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Chemistry along the shock in complex silicate systems

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Defining chemical speciation in a melt/fluid depends strongly on the choice of method one uses to characterize the interatomic bonds. This is an even more daunting task for melts and fluids, which lack periodicity and thus an easy way of determining a series of alternating cations and anions. For fluids, one of the most common ways to define bonding is geometric: we compute the pair distribution functions (PDFs) between all pairs of atoms in that system. Then, by convention, the first local minimum of the PDF marks the radius of the first coordination sphere. Atoms within that distance are considered “bonded”, while atoms outside of that distance are considered not bonded. With this definition, we can determine chemical speciation in a melt, identify coordination polyhedra, track polymerization, calculate volatile speciation, and more. We can even pursue our analysis and monitor the formation of bubbles in natural melts, at low densities/pressures. But are these geometrical methods always right? Or shall we use more sophisticated method, like the electron localization function (ELF) ?

Here, we use and compare these two methods to analyze the behavior of various volatile-bearing complex silicate melts under shocks expected during large and giant planetary impacts. We show how the balance between temperature and pressure affects the chemical speciation along the Hugoniot. We identify the formation of bonds between Fe and C; but their transient character is visible only when performing the full ELF analysis. In a similar way, using both PDF and ELF, we discuss the formation of molecular CO2 and varying oxidizing conditions along the shock trajectory in the case of carbonaceous chondrites. Finally, we discuss in detail the formation of gas bubbles in silicate melts during the release trajectory.