Physical and chemical changes of hydrogen peroxide under high pressures

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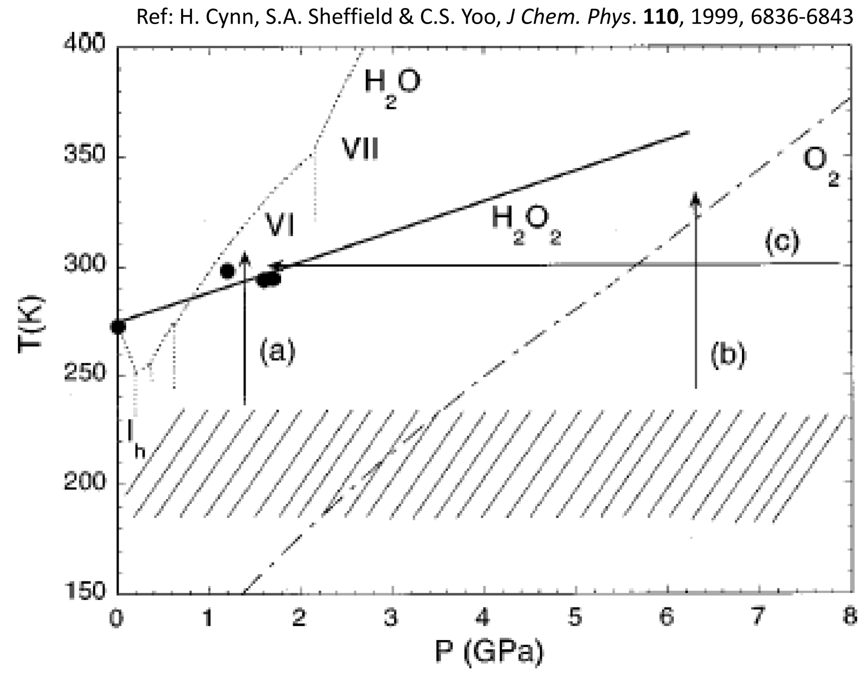
Motivations and Objectives

Ref: H. Cynn, S.A. Sheffield & C.S. Yoo, *J Chem. Phys.* **110**, 1999, 6836-6843

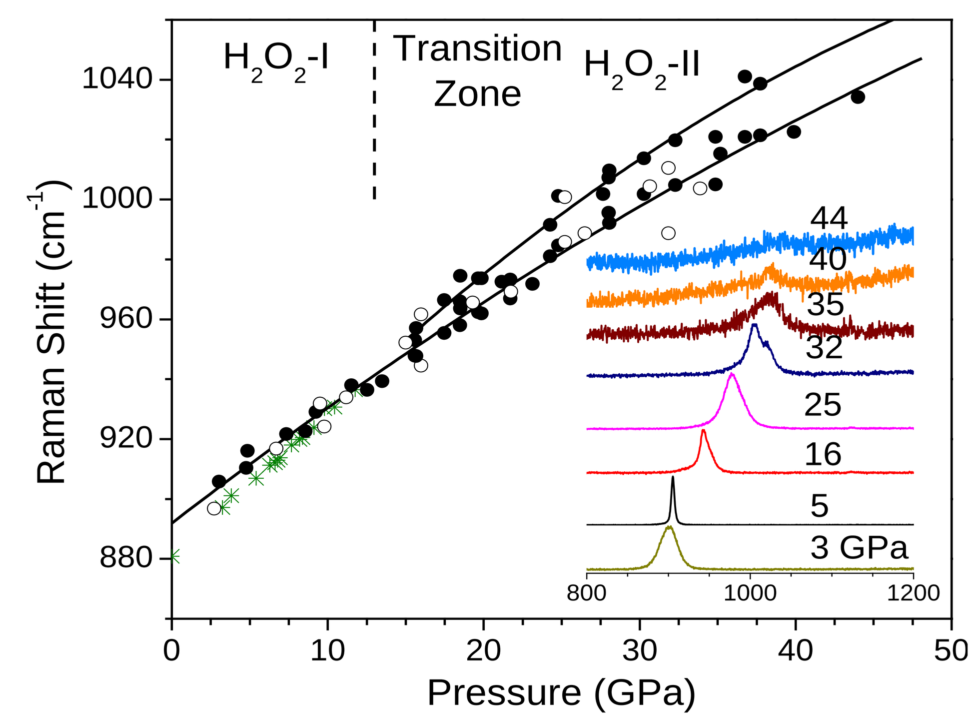


- ❑ H_2O_2 is a strong oxidizer and even explosive, and is often used as IED
- ❑ Stability and behavior of H_2O_2 and water mixtures are not known
- ❑ Shock-induced detonation of concentrated H_2O_2 has been observed at ~13-15 GPa
- ❑ Behaviors of highly concentrated H_2O_2 are not known under static high pressures

