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Carbonatitic glasses and melts

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We perform first-principles molecular dynamics (MD) calculations to study C-bearing melts along the T=3000K isotherm up to high pressure. Then we use the melts to study the quenched glasses. We consider pure forsteritic compositions, atomic C-, CO_2- and $MgCO_3$- bearing compositions. We discuss in detail the behavior of the glass structure under compression and the changes in coordination polyhedra, and we compare the glasses to the equivalent high-temperature melts.

We use several thermodynamic paths to obtain the glasses: (i) instantaneous quench at P=0GPa, then coldly compress, (ii) instantaneous quench at various high pressures and (iii) quench in 1K/MD step at various high pressures. Differences in glass structure and in equations of state develop between the different paths. They become larger at high pressure and are smoothed out by annealing. All glasses exhibit increase in Si-O and C-O coordination numbers, but at a smaller rate than the melts. Important structural rearrangements develop in all glasses around V/V0 compression of about 0.7.