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Pressure-Induced Amorphization in Single-Crystal Ta_2O_5 Nanowires: A Kinetic Mechanism and Improved Electrical Conductivity XUJIE LU, Univ of Nevada - Las Vegas, Carnergie Institute of Washington, QINGYANG HU, George Mason University, WENGE YANG, Carnergie Institute of Washington, LIGANG BAI, Univ of Nevada - Las Vegas, HOWARD SHENG, George Mason University, LIN WANG, Carnergie Institute of Washington, FUQIANG HUANG, Chinese Academy of Science, JIANGUO WEN, DEAN MILLER, Argonne National Lab, YUSHENG ZHAO, Univ of Nevada - Las Vegas — Pressure-induced amorphization (PIA) in single-crystal Ta_2O_5 nanowires is observed at 19 GPa and the obtained amorphous Ta_2O_5 nanowires show significant improvement in electrical conductivity. The phase transition process is unveiled by monitoring structural evolution with in-situ synchrotron XRD, PDF, Raman spectroscopy and TEM. The first principles calculations reveal the phonon modes softening during compression at particular bonds, and the analysis on the electron localization function also shows bond strength weakening at the same positions. Based on the experimental and theoretical results, a kinetic PIA mechanism is proposed and demonstrated systematically that amorphization is initiated by the disruption of connectivity between polyhedra at the particular weak-bonding positions along the a-axis in the unit cell. The one-dimensional morphology is well preserved for the pressure-induced amorphous Ta_2O_5 and the electrical conductivity is improved by an order of magnitude compared to traditional amorphous forms.

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