Thermal and Physical Properties of Titanium Oxide at High Pressure

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We present here pressure dependence of the thermal and physical properties of titanium oxide (rutile) using a semi-empirical approach based on Lindemann's melting law. Rutile is the most common naturally occurring and most stable polymorph of titanium oxide (TiO_2) with a tetragonal symmetry. The amount of rutile found in nature ranges between 0.5% and 0.8% of the total mass of the Earth's crust. It is used in photovoltaic devices, integrated wave guides, gas and humidity sensors, and solar cells. Research on rutile is important to earth scientists because a complete understanding of the composition and thermal state of the Earth's interior depends on information about the elastic properties of this mineral at high pressure and temperature. We have used semi-empirical equations to determine the melting temperature, T_m and Debye temperature, and their pressure dependence. The formalism used to compute $T_m$is based on Lindemann's melting law. In both the cases we have assumed linear dependence of bulk modulus, B and Grüneisen parameter, ξ on pressure. We have applied the formalism to estimate the pressure dependence of viscosity, diffusivity and conductivity of rutile (Titanium oxide, TiO_2). These results show that the pattern of the pressure variation of melting temperature influences the pressure dependence of viscosity, diffusivity and thermal conductivity. The pressure range used in the present study is 0-50GPa. Our analysis shows that the maximum and T_m and maximum Θ_D of rutile are 2695K and 967K at 43GPa and 51.2GPa respectively indicating possible mineralogical phase changes. Viscosity, diffusivity and thermal conductivity at zero pressure and melting temperature are 2.95mPa.s, 4.78 x $10^{-5}cm^2.s^{-1}$ and 7.23 $W.m^{-1}.K^{-1}$ respectively.