Supplementary Information

Structural phase transition and metallization of nanocrystalline rutile investigated by high-pressure Raman spectroscopy and electrical conductivity

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Supplementary Figures

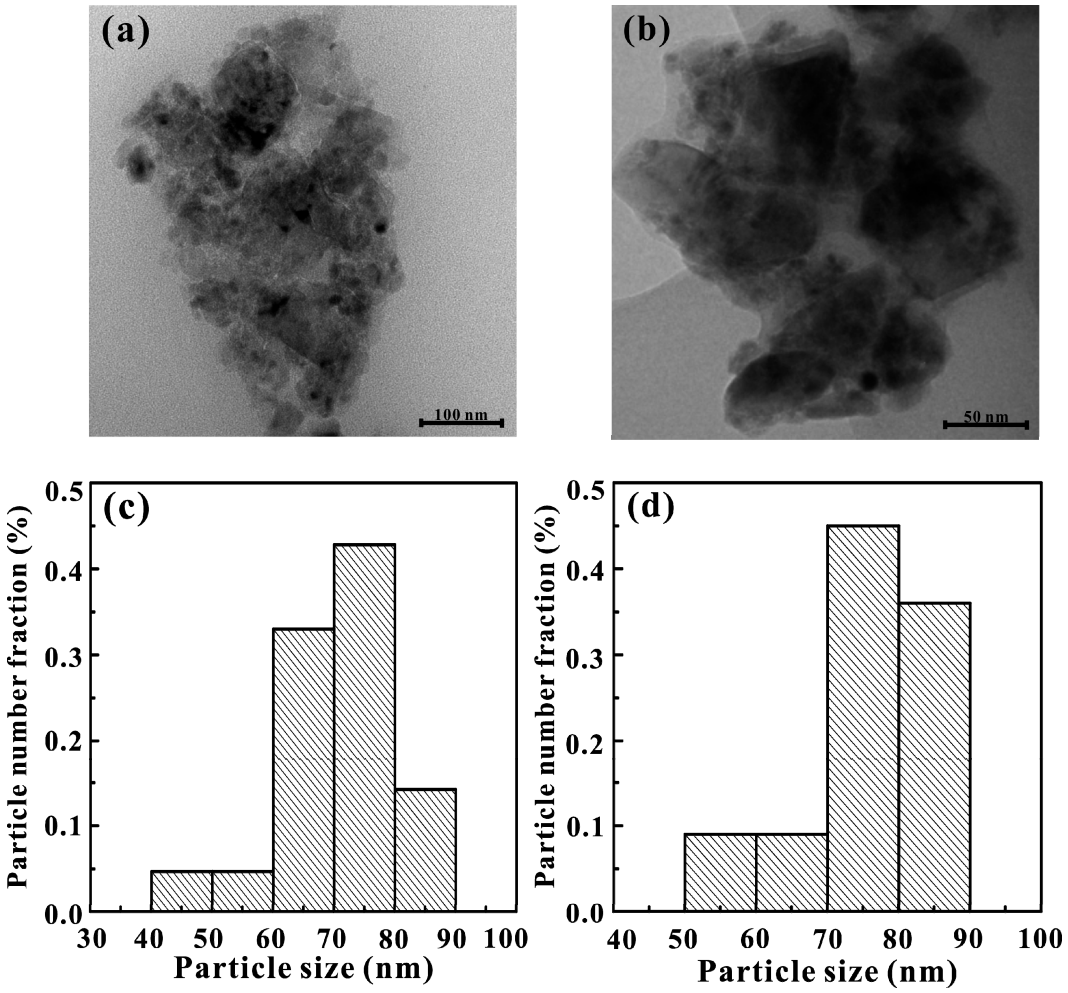

Figure S1. (a) and (b) are the TEM images of the starting sample. (c) and (d) the corresponding histograms of the particle size distribution. It is one of the potentially effective and good methods that the TEM observation can be used to determine the particle size distribution state in our starting sample. As shown in Figure S1 (a) and (b), the starting rutile particles with almost homogenous distribution state. We estimated roughly that there existed at least 20 and 8 particles in Figure S1 (a) and (b), respectively. Figure S1 (c) and (d) represent the corresponding histograms of the particle size distribution for the starting sample, most of the particle size are within the range of 70–80 nm. The average particle size of the starting sample was estimated to be 78 nm, which is in good consistent with the result from XRD.

