

# Supporting information for: Use of a miniature diamond anvil cell in high-pressure single-crystal neutron Laue diffraction

Authors

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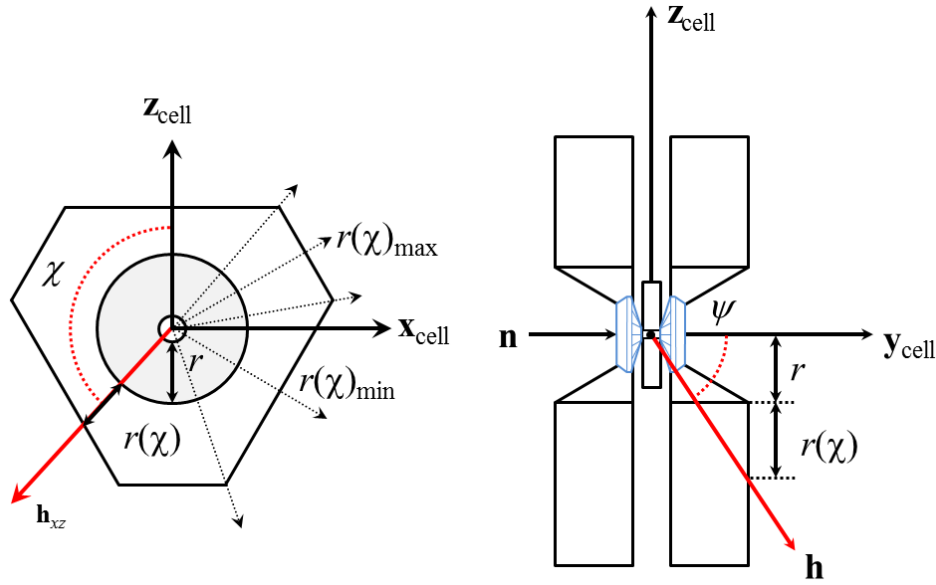
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## Supporting information

### S1. Attenuation correction calculation

The path length of a ray passing through the cell-body was determined in a reference axis system attached to the cell where  $\mathbf{y}_{\text{cell}}$  lies along the cell axis,  $\mathbf{z}_{\text{cell}} \parallel \mathbf{z}$ , and  $\mathbf{x}_{\text{cell}} = \mathbf{y}_{\text{cell}} \times \mathbf{z}_{\text{cell}}$ . The cell has three-fold symmetry about  $\mathbf{y}_{\text{cell}}$  and can be divided into six sectors based on the angle,  $\chi_i$ , between the projection of a reflection  $\mathbf{h}_i$  in the  $\mathbf{xz}_{\text{cell}}$  plane of the cell reference system and the  $\mathbf{z}_{\text{cell}}$  axis (Figure S1).



**Figure S1** (Left) The mini-DAC has three-fold rotational symmetry allowing six sectors to be defined on the basis of angle  $\chi$  (Right) The value of  $r(\chi)$  is used to define a further set of sectors creating limiting values of  $\psi$ . Within each sector a trigonometric expression determines the total path length through the cell body. The thickness of the gasket and sample is exaggerated for clarity.

For the cell rotated to an angle  $\phi$ , the cell axis system of unit vectors is determined by applying rotation matrix  $\Phi$  as in 1 for  $\mathbf{x}_{\text{cell}}$ .

$$\mathbf{x}_{\text{cell}} = \Phi \cdot \mathbf{x} = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad 1$$

The model of the cell is constructed from a  $\chi$ -independent section denoted  $r$  (5.25 mm) and a  $\chi$ -dependent length,  $r(\chi)$ , to account for the change in cell shape with rotation about  $\mathbf{y}_{\text{cell}}$  between upper and lower limits of 6.25 and 3.25 mm. For each reflection, the detector coordinates  $(x_i, z_i)$  and radius  $R$ , determine the ray  $\mathbf{h}_i$  by equations 2 and 3.

