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Phase transitions of VO2 above 200GPa: XRD and first-principles calculations

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It is interesting to compare the phases of VO2 with other dioxides under strong compression. The phase sequence of SiO2 inducing by high pressure were theoretically predicted as CN6 structures (rutile, CaCl2, α-PbO2, pyrite), CN8 (Pnma) and CN9 (P-62m) structures, but only the phases up to pyrite structure in SiO2 were observed experimentally up to now. The CN8 phase and CN9 phases of SiO2 were predicted to be stable at least 650 GPa, which is still challenging to achieve in the static DAC experiment at present. In TiO2, the ambient rutile and anatase phases first transform to α-PbO2 (still in CN6), then to the baddeleyite (CN7) phase, to an orthorhombic (CN8) phase, a Pnma (CN8) phase and P-62m (CN9) phase. The CN9 phase of TiO2 was obtained at the pressure of 210 GPa and the temperature of 4000 K in DAC experiment. In the present study, under strong compression at room temperature, CN6 VO2 transformed to new CN7, then to CN8 phase just at 70 GPa and CN9 at 100 GPa, which is lower than in that of TiO2 and SiO2. Thus, VO2 can be act as a typical material to study the ultra-high phases of other dioxides. Theoretical study predicted the CN10 structure of TiO2 and SiO2 should exist at pressure around 647 GPa and 10 TPa, but the same type of structure in VO2 should stable at just of 350 GPa, which dramatically decrease the difficulty of realization experimentally. In this report, we will present our new XRD and calculations results on VO2 up to 200 GPa.

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