Toroidal Diamond Anvils for Multi-megabar Experiments

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Toroidal anvils and FEA

- In order to improve durability and mitigate diamond anvil failure, toroidal recesses can be machined into diamond anvil surfaces using focused ion beams (FIB)
- Early investigations have indicated that the achievable pressure range can be extended up to 500 GPa
- We have used finite element analysis (FEA) to investigate toroidal anvil geometries and evaluate their applicability to high-pressure research

Simulation Setup

FEA provides a simple yet robust mathematical framework for simulating material properties; boundary conditions are applied to the system and these are iteratively propagated through a solid or surface via finite elements. The implicit simplification in these simulations is that properties such as energy, stress, or temperature are approximately constant within each element but vary across the bulk.

The FEA simulations were performed using the ANSYS software package. This solves the generalized Hooke's law relating the stress vector $\boldsymbol{\sigma}$ to the strain vector $\boldsymbol{\epsilon}$ by the stiffness tensor $\boldsymbol{C}$:

$$\boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\epsilon}$$

The stiffness tensor for cubically symmetric structures is represented in Voigt notation as follows:

$$\boldsymbol{C} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

where the values of the stiffness tensor were taken from Ref. [1] and are shown in Table 1.

Diamond failure frequently occurs during ultra-high pressure experiments and this was accounted for by including stress and strain limits in the simulation. These have been calculated from first principles in Ref. [3] and are shown in Table 2.

The Factor of Safety (FoS) was considered as an indication of where diamond failure was likely. This is generally defined such that a FoS of unity indicates failure and increases above this threshold signify a decrease in failure rate:

$$FoS = \frac{yield\ stress}{current\ stress}$$

The tungsten sample was taken to have an isotropic elastic modulus of 1435 GPa and Poisson ratio of 0.329 as given in Ref. [2].

Note that only a quarter cross-section of the entire assembly was modelled to decrease computational cost; the setup was assumed to be symmetric about the X and Y axes.

C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
2622	1185	1232

Table 1. Elastic moduli of diamond from Ref. [1]

	Stress Limit (GPa)	Strain limit
Compressive	-223.1	-0.28
Tensile	222.5	0.13

Table 2. Compressive and tensile stress and strain limits for diamond from Ref. [3]

