Effect of Impurities on Shock-Induced Phase Transformations in Silica Glasses

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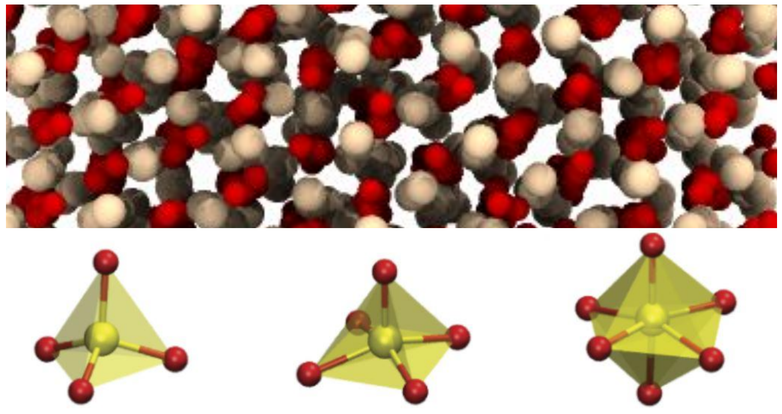
Does NaO_2 concentration affect stishovite formation in soda lime glass?

Objective:

Discover effect of NaO_2 concentration on the formation of high density stishovite in SiO_2 based glasses.

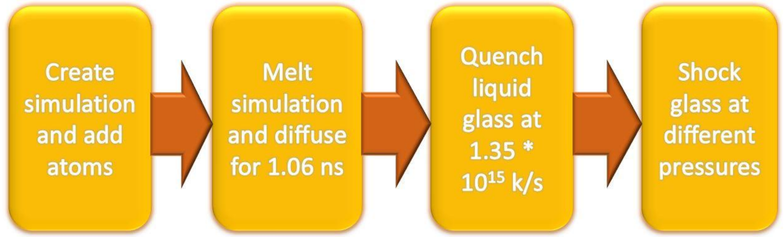


Silica 4 fold Quartz

Silica 5 fold Intermediate

Silica 6 fold Stishovite

Research approach:



MD Force Field:

$$U(r) = \frac{z_i z_j e^2}{r} + D_{ij}\left[\left\{1 - e^{-a_{ij}(r-r_0)}\right\}^2 - 1\right] + \frac{C_{ij}}{r^{12}}$$

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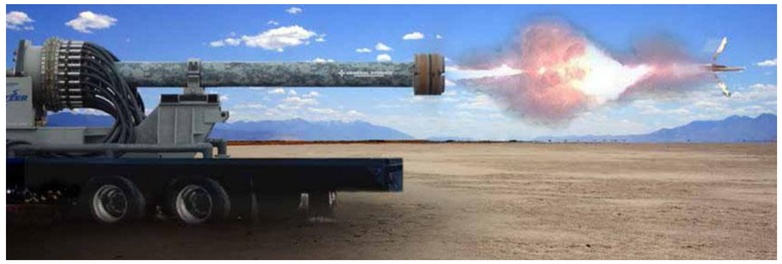
Application:

Understand the response of industrial silica based glasses in warfighter scenarios.

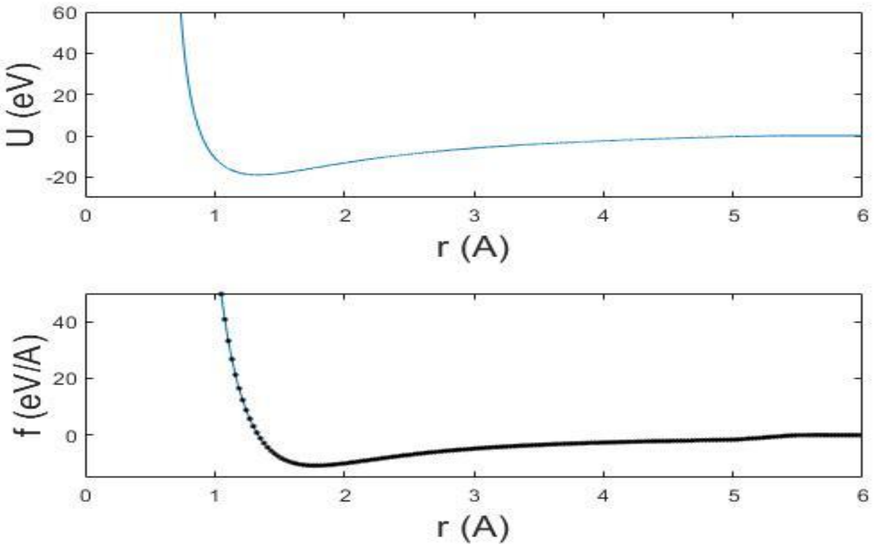


General Atomics Railgun

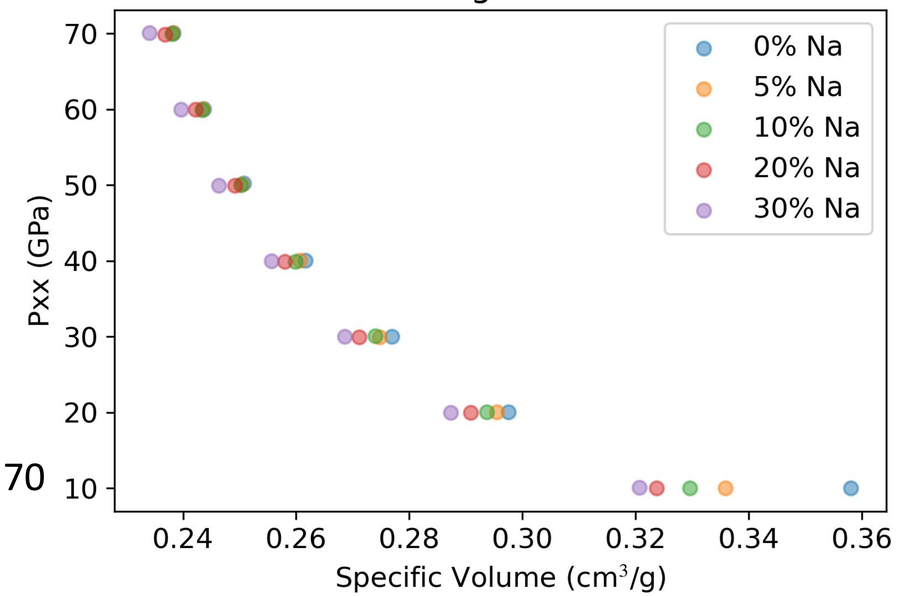
Research Path:

1) Diffusivity test
2) Stishovite with ReaxFF potential
3) ReaxFF potential -> BKS potential
4) Run simulations:
   a) Na concentration (%): 0, 5, 10, 20, 30
   b) Shock values (GPa): 10, 20, 30, 40, 50, 60, 70
5) Post Processing

Potential SiO



Hugoniot



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