Mitigating chemical and shock threats of H_2O_2 requires understanding of the stability of H_2O_2-H_2O mixtures at relevant thermal conditions

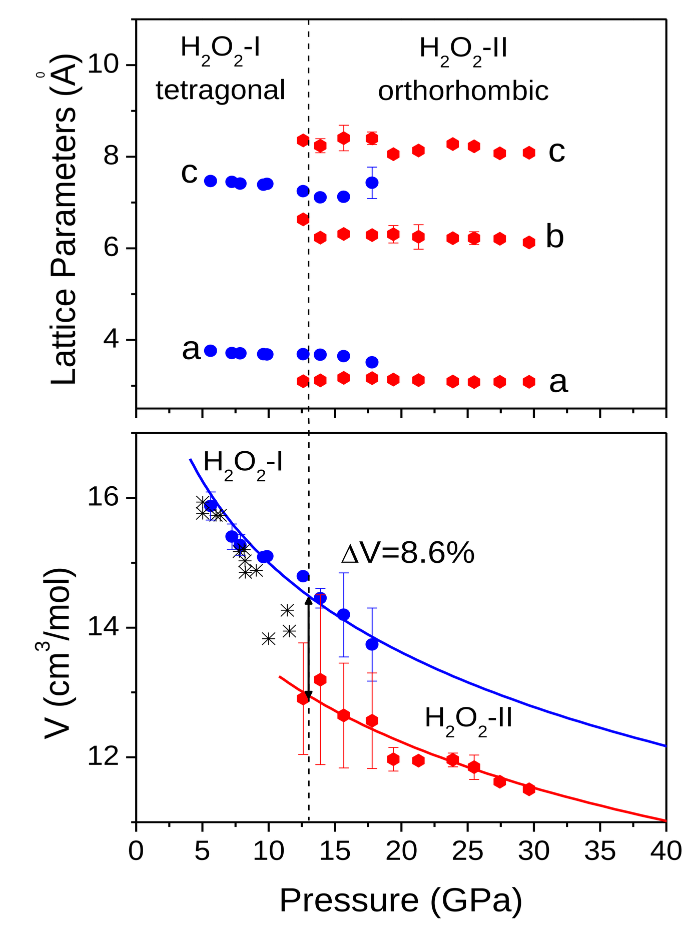
Phase Transitions in H_2O_2

Raman Spectral Evidence



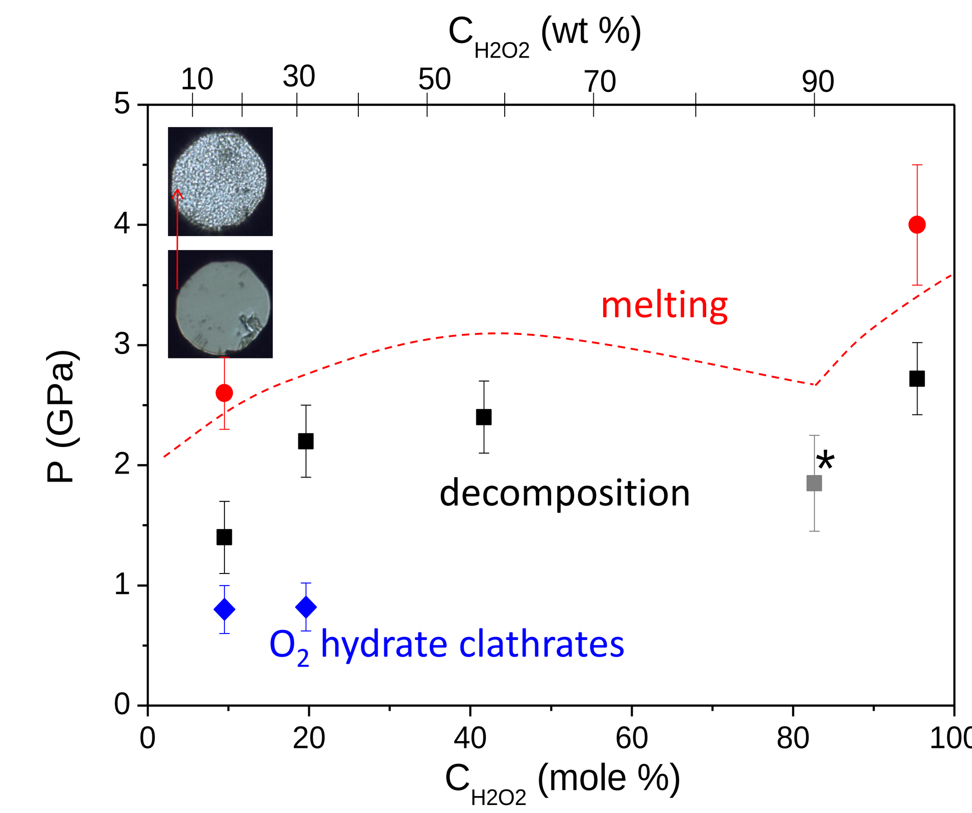
Ref: J.Y. Chen and C.S. Yoo, J. Chem. Phys. 132, 214501 (2010)

