing software, *CX-ASAP*

Unfortunately, structural mapping quickly produces large volumes of data, and manual processing would be inefficient when there are only small changes to the data. Instead, software was developed to automatically process these datasets. It is capable of taking raw frames and providing finalised CIF files with results graphically analysed. This allows for greater insight into these elastic crystals, as more data can be analysed in a reasonable time frame. This software, *CX-ASAP*, consists of a series of independent modules which can be placed together into an auto-processing pipeline. The advantage of this modular approach, is the fact that it is applicable to a wider range of large crystallographic dataset analysis, such as variable temperature experiments. The main consideration of this software is the limit of computer knowledge, as there are key steps during the automation where user input is mandatory for reliable results.

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