Copper phase determination to 290 GPa using laser-shock compression

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Copper is a common pressure calibrant within the high-pressure community due to the availability of accurate shock wave data (Meyers et al., 2003; Murphy et al., 2010; Kraus et al., 2016). It has also been used to calibrate two of the important standards for static x-ray diffraction experiments, ruby and gold (Bell et al., 1986). Copper is useful because it provides more accurate pressure determination than other standards, including Pt, Mo, and W, due to its larger compressibility and lack of phase changes. We examine the crystal structure of copper under shock compression up to 290 GPa. Previous shock studies suggest copper remains in FCC structure from ambient conditions until melting (Hayes et al., 2000). These studies reached peak conditions by utilizing a single shock. Using ramp compression, in which peak conditions are reached through a series of shocks, the ambient pressure FCC phase is observed to be stable to TPa pressures (Fratanduono et al., in press). However, a metastable BCC-structured phase is observed in thin films and is suggested to possibly be stable at higher temperatures (Friedel, 1974). A recent density functional theory computational study by Neogi and Mitra (2017) suggests the possible existence of a BCT or BCC structure at pressures > 100 GPa and 1520 K. We completed a series of laser shock experiments with *in situ* X-ray diffraction using the Dynamic Compression Sector at Argonne National Laboratory in order to study the phase diagram and melting curve behavior of copper (Wang et al., 2019). We observe a BCC structured phase at 240 GPa with a density around 14.02 g/cc. The BCC phase consistently coexists with melt, suggesting a high thermodynamic or possibly kinetic barrier to transformation. Our experimental temperatures are higher than ramp compression studies, and this suggests that the Cu BCC phase is only thermodynamically allowed at high temperatures. The formation of the BCC structured phase may have an effect on the melting temperature of copper. The existence of this BCC structure suggests care should be taken when using the copper Hugoniot to calibrate pressures above 240 GPa.

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