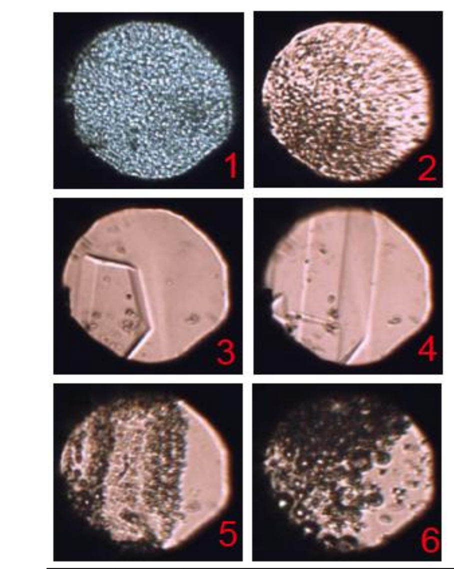
Structural Evidence

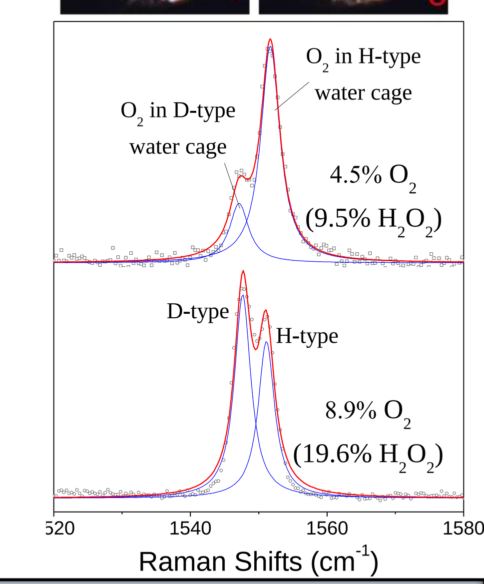


- ❑ Phase transition at 13 GPa from H_2O_2-I to -II, based on Raman and x-ray data
- ❑ It accompanies a volume collapse of ~ 8.6%
- ❑ Pure H_2O_2 is chemically stable to pressures 18 GPa

Behaviors of Binary Mixtures: H_2O + H_2O_2







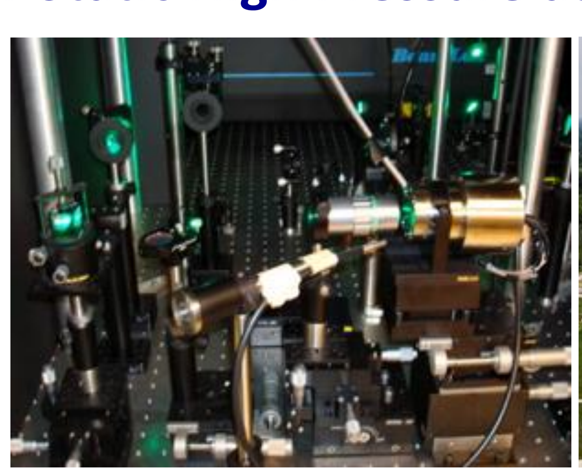
- ❑ Phase transition occurs at lower pressure for diluted samples.
- ❑ Oxygen clathrates are observed at low concentrated mixtures