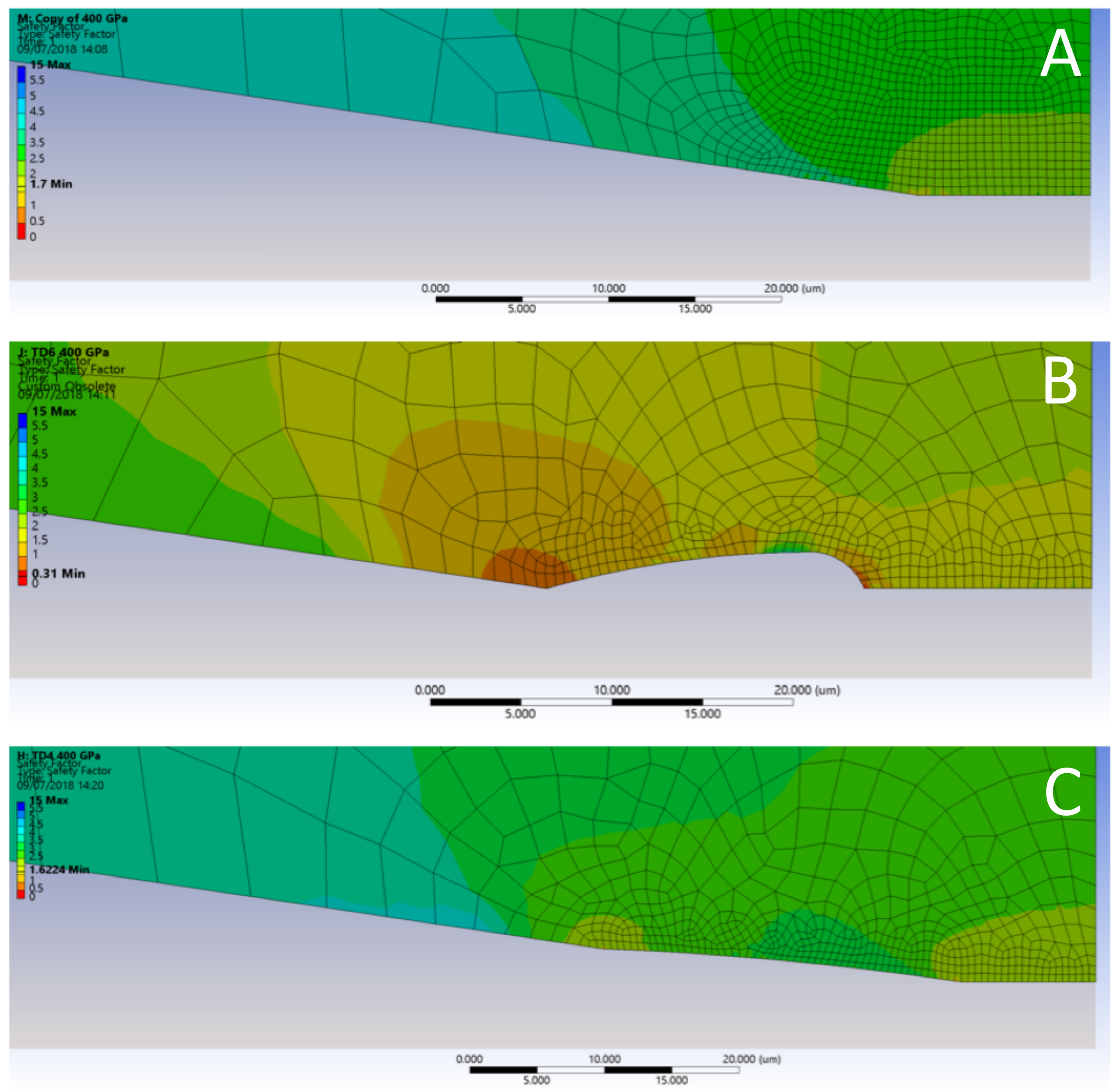

Figure 1. Factor of Safety plots for various diamond anvil geometries with culet pressures of around 400 GPa. (A) displays a standard beveled anvil with a 20 μm culet, (B) shows a toroidal profile machined into a 60 μm culet with a depth of 2 μm, and (C) is a very shallow profile where the culet edge has machined away.

Results

All geometries were tested at a central culet pressure of 400 GPa in order to facilitate comparison against experimental data from Ref. [4].

A regular 250 μm to 20 μm beveled diamond, as used in Ref. [4], was modelled for reference and is shown in Figure 1A. It displays an expected pressure distribution with a sharp peak at the culet and fairly rapid decline in the beveled area, as shown in Figure 2. Failure is most likely at the culet edge but a minimum FoS of 1.7 indicates that the diamond has not failed.

Various toroidal geometries were considered as well. Presented in Figure 1B is a profile inspired by Ref. [5] with a central culet of 13 μm, a tore depth of 2 μm, and a tore radius of 60 μm which reportedly reached pressures of 335 GPa before failing. As expected, at a culet pressure of 400 GPa the FoS at the outer edge of the tore is in fact below 1. It is noteworthy that the failure appears to occur at the edge of the tore, rather than at the culet. This is most likely due to high stress from the gasket material pushing outwards. As seen in Figure 2, this also results in very high pressure on the sample, even higher than that on the culet; the cupping of the diamond likely contributes to this.

Figure 1C shows a concept similar to one proposed in Ref. [6] where the culet edge has been smoothed. This was originally suggested to prevent the culet edges from coming into contact under heavy cupping. Here it also diminishes the outward pressure on the diamond as the gasket material more readily flows outwards.

