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APPLICATION NOTE

The New Diacell® Bragg-XVue Diamond Anvil Cell (DAC) Explained

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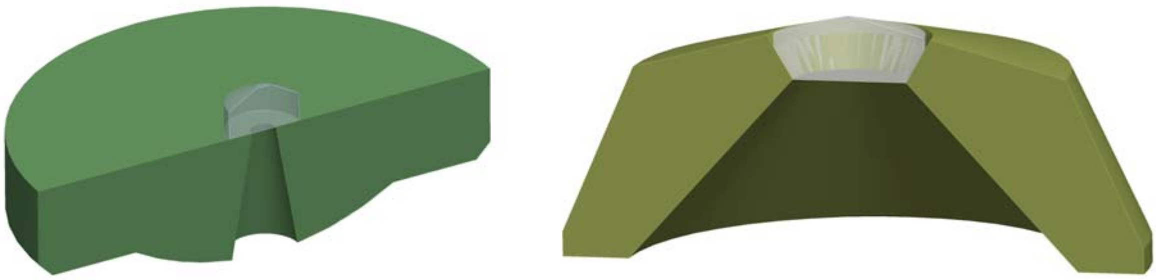
1. Introduction

The Diacell® Bragg XVue DAC is based on developments by Professor Reinhard Boehler of the Max Planck Institute for Chemistry in Mainz, Germany. The novel aspects of this cell will be described below. The cell allows X-ray observations of a sample over a high angle (4θ = 85°), with absorption only by the anvils and not through any "transparent" backing plates.

2. Novel Features

a. Conical Anvils

Figure 1a shows a standard anvil mounted on a beryllium plate for X-ray work, while Figure 1b shows a conical anvil on its special support. In both cases the 4θ angle is 85° and the supports stand over this aperture in the cell base.



(a) (b)

Figure 1: (a) standard design anvil mounted on a beryllium support place; (b) conical anvil on special tungsten carbide support plate.

When force is applied to the culet, the base of the anvil tends to spread while the support tends to contract at the top and spread at the base. In both cases the contraction in the support tends to counteract the spreading in the base of the anvil. However, for the standard anvil this effect is limited to the coefficient of friction between anvil and support and also is localized to the table of the anvil. For the conical anvil the spread is directly opposed by the contraction of the top of the support, and this constraint is carried up the bezel (the conical base of the anvil). Thus the compression in the support of the conical anvil will reduce the hoop and radial stress components in the base of the anvil much more than will the standard support. This enables the conical anvil to span a much larger hole than a standard anvil of similar dimensions will span.

Therefore it is possible to achieve much greater unsupported X-ray angles with a conical anvil. The conical anvil can also be made slightly thinner than a standard one.

Traditionally, beryllium seats have been used for X-Ray diffraction experiments as, unlike other metals, Be has a low mass absorption coefficient so is fairly transparent to X-Rays. Nevertheless, Be support plates always exhibit a diffraction pattern which can be inconvenient for some experiments. The conical support plates solve this problem as there is no absorbing material at the back of the diamond anvils. However, the cone angles of the bezel and the socket in the support must be very closely matched, otherwise the anvil will not be properly supported and could tend to rock. It is not trivial to achieve the degree of matching needed here; but, once accomplished, the lower stress condition of the conical anvil then becomes available.

b. Kinematic Mount

This cell has an unusual way of achieving stability to make the lateral and tilt adjustments to bring the anvil culets into line. Normally a diamond anvil cell will rely on the accurate machining and grinding of a piston and cylinder, or of guide rods and holes, to maintain the alignment of the cell.

The kinematic mount, in contrast, fixes the PCD and spacing in one plate and allows the guides to find their own stable position in channels on the other plate.

c. Plate Deflection

Most diamond anvil cells use a sliding arrangement, either of a piston in cylinder or of a plate along guide rods, to allow the anvils to move towards each other. The Diacell® Bragg XVue sets the two plates a fixed distance apart, and then bends them to bring the anvils into contact. Figure 2 shows the arrangement.

