Stress computation and optimizing the shape of a miniature opposed anvil through finite element analysis

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Abstract. We have demonstrated stress computation of high-pressure apparatus to obtain effective pressure with a miniature opposed anvil cell. The anvils and the gasket were assumed to be made of tungsten carbide (WC) and of stainless steel (SUS 304), respectively. The pressure medium was presumed to be liquid to generate hydrostatic pressure. Considering cell thickness, we set the anvil radius to approximately 6 mm. In order to keep a large space with a diameter of 1 mm, the diameter of 3 mm was fixed on the tip of anvils. Using the stresses found in the analysis, we evaluated the anvil in terms of pressure efficiency and fragility. Calculating pressure in the sample space between anvils and the maximum differential stress of an anvil, we found that the best pressurization efficiency and lowest fragility was achieved with an anvil structure with an angle $\theta$ of 15 degrees and height $h$ of 5 mm.

1. Introduction
High-pressure technique has been recognized as a powerful tools to investigate the physical properties of solids because pressure can distinctly vary physical parameters due to the contraction of its lattice constants. There is the possibility that other property changes may occur, such as structural phase transition and magnetic transition under high pressure[1, 2, 3, 4]. To perform such measurements under high-pressure condition, there is a need to combine a high-pressure cell with other devices that allow modifying parameters such as temperature and magnetic field in addition to pressure in order to explore material properties. However, the size of high-pressure generators is generally limited to combine and use with other instruments. Therefore, it is important to develop space efficient high pressure apparatus to make various experimental techniques accessible to high pressure.

Many trials have been reported using Bridgman anvil cells, diamond anvil cells, and so on[5, 6], where smaller anvil surface areas allow high pressure to be obtained with smaller loads. In general, the pressurizing efficiency of the device is decided based on a variety of factors, such as the compressive strength and tensile strength of the shape of each part. In order to miniaturize the device, the anvil is thinned and the cell thickness is reduced, making this even more difficult. Our aim is to develop a small high pressure cell by optimizing the shapes of the anvil and cells from stress analysis.
2. Basic Construction of the Apparatus
We suppose that the device is being combined with a commercial low-temperature magnetic field generator and set the cell diameter to 20 mm. The basic construction of the anvil was nearly the same as in our previous report[6], as shown in Figure 1. High-pressure generators generally have many large parts, but we attempted to reduce the number of parts in this apparatus as much as possible and simplify the structure of the parts so that pressure can be easily applied. Pressure is generated in a gasket between the anvils made of tungsten carbide (WC). The gasket is made of stainless steel (SUS 304) to maintain pressure. A hole with an internal diameter of 1 mm is made and filled with the material as well as a liquid pressure transmitting medium to increase hydrostatic pressure. The cell body is made of hardened beryllium copper (BeCu). Both ends are closed by screws. The load is applied to the top of upper anvil and the force is blocked by tightening the upper screw of the cell. Considering cell thickness, we set the anvil radius to approximately $R = 6$ mm. In order to secure a test material space with a diameter of 1 mm, the diameter of the upper surface of the anvil was fixed at 3 mm.

![Figure 1. A cross section of the high pressure cell. To simplify the figure, we omitted the screws to fix the anvils after the load is applied.](image)

3. Stress Analysis Through The Finite Element Method
A finite element method (FEM) is a powerful tool to investigate irregular and/or complicated systems. In order to examine the conditions that efficiently produced high pressure gives the above restrictions, we demonstrated stress computation of a part of high-pressure cell between the anvils. The model was implemented using COMSOL Multiphysics 3.4, a commercial FEM solver, and the Geoscience Research Laboratory’s program Easy-Sigma 2D Lite[7].

In order to simplify the analysis, we made the anvils with top/bottom symmetry and bound the center of the anvil to conduct analysis only on the bottom half. Also, taking account of the anvil with vertical-axis symmetry, we performed two-dimensional analysis on one side of the anvil cross-section. We designed a variety of anvils with different parameters for anvil angle $\theta$ and height $h$, and applied loads $F$ up to 10 ton from the upper anvil in the downward direction. The material properties implemented in our simulations are taken from the literature values for WC and SUS 304. A Young’s modulus $E = 580$ GPa and a Poisson’s ratio $\nu = 0.22$ were used for the properties of WC, and $E = 193$ GPa and $\nu = 0.3$ for those of SUS 304[8]. Although a liquid has generally a Poisson’s ratio $\nu = 0.5$, $\nu = 0.4$ was used for the pressure transmitting medium because of the system limitations of the FEM program. $E = 43$ GPa is estimated from $\nu$ and a bulk modulus $B$. Since $B$ of pressure transmitting medium depends on pressure, the value of a water at 5 GPa[9] was used in the present work.
Figure 2. An example of stress distribution of a cross section of a part of high pressure cell. Stresses $\sigma_r$, $\sigma_z$, and $\sigma_\phi$ on cylindrical coordinates are calculated through FEM analysis when the load $F = 3$ ton was applied to an anvil of $\theta = 15^\circ$ and $h = 5$ mm. The unit of stress is GPa.

4. Results and discussion

We calculated stresses when a radial direction $r$ from the central axis of the high pressure cell, that of central axis $z$, and that perpendicular to $r$ and $z$, $\phi$ as coordinate axes of a cylindrical coordinate system. Figure 2 shows an example of a cross section. Here, the load $F = 3$ ton was applied to an anvil of $\theta = 15^\circ$ and $h = 5$ mm. Each stresses $\sigma_r$, $\sigma_z$, and $\sigma_\phi$ is described corresponding to each axes, respectively. It is clear that the magnitudes of every stresses $\sigma_r$, $\sigma_\phi$, and $\sigma_z$ are the highest at the edge on a tip of anvil where an anvil touches a gasket. It is related to the fact that an edge of an anvil is firstly broken in most cases that the load is actually applied.

