High pressure experiments on Zr metal and organic (tert-butyl acetylene: (CH3)3-C≡CH)

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During our recent (and first) beamtime at PETRA III Extreme Conditions Beamline (ECB) P02.2, we performed XRD measurements on metal (Zr) and organic (tert-butyl acetylene: (CH3)3-C≡CH), TBA) samples at high pressures in a DAC. Goal of the study was to: (1) determine strain rates that can be achieved with our gas-membrane DAC, (2) investigate structural evolution in Zr metal under various strain rates, and (3) determine polymerization thresholds and reaction kinetics in TBA under pressure-jump conditions. As shown in Fig. 1, based on the pressure marker used in the experiment, during initial experiments we were able to achieve strain rates of $10^{-2}$/s, and furthermore we were able to continuously collect XRD patterns showing structural evolution in Zr from ambient pressure up to 42 GPa (Fig. 2), and polymerization in TBA in the pressure range up to 10 GPa (Fig. 3).

Currently, we are still in the process of analyzing all of the data collected during our beamtime – in all we performed 12 experiments and collected over 30000 diffraction files. Our initial data analysis is allowing us to plan our next experiment, which will allow us to further improve our experimental technique in order to achieve higher strain rates with our diamond anvil cell. Furthermore, continued analysis of data we previously collected will allow us to gain further insight into the structural evolution in Zr metal and polymerization in TBA, and also extract additional information on the kinetics of phase transition, stress distribution in the sample chamber, and overall performance of our DAC over the pressure range and loading conditions of the experiment.

Fig. 1. Typical pressure-jump profile generated, as shown from data collected on Pt
Fig. 2. (a)-(c) ADXD patterns collected during pressure increase, showing $\alpha \rightarrow \omega \rightarrow \beta$ structural evolution in Zr from 0 to 42 GPa.

Fig. 3. TBA ramp compressed to $> 10$ GPa (at $\approx 1$ GPa/s), with 1 sec exposures.

So far, results obtained from the experiment have been presented at various venues:

1. American Physical Society March meeting 2012, Presentation (B25.00002), Raja Chellappa, Dana Dattelbaum, Stephen Sheffield

2. Dynamic Compression Sector (DCS) at the Advanced Photon Source (APS) workshop, Argonne National Laboratory, Argonne, IL, Jan. 19, 2012.