Raman frequencies of diamond under non-hydrostatic Pressure

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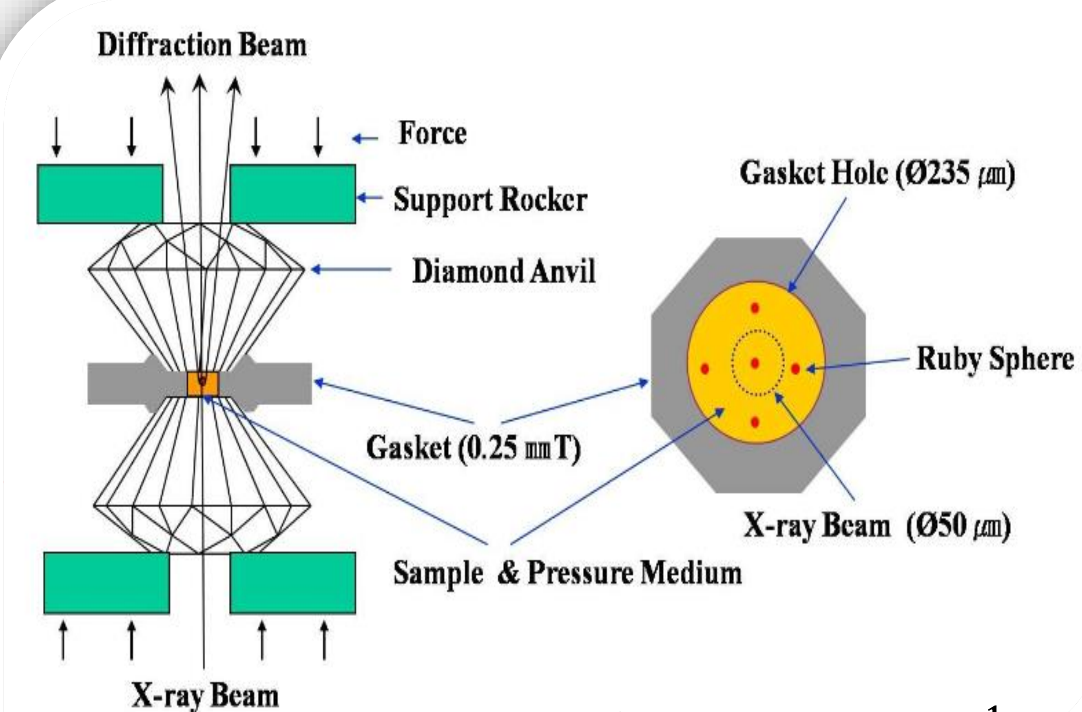
Introduction

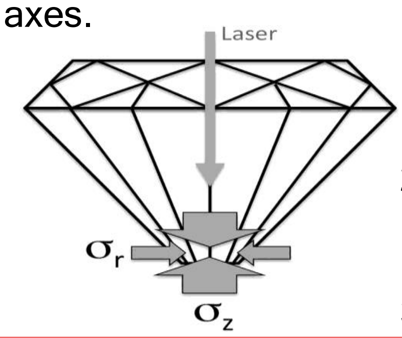
- Advances in the design and assembly of diamond anvil cells are pushing the boundaries of static high-pressure experiments to multimegabar pressures.
- Accurate determination methods of pressure under these conditions are challenging.
- The Raman edge as a pressure determination method, **b**ased on **the shift** of the **high-frequency edge** of the **Raman band** of the diamond.



Schematic diagram of the Diamond Anvil Cell[1].

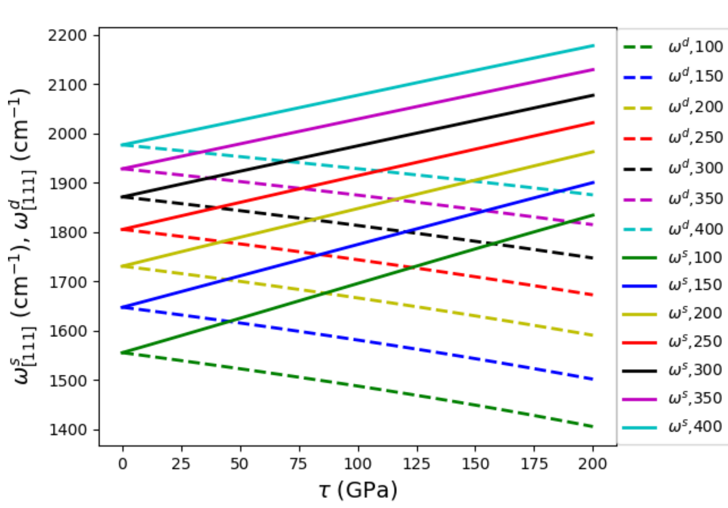
Objectives

1. Determining with first-principle methods the Raman frequencies of the diamond which are subjected to non-hydrostatic uniaxial stress along the [001] and [111] crystallographic axes.



