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Origin, properties, and structure of breyite: The second most abundant mineral inclusion in super-deep diamonds

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Abstract

Earth's lower mantle most likely mainly consists of ferropericlase, bridgmanite, and a $CaSiO_3$-phase in the perovskite structure. If separately trapped in diamonds, these phases can be transported to Earth's surface without reacting with the surrounding mantle. Although all inclusions will remain chemically pristine, only ferropericlase will stay in its original crystal structure, whereas in almost all cases bridgmanite and $CaSiO_3$-perovskite will transform to their lower-pressure polymorphs. In the case of perovskite structured $CaSiO_3$, the new structure that is formed is closely related to that of walstromite. This mineral is now approved by the IMA commission on new minerals and named breyite. The crystal structure is triclinic (space group: $P\overline{1}$) with lattice parameters a_0 = 6.6970(4) Å, b_0 = 9.2986(7) Å, c_0 = 6.6501(4) Å, α = 83.458(6)°, β = 76.226(6)°, γ = 69.581(7)°, and V = 376.72(4) Å. The major element composition found for the studied breyite is $Ca_{3.01(2)}Si_{2.98(2)}O_9$. Breyite is the second most abundant mineral inclusion after ferropericlase in diamonds of super-deep origin. The occurrence of breyite has been widely presumed to be a strong indication of lower mantle (>670 km depth) or at least lower transition zone (>520 km depth) origin of both the host diamond and the inclusion suite.

In this work, we demonstrate through different formation scenarios that the finding of breyite alone in a diamond is not a reliable indicator of the formation depth in the transition zone or in the lower mantle and that accompanying paragenetic phases such as ferropericlase together with $MgSiO_3$ are needed.

Keywords: Breyite, diamonds, super-deep diamonds, Earth's mantle, transition zone, lower mantle, walstromite, $CaSiO_3$