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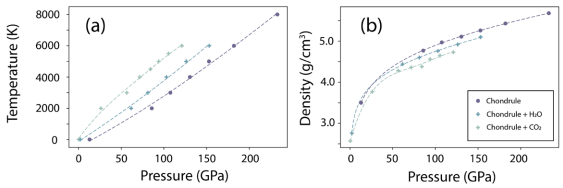

Ab initio simulation of volatiles bearing chondrite during giant impacts

ADRIEN SAURETY[1] AND RAZVAN CARACAS[2]

[1]Caltech

[2]Institut de Physique du Globe de Paris, Universite Paris Cite, CNRS

The volatile budget of terrestrial planets is primarily inherited from the accretion process. At this stage, impacts played a significant role in delivering or removing volatiles from the silicate of young planets. Among those volatile elements, hydrogen and carbon are particularly interesting as they are thought to be abundant in the early solar system but depleted in the mantles of the terrestrial planets.

In this study, we investigate the shock response of hydrated and carbonated silicate representative of the early solar system using ab initio molecular dynamics. We calculate the Hugoniot and evaluate how the addition of volatiles affects transport, structural, and thermodynamic features under shock compression. We found that H2O or CO2 addition in the silicate decreases its initial density, which contributes to modifying the Hugoniot curve. At constant shock pressures, the addition of H2O or CO2 raises peak temperatures, altering volatile loss and melting behavior. The enhanced heating and melting caused by water imply that hydrated materials may have played a role in shaping the evolution of planetesimals.

We used the radius of the first coordination sphere to compute the speciation of C in the melt along the Hugoniot curve. We note the formation of iron and silicon carbide under certain conditions during the AIMD run. To further investigate the chemical bonding between C and Fe, as well as between C and Si, we computed the electron localization function. This analysis revealed that C-Fe and C-Si are covalently bonded. A similar analysis of the hydrated melt supports the presence of bonded Si–H and Fe–H species along the Hugoniot. The proportions of hydrides and carbides depend on the shock conditions and can affect the melt's redox state.

Our results suggest that even a small amount of volatiles in silicates influences the thermodynamics and chemical behavior during planetesimal impacts. These transformations should be considered in models of vapor formation and volatile depletion of early planetary bodies.

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