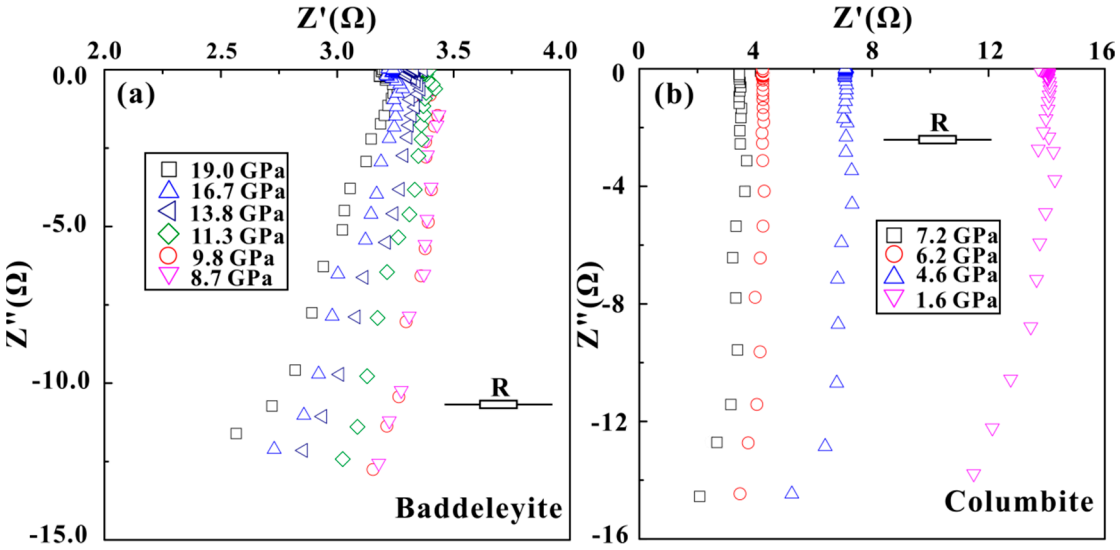

Figure S2. (a) The Nyquist diagram of the impedance spectra for baddeleyite phase at the pressure range of 19.0–8.7 GPa during decompression. (b) The Nyquist diagram of the impedance spectra for columbite phase at the pressure range of 7.2–1.6 GPa during decompression, the equivalent circuit of R stands for the resistance.