The presence of water stabilizes the H_2O_2 mixtures by forming stronger hydrogen bonds

Experimental Approach

Under Static High Pressure at WSU

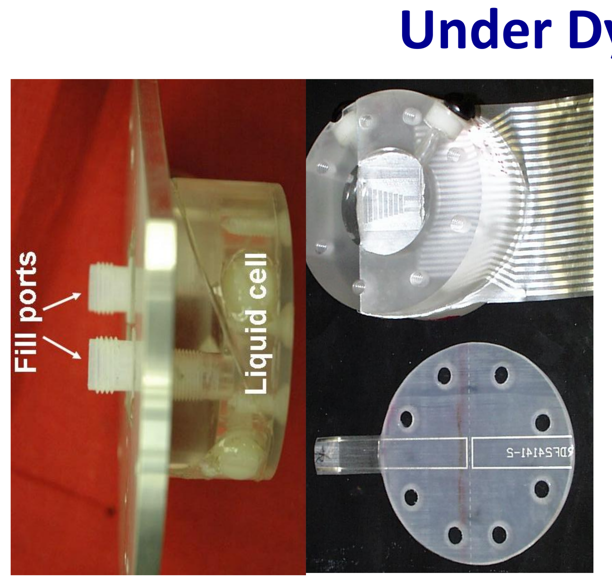
Diamond anvil cell
Pressurizing



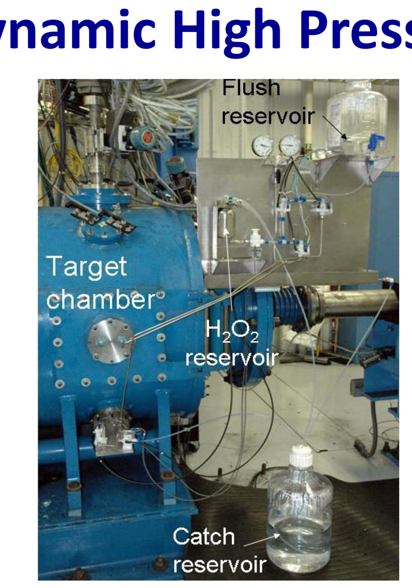
Confocal micro-Raman
Phase mapping

Synchrotron x-rays
Characterization

Under Dynamic High Pressure at LANL