$$\gamma = \frac{x_i}{R} \quad 2$$

$$\mathbf{h}_i = \begin{pmatrix} R/\sin \gamma \\ R/\cos \gamma \\ z_i \end{pmatrix} \quad 3$$

The angles  $\chi_i$  and  $\psi_i$  and consequently value of  $r(\chi_i)$ :

$$\chi_i = \arccos\left(\frac{\mathbf{h}_{xz,i} \cdot \mathbf{z}_{cell}}{|\mathbf{h}_{xz,i}| |\mathbf{z}_{cell}|}\right) \quad 4$$

$$\psi_i = \arccos\left(\frac{\mathbf{h}_i \cdot \mathbf{y}_{cell}}{|\mathbf{h}_i| |\mathbf{y}_{cell}|}\right) \quad 5$$

For example, in the range  $0^\circ < \chi < 45^\circ$   $r(\chi)$  is given by A6,  $r(\chi)_{\min}$  is determined at  $0^\circ$ ,  $r(\chi)_{\max}$  at  $60^\circ$ . The other limiting angles are  $\chi = 75^\circ$ ,  $120^\circ$ , and  $165^\circ$  between which similar expressions are used with  $r(\chi)_{\min}$  or  $r(\chi)_{\max}$  as appropriate.

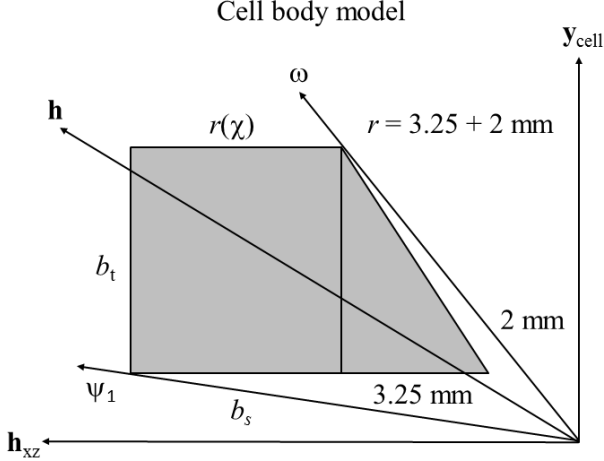
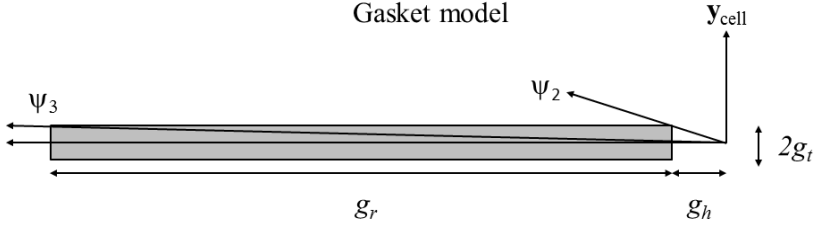
$$r(\chi_i) = \frac{r + r(\chi)_{\min}}{\cos \chi_i} - r \quad 6$$

For the backing-plate thickness, cell body separation, gasket dimensions, and  $r(\chi_i)$ , a set of limiting  $\psi_i$  angles are calculated to determine whether the diffracted ray passes through the diamonds, gasket, and cell body.