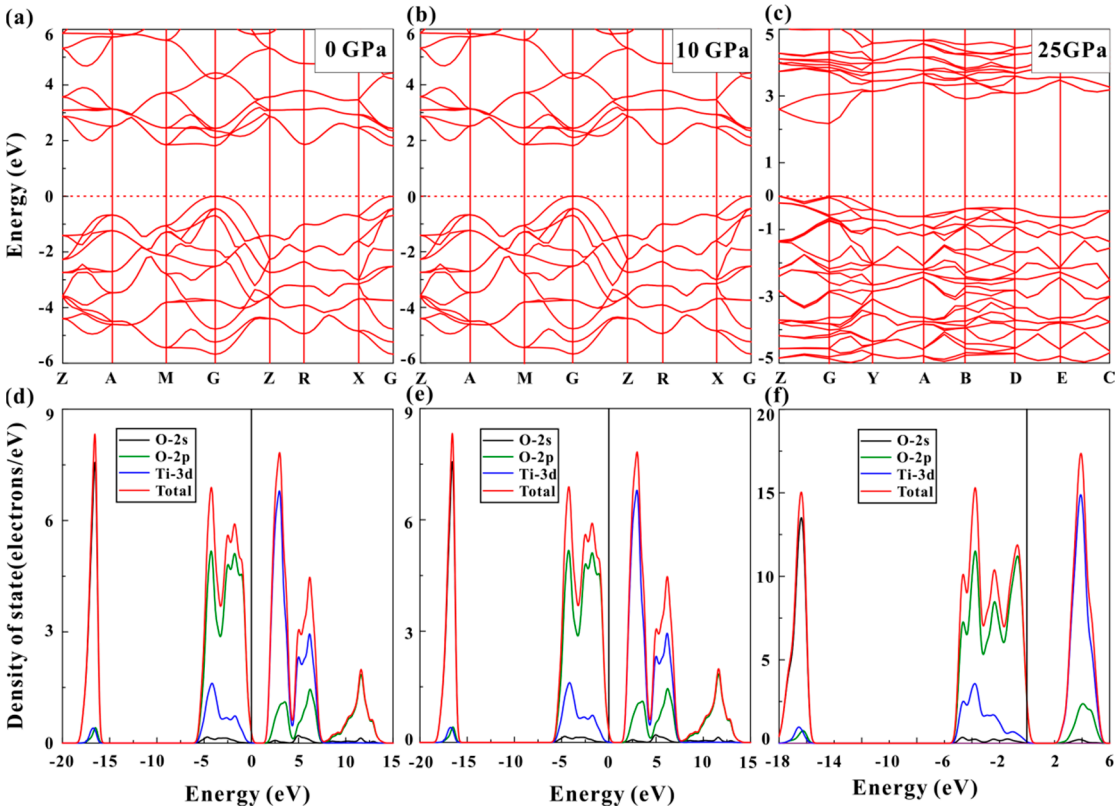

Figure S3. (a) and (b) Calculated band structure for rutile phase at the pressures of 0 GPa and 10.0 GPa. The bandgap energy for rutile phase are 1.99 eV and 1.96 eV at the pressures of 0 GPa and 10.0 GPa, respectively. (d) and (e) The corresponding total density and projected density at the pressures of 0 GPa and 10.0 GPa for rutile phase. (c) Calculated band structure for baddeleyite phase at 25.0 GPa. The bandgap energy for baddeleyite phase is 2.17 eV at 25.0 GPa. (f) The corresponding total density and projected density at 25.0 GPa for baddeleyite phase.

