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Simulating Pressure-Driven Solid–Solid Phase Transformations Across Crystal Structure Types HONGJIN DU, HILLARY PAN, JULIA DSHEMUCHADSE, Cornell University — Materials' properties can vary widely based on the pressure at which they are formed and the crystal structure that they adopt—an example being the graphite and diamond allotropes of carbon. Many materials undergo structural transitions if they are put in a pressurized environment. Here, we investigate the high-pressure behavior of sixteen known, self-assembled structures under isotropic compression. We model these systems with molecular dynamics simulations of particles that interact via simple pair potentials. Particles, which spontaneously self-assemble into these different crystal structures, are initialized and then pressurized through a successively decreasing simulation box size. We observe pressure-driven solid–solid phase transitions across structure types, as well as a variety of other transformation behaviors as a function of pressure. We compare our findings with the pressure-dependent structural behavior that is known from atomic systems. Our work expands current knowledge on relationships between structure and pressure, and paves the road toward switchable materials.

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