H_2O_2 target with stress gauge

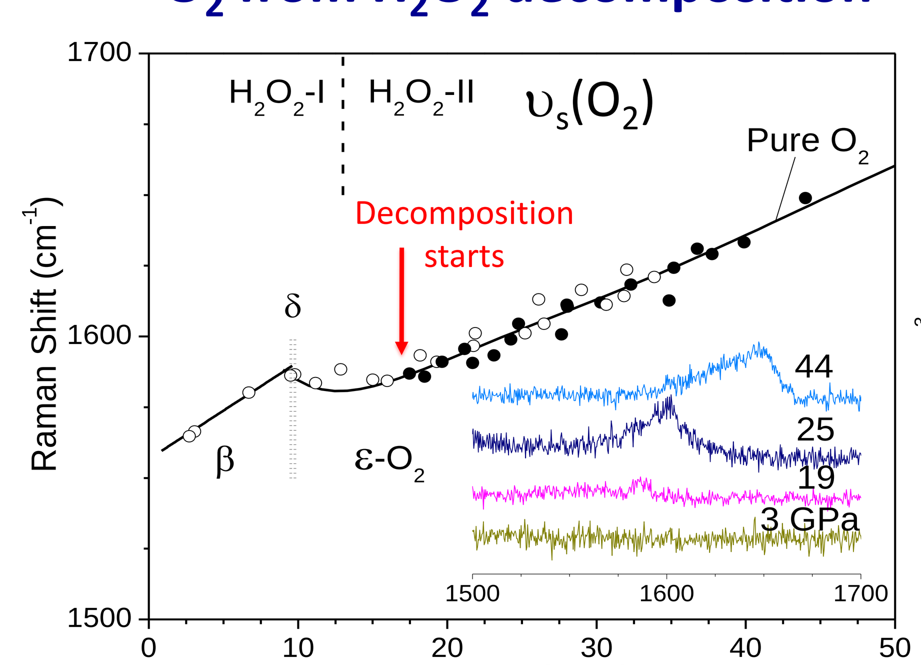


Loading H_2O_2

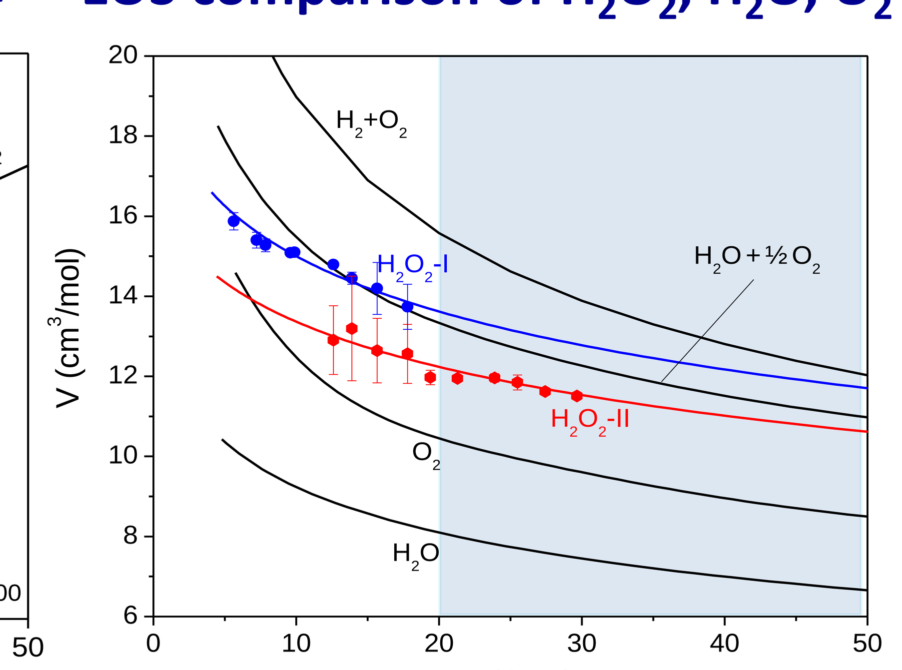
2-Stage gas gun

Chemical Decomposition of Compressed H_2O_2

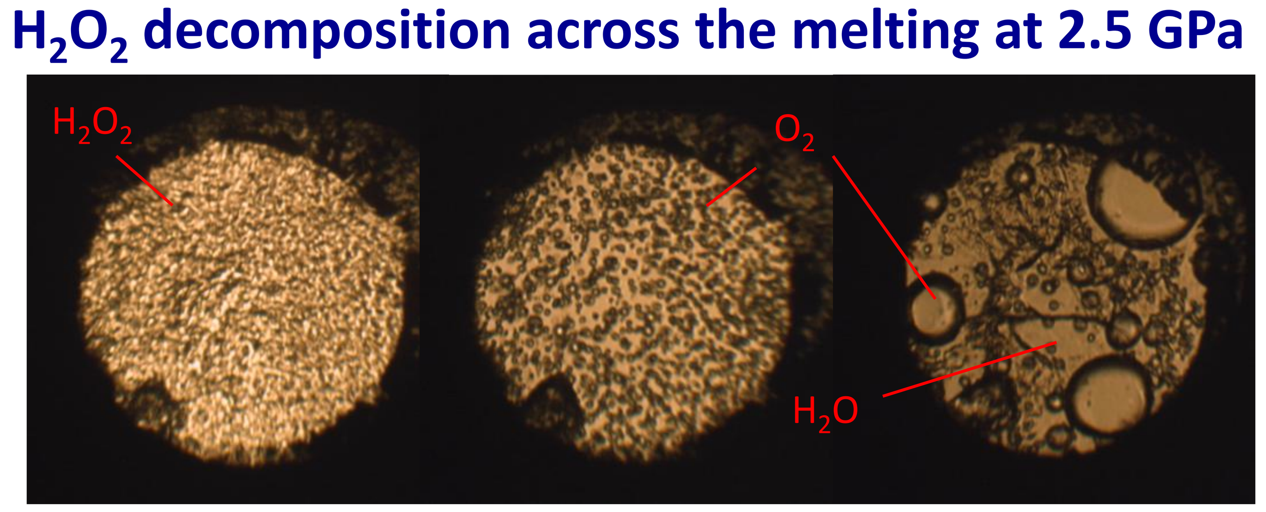
O_2 from H_2O_2 decomposition



EOS comparison of H_2O_2, H_2O, O_2



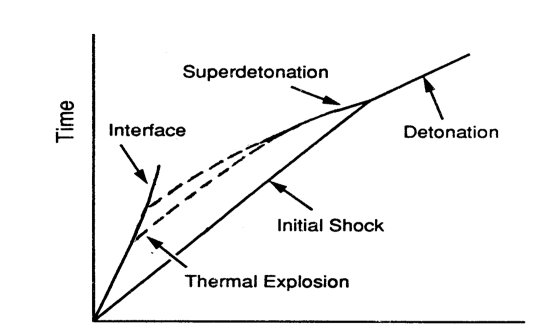
H_2O_2 decomposition across the melting at 2.5 GPa

