Observation of nine-fold coordinated amorphous TiO2 at high pressure

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Understanding pressure-induced structural changes in amorphous dioxides (a-AO2) is of great importance in many fields of science. Here we report new experimental results of high pressure polyamorphism in amorphous TiO2 (a-TiO2) with the Ti-O coordination number (CN) close to 9. Our experimental data show that CN increases from 7.2 at 15.7 GPa, to 8.8 at 70.2 GPa, and finally reaches a plateau ~8.9 at pressures up to 85.7 GPa. We find that CN of both crystalline TiO2 and a-TiO2 follows a similar and systematic dependence on the ratio (γ) of the ionic radii of Ti and O. The γ of a-TiO2 is 0.614 at 15.7 GPa, which is similar to that of baddeleyite-type TiO2 (~0.61), and increases continuously with pressure. At 70.2 GPa, γ of a-TiO2 is 0.701, which is similar to that of cotunnite-type TiO2 (~0.693). It appears that the CN≈9 plateau of a-TiO2 correlates to the cotunnite-type and Fe2P-type polymorphs, which have the same CN=9 but correspond to different γ values. This CN-γ relationship is applicable to other a-AO2 of a-SiO2 and a-GeO2. All three compounds show surprisingly consistent between CN and γ, implying a unified relation between CN and γ in a-AO2. The established CN-γ relationship may be used to predict the compression behavior of a-AO2 compounds to extreme conditions.