Shock Compression of Forsterite (Mg_2SiO_4) to 950 GPa.

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Introduction: Planetary collision processes, such as moon formation [1] and impact melting [2] depend on the properties of mantle materials at extreme conditions. Additionally, the recently discovered super-Earths have interior pressures exceeding several hundreds of GPa [3]. Simulating impacts and planetary interiors requires an accurate description of mantle materials at extreme pressures and temperatures. However, the equation of state (EOS) of minerals at the pressure and temperature states encountered in impacts and super-Earths are often not well constrained and the phase state is unknown.

To better understand the behavior of mantle materials at extreme conditions, we combine high precision experiments with density functional theory (DFT) based quantum molecular dynamics (QMD). We use Sandia National Laboratories' Z – Machine [4] to shock compress relevant mantle minerals up to 1200 GPa [5]. The ability to generate steady planar shocks with well-characterized impactors and targets is critical for developing accurate EOS models. In addition, we performed laser-driven decaying shock experiments using the Omega Laser Facility. While the experiments provide continuum level data, such as Hugoniot pressure and temperature, to fully address the physics relevant to planetary science we use QMD methods to examine phase state.

Here, we show recent results on forsterite (Mg_2SiO_4) [6], the Mg end member in the olivine series. Along the Hugoniot, Mg_2SiO_4 has several phase transitions below 200 GPa [7]. Above 200 GPa, recent work, based on continuum level measurements, proposed Mg_2SiO_4 melts incongruently with solid MgO forming from the liquid Mg_2SiO_4 [8]. However, subsequent work using decaying shocks did not observe evidence of phase transitions above 200 GPa [9]. These contradictory results demonstrate the need for high precision measurements and QMD calculations to determine the Mg_2SiO_4 phase state and to constrain the EOS at conditions relevant for planetary studies.

Approach: The Z machine is a pulsed power system capable of delivering ~20 MA of current over a few 100 ns to a target load. The large current produces a strong magnetic field and the combined current and magnetic field creates a Lorentz force that can accelerate aluminum flyer plates up to 40 km/s [10]. The current pulse is tailored so that the flyer plates are shock-lessly accelerated toward the target and maintain a large solid density layer at impact. Impact produces steady shocks in the samples. The technique produces precision Hugoniot measurements that are consistent with traditional shock compression methods. A velocity interferometry measures the flyer plate velocities and sample shock velocities, from which we calculate the Hugoniot state. A streaked optical pyrometer (SOP) system measures sample emission during the shock wave transit. We compare the sample's emission to the emission from a quartz standard [11] to determine temperature.

Decaying shock experiments were performed at the OMEGA Laser Facility [12]. OMEGA produces strongly decaying shock waves by careful tuning of the driving laser pulse. These experiments measure shock velocity and thermal emission, which are calibrated in time. The Hugoniot temperature is determined using the measured reflectivity and comparison to the quartz standard [13]. The OMEGA measured reflectivity is used in determining the Z experimental temperatures.

To elucidate the phase state of Mg_2SiO_4 along the Hugoniot, we performed QMD calculations along the Hugoniot using the VASP code [14-16]. The Hugoniot state is determined by satisfying the Rankine-Hugoniot (RH) energy equation: $E\text{-}E_0 = 0.5(P+P_0)(V\text{-}V_0)$ where the subscript 0 identifies the initial state energy, pressure, and specific volume (1/ρ). We simulate a pure liquid Mg_2SiO_4 system at several temperatures for a specific density and interpolate the calculated E and P until the RH equation is satisfied [5,6].

