Decoding the Effect of Temperature and Pressure on Glass

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Abstract Body: When subjected to variations in temperature or pressure, silicate glasses can exhibit drastically different behaviors, which are encoded in their atomic structure. However, decoding the effect of temperature and pressure on the atomic structure of silicate glasses is experimentally challenging. On the other hand, although molecular dynamics (MD) simulations offer a direct access to glasses' structure, they are limited to very high cooling rates. Here, we demonstrate that force-enhanced atomic refinement (FEAR) simulations can yield glass structures that simultaneously exhibit excellent agreement with experimental data and high thermodynamic stability. This allows us to explore how the atomic structure of glasses governs their response to changes in temperature and pressure.