Charge-density Wave in the Incommensurate Phase of Metallic Sulfur at Megabar Pressure

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Recent discoveries of incommensurate (IC) host-guest and/or modulated phases in elemental metals at high pressure suggest that aperiodic structures are a common phenomenon among the elements under pressure. However, the driving force for development of the incommensurability and structural modulations in these elemental systems is poorly understood.

Using synchrotron x-ray diffraction and diamond anvil cells, we show that the metallic phase of sulfur stable above 83 GPa, has an IC modulated crystal structure with a monoclinic average cell and a modulation wavevector q = <0 0.281 0> at 100 GPa. We observe a strong pressure dependence of the modulation up to 135 GPa, where the modulation disappears.

We perform first-principles calculations using the density-functional theory to analyze the average structure of the IC phase. We obtain a simple Fermi surface (FS) that exhibits parallel zones, indicating a nesting, characterized by a wavevector close to the experimental modulation. The phonon dispersion shows a softening with a minimum at the same wavevector as the FS nesting vector. These indicate that the IC structure in metallic sulfur at megabar pressures is due to a charge-density wave.

Keywords: high pressure, incommensurate modulated structures, electronic band structure calculations