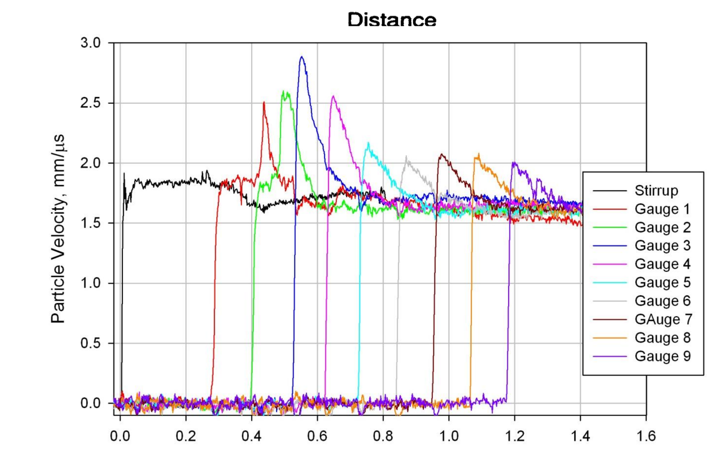


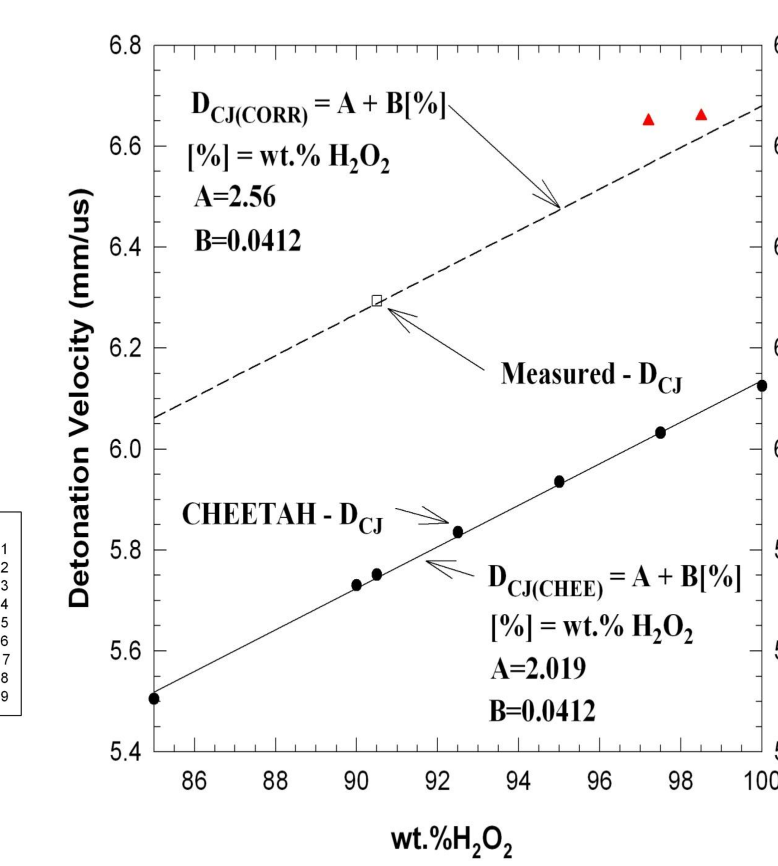
Decomposition of H_2O_2 is driven by densification and melting

Detonation in Shocked H_2O_2

Homogenous detonation model







- ❑ 98 % H2O2 detonates at 6.7 Km/s (13-15 GPa).
- ❑ It seems to follow homogenous detonation model based on the spatially resolved wave profile measurement
- ❑ The work has been done in collaboration with D. Dattelbaum and S. Sheffield In LANL

Is shock-induced detonation different from the static pressure-induced decomposition ?

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