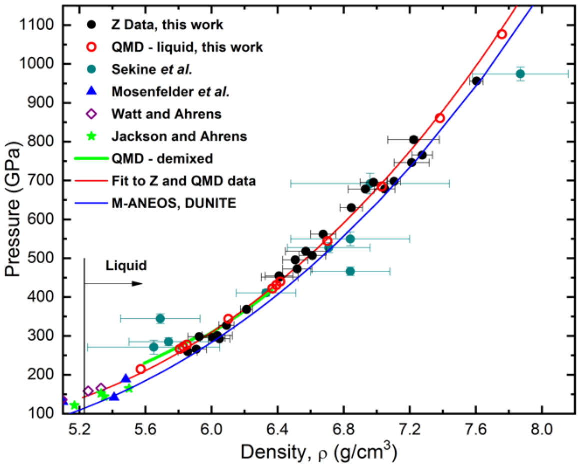

Figure 1. Mg_2SiO_4 Hugoniot in P-ρ space including data from Refs. [7,8,18,19] and M-ANEOS [17].

Results: Figure 1 shows the experimental Hugoniot and QMD calculated Hugoniot for Mg_2SiO_4 compared to previous data. The Z experimentally measured pressures range from 260 GPa to 950 GPa. The QMD results on pure liquid Mg_2SiO_4 are in agreement with the Z experimental data. Contrary to Ref. [8], our data does not exhibit any slope changes in the pressure range from 250 GPa to 450 GPa. For comparison, we plot the M-ANEOS DUNITE Hugoniot [17], which is often used in planetary simulations. The Hugoniot from the M-ANEOS is in reasonable agreement in P-ρ over the range we examined. This was not expected since M-ANEOS was constructed without data above 200 GPa.

Figure 2 plots the Hugoniot in T-P space over the range we studied. We find that the temperatures from the Z experiments, the OMEGA experiments, and the QMD calculations are all in agreement. The temperature increases monotonically with pressure and does not exhibit any signatures of a phase transition or demixing along the Hugoniot. The data from Bolis *et al.* [9] consistently trends toward higher temperatures. While the M-ANEOS reasonably matches the Hugoniot in P-ρ, it overestimates the temperature along the Hugoniot. This can affect modeling of planetary impact processes that depend on entropy, such as vaporization.

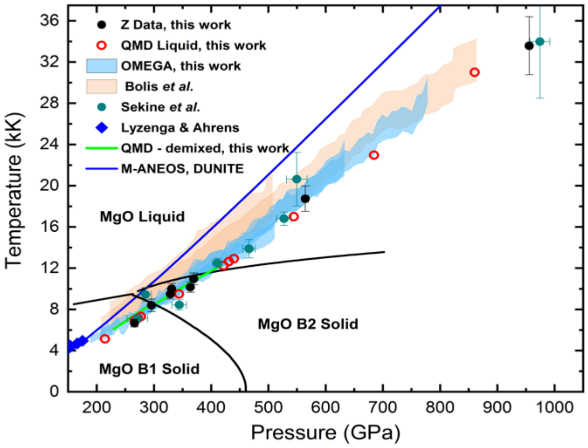

Figure 2. Mg_2SiO_4 Hugoniot in T-P space compared to the MgO phase boundaries [5].

To determine whether incongruent melting occurs along the Hugoniot, we calculated the Hugoniot states for a demixed assemblage of solid MgO + liquid Mg_2SiO_4, including both B1 and B2 phases of MgO. In P-ρ space, the demixed Hugoniot is indistinguishable from the calculated pure liquid Mg_2SiO_4 Hugoniot and is within the uncertainty of the experimental data. In T-P space, which is often sensitive to phase changes, we again find that the demixed Hugoniot is indistinguishable from the pure liquid and lies within the experimental temperature uncertainties. The demixed Hugoniot does show a 200K change in temperature due to the MgO B1-B2 transition, however, this is within all experimental uncertainties and significantly smaller than Sekine *et al.* [8] observed.

Summary: We have experimentally measured and calculated the Mg_2SiO_4 Hugoniot over the range from 200 GPa to 950 GPa. The Z, OMEGA, and QMD results exhibit a continuous, monotonically increasing Hugoniot without evidence of phase changes or demixing. On the continuum scale, the demixed Hugoniot and the pure liquid Hugoniot are indistinguishable and we cannot definitively state whether demixing occurs. These results provide new constraints on the forsterite EOS in pressure-temperature regimes important for planetary impacts and for planetary interiors.

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