2. Theoretical predictions are compared to experimental data and used to re-calibrate the pressure scale used in experiments.
3. Understanding the stress-strain state of the diamond anvil cell.

Results and Discussion



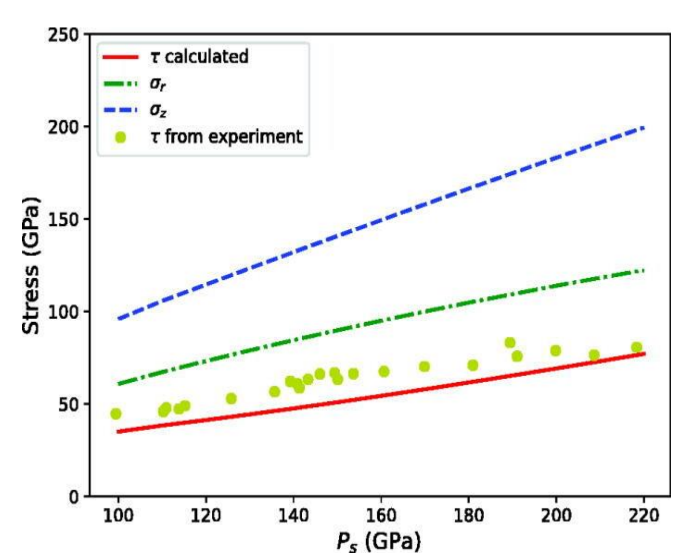
- If both ω^d and ω^s are known from experiments, the stress state (σ_{AV},τ) of the diamond anvil can be extracted by inverting Eq. 1.

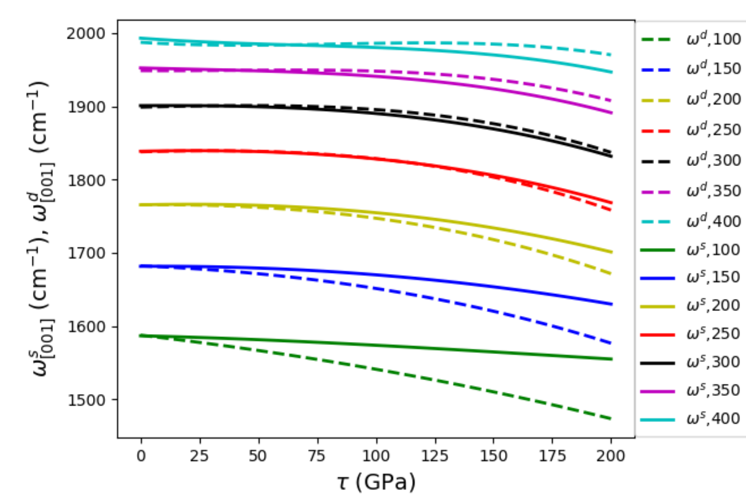
$$\omega(\sigma_r, \sigma_z) = \omega_H(\sigma_{AV}) - (a_0 + a_1(\sigma_{AV}-300) + a_2(\sigma_{AV}-300)^2)\tau - (b_0 + b_1(\sigma_{AV}-300) + b_2(\sigma_{AV}-300)^2)\tau^2 - (c_0 + c_1(\sigma_{AV}-300) + c_2(\sigma_{AV}-300)^2)\tau^3,$$

Eq. 1

The Raman frequency of diamond :

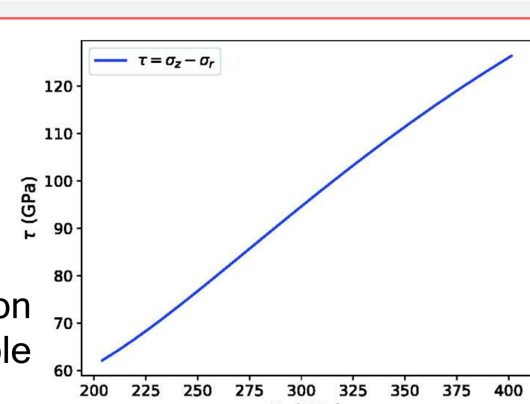
- In the absence of stress, it is triply degenerate.
- Under stress, it splits into a doublet (ω^d) and a singlet (ω^s).
- Proposed an analytical form.





Calculated values of the stress along the loading axis (σ_z) and along the radial direction (σ_r), and shear stress τ, as a function of the pressure P_s in the sample, for the diamond-anvil cell loaded along the [111] diamond axis. The experimental data for the shear stress τ reported in Ref. 2 are also shown.

Summary



Shear stress τ as a function of the sample pressure P_s.

1. We were able to determine the stress state of the diamond anvil in ultra-high-pressure experiments by combining theoretical and experimental data.
2. The maximum shear stress determined for loading along [001] is large but still considerably below the theoretical limit for the onset of an elastic instability (τ_{max} = 200 GPa) for uniaxial compression along the cubic axis[3].
3. We found that shear stresses close to the tip of the anvil can reach values exceeding 1 Mbar.

References

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