Shock-Compressed Silicon: Hugoniot and Sound Speed to 2100 GPa

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The behavior of silicon (Si) above millions of atmospheres >100 GPa is important to understand the structure and evolution of terrestrial planets,[1–4] as well as the performance of inertial confinement fusion (ICF) capsule designs.[5–8] In rocky planets, Si is thought to be intrinsically paired to oxygen and, to a lesser extent, metals since they are prevalent on Earth's surface. However, it is likely that atomic bonding and compound formation are quite different at the extreme pressures expected in super-Earth-like planets.[9] In direct-drive ICF target designs, materials are selected based on a variety of properties at pressures exceeding several TPa (Ref. 5). Si has been proposed as a dopant for plastic shells[8] to mitigate laser imprint and Rayleigh–Taylor instabilities. While there has been significant work understanding the behavior of carbon[10–13] at TPa pressures, very little is understood about its group-14 analog, Si, at these extreme conditions.

Principal Hugoniot and sound-speed data are presented for silicon shocked to 320 to 2100 GPa. These Hugoniot data exhibit a different u_s–u_p slope ($S = 1.26 \pm 0.06$) from the measurements of Ref. 14 ($S = 1.80 \pm 0.10$) at lower pressures (80 to 200 GPa). A change in Hugoniot slope can point to a significant structural change in the material, e.g., solid–solid phase transitions or melting,[15,16] dissociation,[17] or ionization.[18,19] Quantum molecular dynamics (QMD) simulations performed at various points along silicon's principal Hugoniot predict an increase in ionic coordination and ionization of the $3s^2$ electron that is concurrent with the observed change in slope. Sound speeds were determined by time correlating the arrival of imposed acoustic perturbations at the shock front. The isentropic sound speed c_s of shock-compressed silicon was determined to be 15 to 23 km/s in the 5.7- to 7.6-g/cm^3 density range.

Experiments were conducted on the OMEGA EP Laser System.[20] Targets were irradiated by one to four 351-nm laser beams directly onto a parylene-n (CH) ablator, producing strong shock waves that compress the planar samples. These experiments used laser intensities of 30 to 305 TW/cm^2 produced by 4- and 5-ns temporally square and ramp-top laser pulses with spot sizes of approximately 1100 or 1800 μm. A portion of these experiments had preimposed acoustic perturbations on adjacent sides of the target stack, enabling a sound-speed determination.

The Hugoniot results are plotted in Fig. 1. Shock and particle velocity data from this work and four data points from Ref. 14 are fit separately using a weighted linear regression (method described in Ref. 21). This study is restricted to the high-pressure, single-wave regime, where shocked silicon does not form elastic and inelastic precursors; only Hugoniot data with pressure greater than 80 GPa are included in the fit. Functional forms were compared through a general linear F-test criterion, evaluated at the 1σ probability cutoff. An additional Bayesian statistical inference method was used for model selection, comparing a bilinear model against global linear and quadratic models through the Bayes factor. Accordingly, the bilinear model best represents silicon's

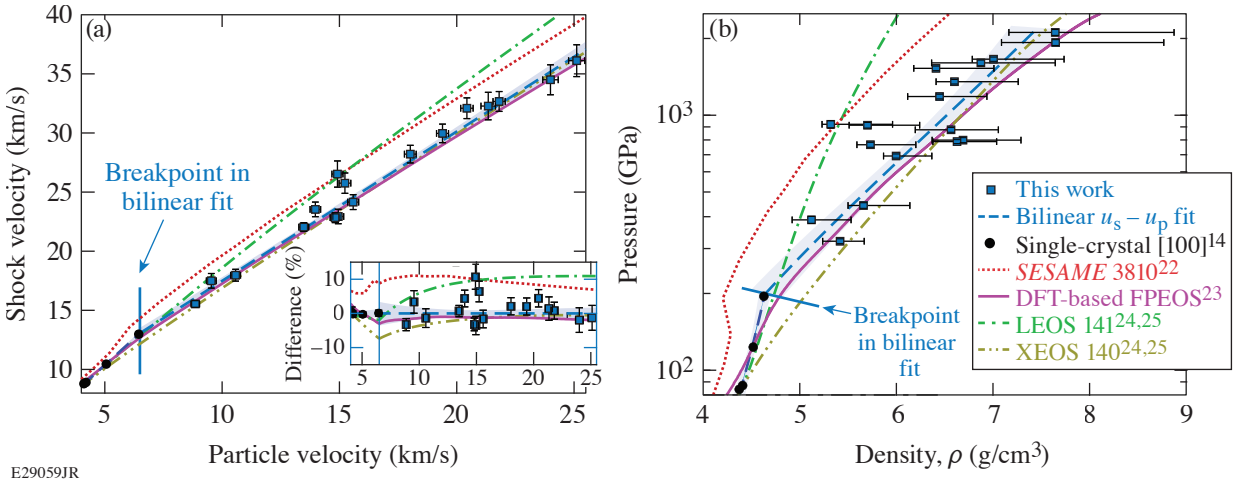

Figure 1
Silicon principal Hugoniot in (a) shock velocity u_s versus particle velocity u_p space and (b) pressure P versus density ρ space. Only dynamic compression data above 80 GPa, the single-wave compression regime in shocked silicon, are shown. Experimental data from this work (blue squares) and Ref. 14 (black circles) are fit with a bilinear functional form (dashed blue line) with a breakpoint at u_p = 6.5 km/s (solid blue line). A 1σ functional prediction band is shown as the shaded region surrounding the fit. Data is compared with Hugoniots from *SESAME* 3810 (red dotted curve),[22] DFT-based FPEOS (pink curve),[23] LEOS 141 (dashed–dotted green curve) and XEOS 140 (dashed–dotted yellow curve).[24,25] Inset in (a): Percent difference in shock velocity with respect to this work's u_s–u_p fit. FPEOS shows the best agreement with the experimental Hugoniot. The legend in (b) also corresponds to (a).

response to shock compression for shock pressures greater than 80 GPa. Using a χ^2 minimization, the breakpoint between the two linear regions was found at $u_{p,break}$ = 6.5 km/s.

Theoretical calculations have played an important role in explaining observed changes in physical properties of high-energy-density materials.[26–34] Changes in the Hugoniot slope are typically associated with ionic or electronic rearrangement. To better understand the physical mechanisms driving the change in Hugoniot slope for liquid silicon, density functional theory (DFT)-based QMD simulations were performed to examine changes in ionic coordination under shock compression. DFT-based QMD simulations suggest that the experimentally observed change in Hugoniot slope is coincident with an increase in ionic coordination and ionization of the $3s^2$ electron.

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