For rays passing through the cell body, the path length is determined by calculating points of intersection with the cell faces. Path lengths through the gasket are calculated by a simple trigonometric expression. Once the path lengths through the cell body  $l_{i,cb}$ , diamonds  $l_{i,d}$ , and gasket  $l_{i,g}$ , are determined, the attenuation for each reflection  $i$  is then calculated using the expression 7. Since the attenuation due to the diamonds is so low relative to the gasket and cell body, this term is omitted for  $\psi > \omega$ . The guide pins (Cu-Be) and screws (Fe) are omitted from the model. The gasket was circular in shape simplifying the correction term. Details are given in Table S1.

$$a_i(\psi_i, \chi_i, \lambda_i) = \frac{I}{I_0} = e^{-\mu_{cb}(\lambda_i)l_{i,cb}(\psi_i, \chi_i)} e^{-\mu_g(\lambda_i)l_{i,g}(\psi_i, \chi_i)} e^{-\mu_d(\lambda_i)l_{i,d}(\psi_i, \chi_i)} \quad 7$$

**Table S1** Expressions for determining angular limits and path length  $l_i$ . Calculations are carried out in the plane containing the diffracted beam  $h$  and the cell axis  $y_{\text{cell}}$ .  $b_t$  is the cell body thickness (5 mm),  $b_s$  is half the cell body separation (1.625 mm),  $r$  is the fixed cell radius (5.25 mm) which is the sum of the radius of the cell opening  $d_r$  (2 mm) and the inner cone radius  $r_{\text{cone}}$  (3.25 mm),  $r(\chi)$  is the  $\chi$ -dependent cell radius (maximum value 6.25 mm, minimum value 3.25),  $g_t$  is half the gasket thickness,  $g_h$  is the gasket hole radius and  $g_r$  is the gasket radius. The diamond height,  $d_h$  is 3 mm, set into the body by 1.5 mm,  $d_r$  is the radius of the cell opening (2 mm).

$\psi$ limits for cell body	
$\omega = \text{atan}\left(\frac{r}{b_t + b_s}\right)$	Cell-opening angle.
$\psi_1 = \text{atan}\left(\frac{r + r(\chi)}{b_s}\right)$	High-angle limit of cell body.
<p style="text-align: center;">Cell body model</p> 	
<p style="text-align: center;">Gasket model</p> 	
$\psi$ limits for gasket	
$\psi_2 = \text{atan}\left(\frac{g_h}{g_t}\right)$	Low-angle limit of gasket
$\psi_3 = \text{atan}\left(\frac{g_r + g_h}{g_t}\right)$	High-angle limit of gasket
$\psi$ range	Expression for $l_i$
$\psi \leq \omega$	$l_{i,d} = \frac{d_h}{\cos \psi}$

$$\omega < \psi \leq \psi_1$$

Diffacted ray has equation

$$y_h = \frac{x}{\tan(\psi)}$$

Intercepts are determine between  $y_h$  and the two possible entry points:

Conic opening face:

$$y_{cone} = \left(\frac{b_t}{r_{cone}}\right)x + b_s - \left(\frac{b_r d_r}{r_{cone}}\right)$$

Cell rear face:

$$y_r = b_s$$

The point furthest from the origin is the first intercept. The second set of intercepts is determined between:

Cell front face:

$$y_f = b_s + b_t$$

Cell side wall:

$$x = r + r(\chi)$$

The point closest to the origin is the second intercept. The path length  $l_{i,cb}$  is the distance between these points.

$$\psi_1 < \psi \leq 90^\circ$$

Ray passes between cell bodies, gasket attenuation only.

Gasket terms	Expression for $l_i$
$\psi_2 < \psi \leq \psi_3$	$l_{i,g} = \frac{g_t - (g_h \tan(90^\circ - \psi))}{\sin(90^\circ - \psi)}$
$\psi_3 < \psi \leq 90^\circ$	$l_{i,g} = \frac{g_r}{\sin(\psi)}$
<b>Linear attenuation functions <math>\mu(\lambda)</math></b>	
Diamond	$\mu_d(\lambda) = 0.0005\lambda$
BERYLCO-25 (Cu <sub>0.87</sub> Be <sub>0.13</sub> , density 8.249 g cm <sup>-3</sup> )	$\mu_{cb}(\lambda) = 0.1611\lambda + 0.042$
Iron	$\mu_g(\lambda) = 0.1208\lambda + 0.0332$