Poster

Centring of Diamond Anvil Cells Using an Optical Sensor

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High pressure is a great tool to be used for studying the crystallographic properties of molecular materials, which has developed remarkably in the past few decades and becomes a well-established technique to be widely applied [1]. And thanks to the invention and developments of the diamond anvil cell (DAC) (Fig. 1) in the 1950-60s [2-4], the generation of high static pressures in the laboratory is greatly facilitated, lowering the technical threshold of studying materials under extreme conditions. This also raised the awareness of scientists regarding the use of pressure to scrutinise the relationship between molecular structure and material properties.

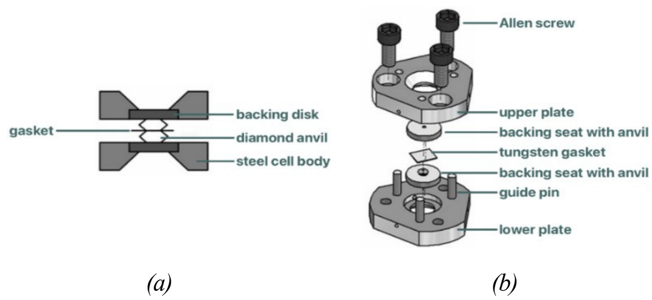

Figure 1. *(a)* An illustration of the cross-section through a diamond anvil cell (DAC). *(b)* Merrill-Bassett DAC [5].

While the practicality of DAC has been unarguably demonstrated and testified over the years, with respect to the high-pressure work by X-ray diffraction, the centring of the cell onto the diffractometer can still be an arduous task. In this study, the standard experimental approaches for setting up the Merrill–Bassett DAC were followed, while a confocal system (Micro-Epsilon IFS2406-3 confocal device with Confocal DT2421 control unit) was used to optically centre the cell with the diffractometer. The optical system can project polychromatic light onto the target surface, in this case, the crystal mounted on the goniometer head, and with the reflected light from target surface received by the sensor and transferred to the controller, a distance measurement can be performed to determine whether the target and the X-ray source are aligned. This user-friendly system with high-precision measurements provided certain convenience in centring the pressure cells.

This work aims to examine the crystallographic properties of glyphosate [6] (Fig. 2) using single-crystal X-ray diffraction, and compare the effect of applying different offsets during the centring process on the collected data. Two types of X-ray sources were applied: molybdenum (Mo) Kα radiation and silver (Ag) Kα radiation. With the increase number of offsets introduced to the DAC centring, the *R* factors increase accordingly, in general, thus validating the influence of offset on the quality of crystallographic data.

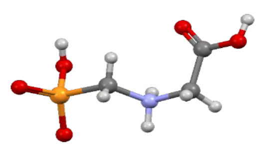

Figure 2. The zwitterionic molecular structure of glyphosate

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