A046-02-250823 **Diffraction studies in dynamic compression experiments**

Dynamic compression of bismuth at the European XFEL results from Exp. 3076

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Bismuth (Bi) has a rich phase diagram at relatively low pressures and temperatures with a variety of crystal structures accessible below 10 GPa. At ambient temperature, Bi undergoes the following sequence of structural phase transitions, Bi-I (hR2) transforms to Bi-II (mC4) at ~2.55 GPa. Bi-II transforms to the complex host-guest incommensurate structure at ~2.7 GPa and above ~8 GPa (depending on the reference) Bi-III transforms to Bi-V a high symmetry bcc phase [1]. The high-pressure behavior of Bi has been extensively studied using a variety of high-pressure techniques and diagnostics. Static DAC techniques combined with x-ray diffraction [1,2,3], dynamic diamond anvil cell (dDAC) with x-ray diffraction [4,5], and dynamic laser ramp and shock compression with x-ray diffraction and /or VISAR [6,7,8, 9, 10].

Early shock compression studies found that the phase transition pressures were consistent with the phase transition pressures reported from static compression studies [11-13]. However, these studies did not utilize techniques which yielded crystal structure information. Structural determination under dynamic compression has been carried out recently using time resolved X-ray diffraction techniques at XFELs and synchrotrons where significant deviations from the equilibrium phase diagram were observed [6,7,9]. Interestingly incommensurate Bi-III was not observed in any of these experiments on compression, and instead Bi-V was observed alongside an unidentified metastable phase Bi-M at pressures as low as 3 GPa [6,7]. Additionally, the observation of Bi-V at lower pressures in shock experiments when compared to static compression experiments is surprising, since kinetic hinderance typically results in over-driving of the phase transition boundary [8].

To resolve these discrepancies, we carried out a series of dDAC experiments at the High Energy Density (HED) instrument at the European X-ray free electron laser (EU-XFEL) facility. A ~15 µm beam size at 18 keV was used. We utilized the long pulse trains where we collected data for 550 µs with a time resolution of ~1.78 µs. This mode allowed us to collect diffraction data across the entire compression ramp of the dDAC. A new triggering scheme was also developed which allowed us to collect diffraction data on the hold and decompression parts of the ramp.

Before each ramp we carried out dry runs to assess heating of the sample and reduced the X-ray fluence until minimal heating was observed. In all the runs we observe the phase transition sequence that has been established from static compression experiments Figure 1. Hence, we do not skip Bi-III in these runs and our preliminary analysis suggests that the Bi-III stability field may be shrinking at these compression rates. Notably, the compression rates we achieved in these runs are much slower than those reported in [6]. Experiments carried out during Exp. 3076 demonstrated that the long pulse trains can be used to cover the entire compression part of the dDAC ramp, and that structural information can be obtained at these extreme compression rates with unparalleled time resolution.

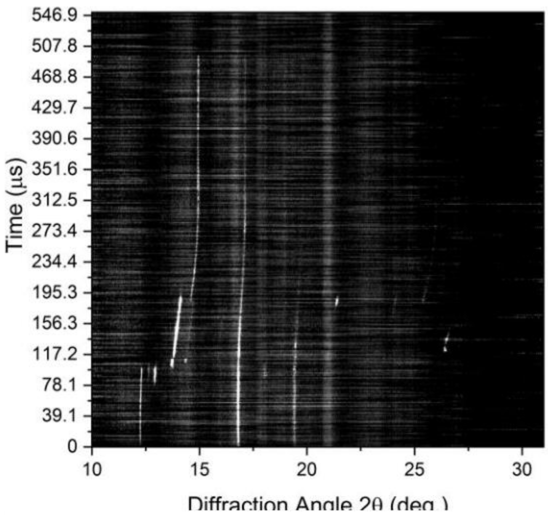

Figure 1. Run 378 showing compression from Bi-I to Bi-II to Bi-III and finally into Bi-V at an average compression rate of 61 TPa/s.

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