Density of minerals V: Coordination

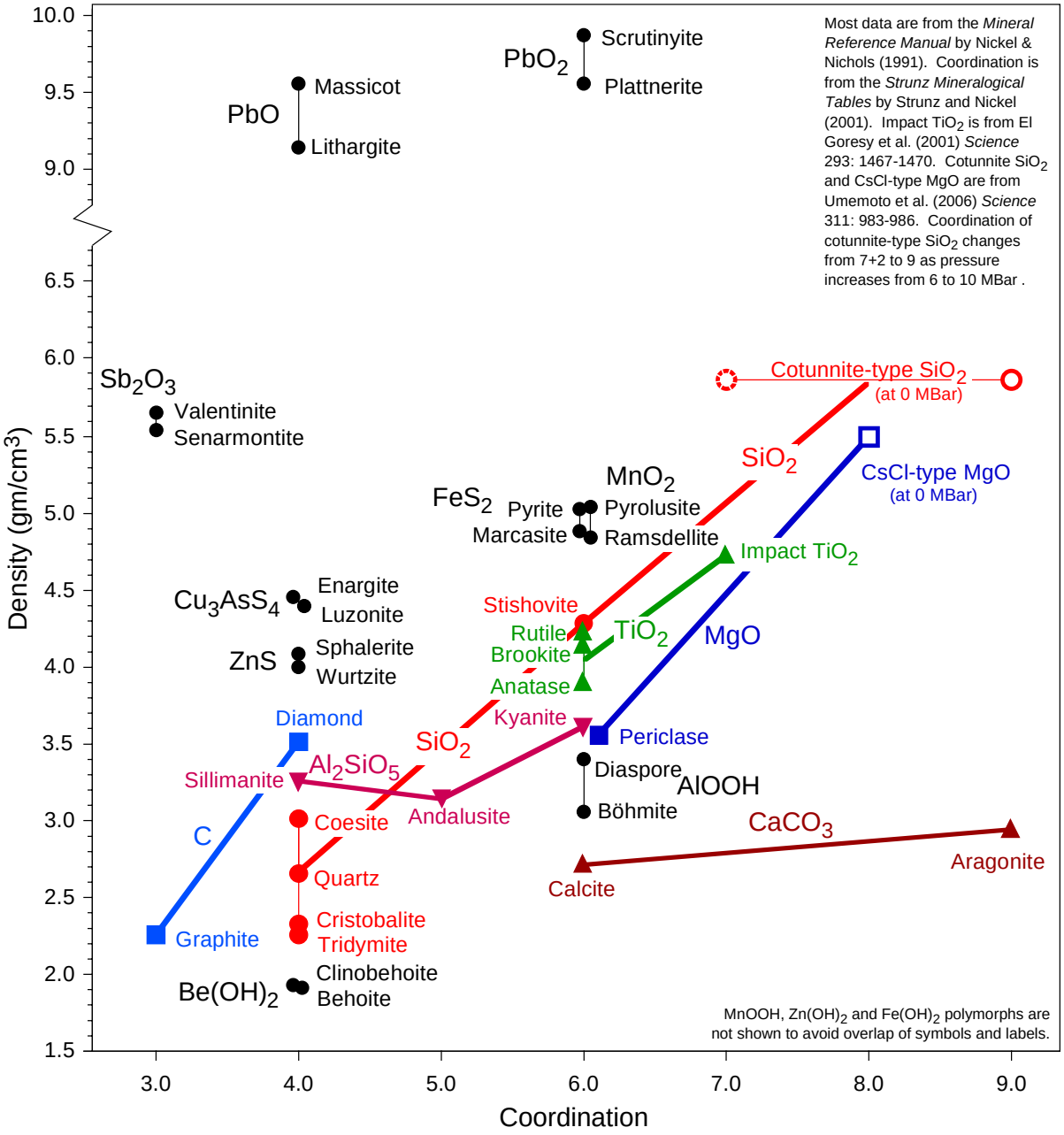
The plot at right shows the density of minerals that are polymorphs. Colored symbols indicate polymorphs that differ in coordination of cations (for example, ^{VI}Ca in calcite and ^{IX}Ca in aragonite) or atoms (for example, ^{III}C in graphite and ^{IV}C in diamond). Black symbols show polymorphs in which coordination is the same. Filled symbols indicate minerals; open symbols indicate substances not found on earth but hypothesized to exist in the interiors of larger planets.

The most obvious observation is that almost all the colored lines have an upward trend, and thus density almost always increases wtih coordination. For the coordination of oxygen around cations, that pattern seems to exist because the oxygens can be squeezed together. "The oxygen atom is more compressible than the cations. Total electron density calculations for coesite and stishovite show that the bonded radius of the oxygen atom decreases by 0.20Å while the radius of the Si atoms decreases by 0.02Å with the change in coordination . . . . . The reason that oxygen is more compressible than the cations is not related to the size of the atoms [it's not that the larger O atom has more to give] but rather to the slope of the electron density in the bonding region. The electron density of oxygen [which in its 2- state has two "extra" electrons] falls off rather rapidly compared to the electron densities around cations . . ." .[1]

The implication of all this for the natural occurrence of minerals is that polymorphs with greater coordination are commonly found in higher-pressure environments, either deeper in the Earth (as in the case of kyanite) or in bolide impacts (as with stishovite).

A second observation is that the slope of the colored lines depends on the relative abundance of the atom that undergoes a change in coordination. The steepest slope is that between graphite and diamond, where every atom undergoes an increase in coordination. In contrast, the slope is least steep for $CaCO_3$, where only one atom in five undergoes the increase in coordination from 6 to 9.

Finally, differences in density between polymorphs are generally proportional to density. For example, the densities of the $Be(OH)_2$ polymorphs are small and the difference between them is small. At the other extreme, the densities of PbO and PbO_2 polymorphs are large, and the difference between them is large.



[1] Prewitt, C.T., & Downs, R.T., High-pressure crystal chemistry, in Hemley, R.J., ed., Ultra-high Pressure Mineralogy: Reviews in Mineralogy v. 37, p. 283-317)