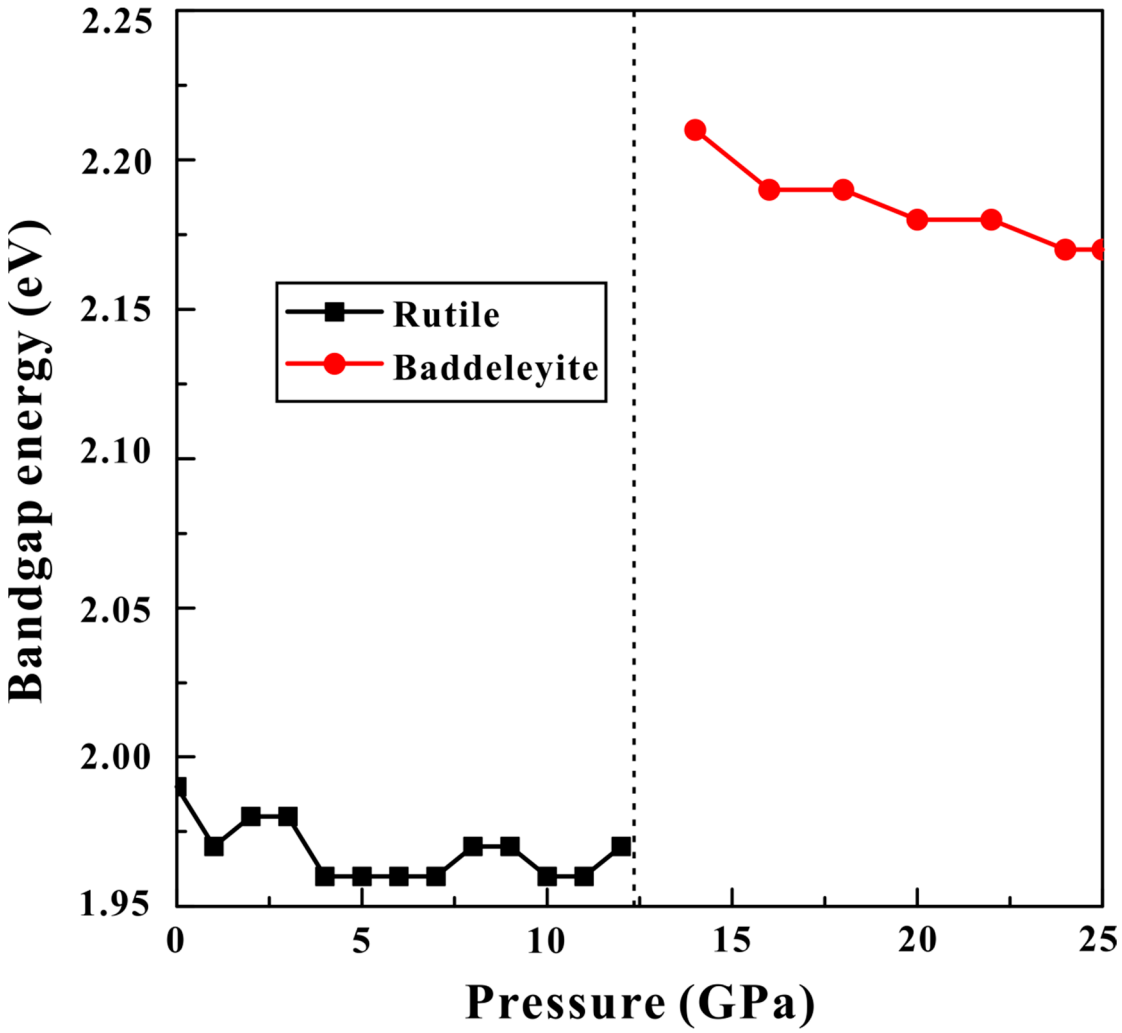

Figure S4. The calculated bandgap energy of rutile phase at the pressure range of 0–12.0 GPa and the baddeleyite phase within the pressure range of 14.0–25.0 GPa.

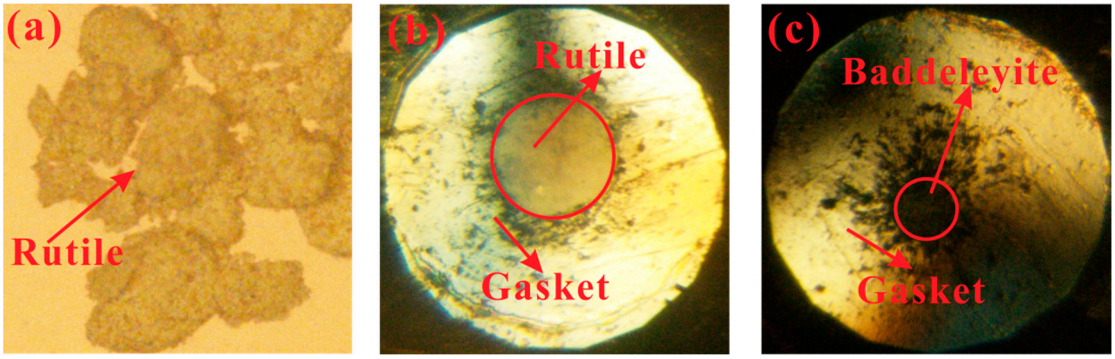

Figure S5. (a) The optical microscope image of the starting material for nanocrystalline rutile. (b) and (c) The optical microscope images of the nanocrystalline rutile at the pressure points of 10.0 GPa and 15.0 GPa using the diamond anvil cell, respectively.