Poster Presentation

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Phase transitions and enhanced conductivity of CaC2 under high pressure

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Calcium carbide is widely used in the industry for the production of acetylene and other purposes. Its phase transitions under ambient pressure have been studied since 1930s [1]. In recent years, with the development of high pressure science, its phase transitions under high pressure attracted more attentions [2], and its physical properties such as conductivity and superconductivity were focused [3]. Up to now, most of the researches on CaC2 under high pressure are theoretical, and experimental investigations are expected to figure out the structural transitions. In this work, we investigated the structural transitions of CaC2 (phase I, tetragonal, I4/mmm) up to ~30 GPa by powder XRD, neutron diffraction, and neutron PDF analysis on the recovered samples, and measured the conductivity of CaC2 up to ~20 GPa. XRD data are employed to refine the unit cell parameters, based on which the equation of state is fitted. As identified by series of fittings, the tetragonal phase stabilizes up to 10 GPa, above which it has a minor phase transition. The crystal structures were refined by the structural model of phase I with in-situ neutron diffraction data. Both of the bond length of C-C triple bond and the nearest intergroup C…C distance show a turning point at around 10-12 GPa. The critical pressure is in consistent with the predicted phase transition from phase I to phase VI (monoclinic, I2/m), though the phase VI can't be identified and refined with the data under the current resolution. The resistivity of CaC2 decreases from 1000 Ω•m at 2 GPa to 0.0001 Ω•m at 22 GPa, which can be attributed to the compression of intergroup C…C distance from 0.335nm to 0.315nm. The resistivity-pressure curve also shows a turning point at ~10GPa, corresponding to the phase transition. Above 18 GPa, CaC2 starts to amorphize, which is reversible but sluggish. The C22- may get connected to each other, as observed in the neutron PDF data of the recovered sample.

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