At the part of a pressure transmitting medium, on the other hand, all values of $\sigma_r$, $\sigma_\phi$, and $\sigma_z$ are almost same within $\pm0.1$ GPa. It indicates that the sample can be compressed by the pressurization of a hydrostatic pressure in the pressure transmitting medium. Here, we estimated the pressure $P$ in sample space as a deviatoric stress which is an average of $\sigma_r$, $\sigma_\phi$, and $\sigma_z$. In the case of Figure 2, the magnitude of $P = 1.2$ GPa is much smaller than that in the experimental result, where $P = 4$ GPa is developed by applying the load $F = 3$ ton[6]. It may come from the fact that the parameters used in the FEM analysis are different from the actual value because a 1:1 mix of Fluorinert FC70 and FC77 is used as a pressure transmitting medium in the previous report. Moreover, both $E$ and $\nu$ depend on pressure, and a liquid pressure transmitting medium
freeze solid and a bulk modulus increases sharply as increasing pressure. To calculate $P$ using exact values of the parameters in the FEM analysis, the measurement of the compression curve of a pressure transmitting medium is planned in future.

Using the stresses found in the analysis, we evaluate the anvil in terms of pressure efficiency and fragility. First, we examine how changes to $\theta$ and $h$ affect $P$ in a pressure transmitting medium. Next, to evaluate the fragility, we defined a differential stress $Y$, which is the difference of the anvil between a maximum main stress $\sigma_z$ and a minimum main stress $\sigma_r$. As $Y$ increases, the anvil becomes more fragile. In all high pressure cells we calculated, the maximum differential stress $Y_{\text{max}}$ is the value at the edge on the tip of the anvil. Since it is consistent with the fact that an edge of an anvil is firstly broken in most cases that the load is actually applied, it is reasonable to evaluate the fragility of the anvil by examining how changes to $\theta$ and $h$ affect $Y_{\text{max}}$.

Figures 3 and 4 show $P$ and $Y_{\text{max}}$ as a function of applied load $F$, respectively. One condition for breaking the material is when $Y_{\text{max}}$ exceeds the compressive strength of the material. For example, when the anvils are made by submicron cemented carbide grades (Sandvik Co. Ltd.) where the compressive strength is about 8 GPa, the pressure cell can be applied the load up to about 10 tons. Both $P$ and $Y_{\text{max}}$ increases proportionally as increasing $F$, while pressure calibration curve is not actually quite simple in a commercial Bridgman anvil cells[6]. Although it comes from the fact that we simplified the structure of a high pressure cell for the FEM analysis, it is possible to evaluate the best pressurization efficiency and lowest fragility at least qualitatively.

![Figure 3](image1.png)  
**Figure 3.** Pressure $P$ of a sample space as a function of the load $F$ ($\theta=15^\circ$).

![Figure 4](image2.png)  
**Figure 4.** The maximum differential stress $Y_{\text{max}}$ as a function of the load $F$ ($\theta=15^\circ$).

Figure 5 shows pressure $P$ of a sample space as a function of the angle $\theta$ of the anvils when a 10 ton load is applied. $P$ reaches a maximum when $\theta$ is 15 degrees. This is due to the fact that at the angle increases between 5 to 15 degrees, stress is concentrated on the tip, raising $P$. Above 15 degrees, more stress escapes in the horizontal direction and $P$ decreases. On the other hand, as shown in Figure 6, $P$ tends to be enhanced below $h = 10$ mm for all angles $\theta$. These results may come from the fact that vertical direction stress $\sigma_z$ reaches its extreme.

Figure 7 shows the maximum differential stress $Y_{\text{max}}$ as a function of angle $\theta$ of the anvils when a 10 ton load is applied. $Y_{\text{max}}$ decreases monotonically as $\theta$ decreases, and tends to saturate
Figure 5. Pressure $P$ of a sample space as a function of angle $\theta$ of the anvils when a 10 ton load is applied.

Figure 6. Pressure $P$ of a sample space as a function of height $h$ of the anvils when a 10 ton load is applied.

Figure 7. The maximum differential stress $Y_{\text{max}}$ as a function of angle $\theta$ of the anvils when a 10 ton load is applied.

Figure 8. The maximum differential stress $Y_{\text{max}}$ as a function of height $h$ of the anvils when a 10 ton load is applied.

below 15 degrees. On the other hand, as shown in Figure 8, $Y_{\text{max}}$ tends to be suppressed below $h = 10$ mm for all angles $\theta$. These results indicate that it is hard to break when the low anvils were used in the pressure cell.

From these results about $P$ and $Y$, we consider the optimal anvil structure using calculation results. First, because $P$ was highest at 15 degrees, a value of 15 degrees is suitable for $\theta$. While smaller values of $\theta$ are better for $Y_{\text{max}}$, Figure 7 shows that there is no significant difference in values between 5 and 15 degrees. Thus, we prioritize pressurization efficiency and set the optimal angle at 15 degrees. Next, we found that $P$ was largest and $Y_{\text{max}}$ was smallest when $h$
= 5 mm. This means that pressurization efficiency was suitable and the anvil was less fragile, so we set the optimal value of $h$ at 5 mm.

5. Summary
In the present work, a FEM analysis was performed to optimize the shape of an anvil of opposed anvil cell. We found that the best pressurization efficiency and lowest fragility was achieved with an anvil structure with an angle $\theta$ of 15 degrees and height $h$ of 5 mm. In future, we will conduct stress analysis of the overall pressure cell, including the anvil, used to maintain pressure within the sample space. Specifically, we must examine the optimal shape of the overall cell to examine the optimal anvil diameter, cell thickness for maintaining high pressure and the necessary overall cell height.

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