Structural Stability and Transport Properties of TiZrNi Quasicrystals under High Pressure

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Quasicrystals (QCs) are characterized by long-range order with five-fold rotational symmetry, which is forbidden in conventional crystalline materials. Among known QCs, Ti-based systems constitute the second largest class after Al-based ones. In particular, TiZrNi quasicrystals have attracted significant attention due to their high hydrogen storage capacity, which increases with applied pressure.

In this study, we investigated the structural and transport properties—including superconductivity, electrical resistivity, and magnetization—of $Ti_{53}Zr_{27}Ni_{20}$ quasicrystals under high pressure using a diamond anvil cell. These properties are systematically compared with those of hydrogenated samples. Synchrotron X-ray diffraction measurements reveal that $Ti_{53}Zr_{27}Ni_{20}$ quasicrystals absorb up to 3.4 wt.% hydrogen at 5.08 GPa without undergoing a structural phase transformation. Upon decompression, approximately half of the absorbed hydrogen is released, highlighting the potential of TiZrNi quasicrystals for practical hydrogen storage applications. Notably, the 1/1 approximant phase of TiZrNi transforms into a quasicrystalline phase during decompression from pressures exceeding ~20 GPa.

The superconducting transition temperature (Tc) of the pristine powder is 1.94 K at 0.78 GPa and increases monotonically to 6.47 K at 75 GPa. Hydrogenated samples exhibit a similar pressure dependence of Tc, although with an approximately 0.8 K lower transition temperature compared to the pristine material across the investigated pressure range.