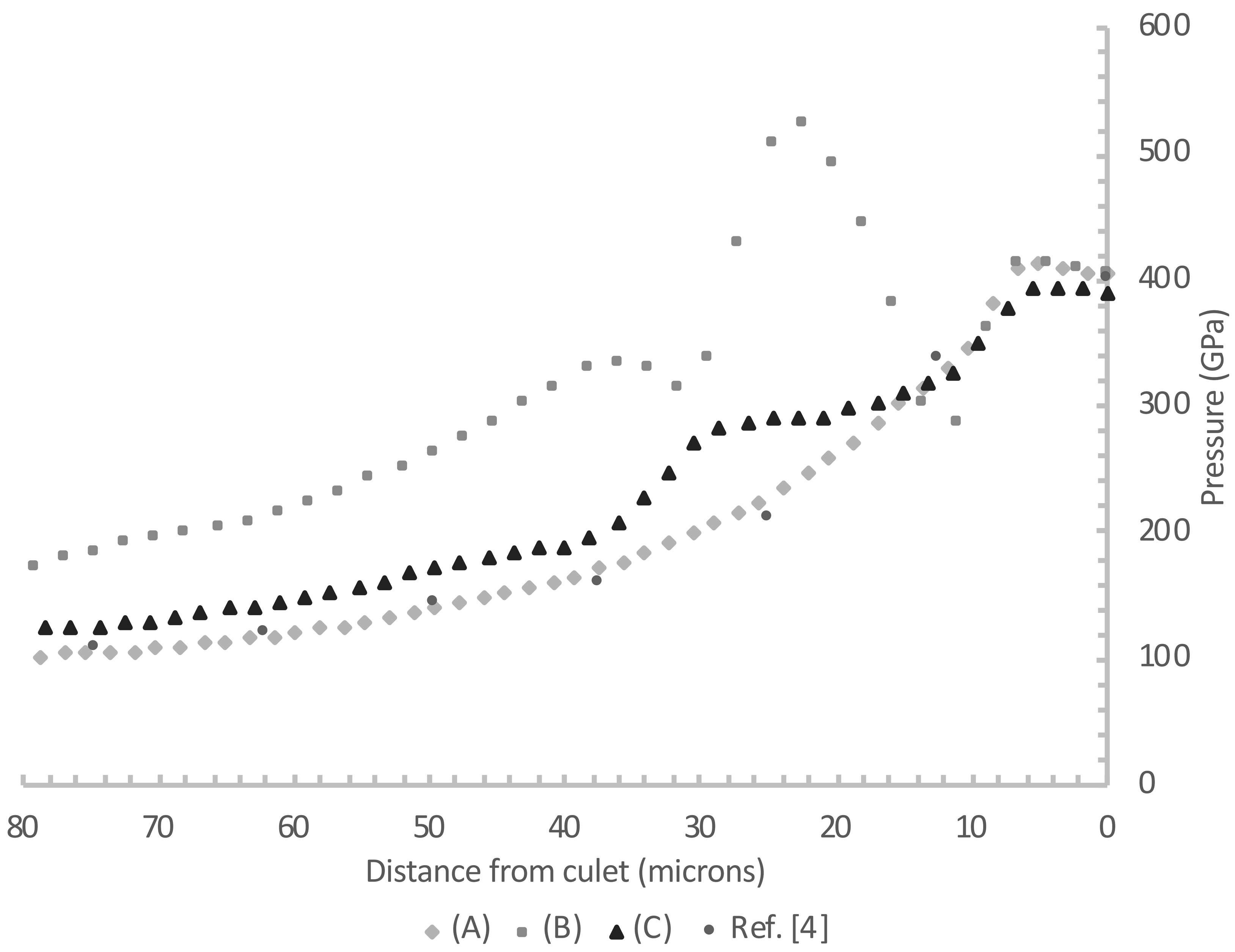

Figure 2. Pressure distributions as a function of distance from the culet centre. The profile used in (A) closely matches the experimental data from Ref. [4] as anticipated; (B) shows a slight increase in pressure around 30 μm where the diamond bevel begins; (C) shows an exceptional spike at 22 μm which appears to be a result of additional compression as the sample is pushed outwards.

References

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Acknowledgements

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Next Steps

- Use our insights regarding the efficacy of toroidal diamonds anvils to begin creating our own geometries in-house
- Develop techniques for preparing and loading toroidal diamond anvil cells
- Study a wide range of elements at multi-megabar pressures
- Particularly focus on the alkali metals and light alkaline earth metals