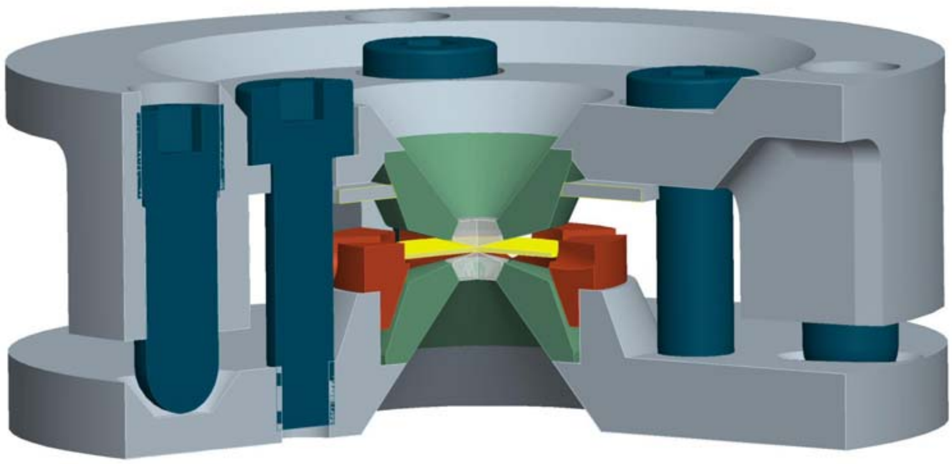


Figure 2: Cross section of Diacell® Bragg XVue.

The plates are held apart by the tilt adjustment screws toward the edge, while the clamping screws toward the centre force the anvils together. A disadvantage is the extra force required to bend the plates, in addition to the usual force needed to press the anvils together. This disadvantage is partly overcome by the fourth innovation, the gearbox.

d. Gearbox

In a cell whose alignment is maintained through three screws at the edge, locating a pair of plates which are bent towards each other, it is important to make sure that the plates will bend symmetrically with respect to the support positions. The clamping screws have the same symmetry as the supports, but the tightening of the screws must also preserve the same symmetry. If one screw is tightened more than the other two, this is likely to upset the alignment of the anvils. The gearbox ensures that all three screws are tightened equally. By using a gear ratio of 4 to 1, the leverage needed to tighten all three screws together is reduced to less than is needed for a single screw at a time. To achieve sufficient force to generate the highest pressures, a holder for the cell is also available, so that the round cell can be gripped more securely as shown in Figure 3.

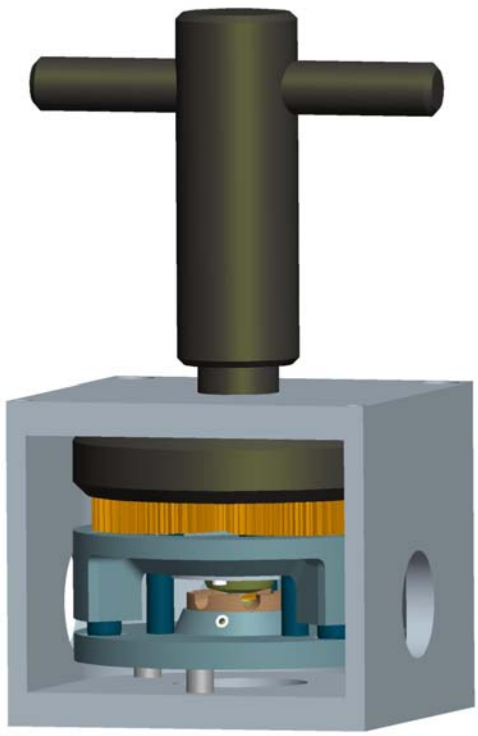


Figure 3: Diacell® Bragg XVue in its holder. This holder is unique to the Bragg XVue and greatly facilitates the process of applying pressure to the cell.

3. Operation

a. Alignment

The tilt adjustment screws (see Fig. 2) have a triple function:

1. adjusted individually, they allow the anvil culets to be made parallel
2. collectively, they determine the anvil spacing before loading is applied
3. through the kinematic mount, they locate the anvils laterally, allowing stable fine adjustment by the lateral adjustment screws

b. Pressure Generation

The gasket may be pre-indented by applying the expected maximum load for the experiments. The hole for the sample, pressure medium and calibrant (such as ruby; *c.f.* Optiprexx PLS) is drilled in the centre of the indentation (*c.f.* Boehler µDriller). The sample is then loaded into the hole and sealed by tightening the clamping screws (using the gearbox) until the culets are in contact with both sides of the gasket. The Diacell® Bragg XVue is now ready for experimental pressures to be applied.

The cell, with the keys of the gears in the sockets of the clamping screws and the gearbox plate holding the gears together, is inserted into the holder with one of the tilt screw pillars sliding between the pegs. The gearbox handle is inserted into the hole of the holder, so the pinion on the handle meshes with the gears, as in Figure 3. Load can now be applied using the gearbox to turn the clamping screws. The anvils can still be seen through the sight-holes in the holder and the gasket holder. If necessary the holder can be clamped in a vice to apply high loadings – but in any case it serves as an invaluable aid to facilitate the whole process of applying pressure to the Diacell® Bragg XVue.

4. References

- Reinhard Boehler *et al.*, New Anvil Designs in Diamond Cells, High Pressure Research, **24**, 291, 2004.
- Reinhard Boehler, New Diamond Cell for Single Crystal X-Ray Diffraction, Review of Scientific Instruments, **77**, 115103 (2006).