Non-empirical equation of state for polymethyl methacrylate (PMMA) based on atomistic simulations

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Based on calculations using density functional theory methods, the thermodynamic properties of polymethyl methacrylate were determined in the region of monomer, solid phase, chemical decomposition zone, and warm dense matter state. The considered range of thermodynamic quantities has been significantly expanded compared to previously used atomistic modeling methods by the use of the extended first principles molecular dynamics method.
The calculated equation of state covers the density range of 0.5–6 g/cm^3, temperatures of 0–20 MK, and pressures of 0–570 Mbar. This allows directly compare the results of first-principles simulation with calculations using one-center models. The dependence of the calculated shock-wave properties of the investigated system in the low-pressure region on the initial approximation used to represent the original substance was analyzed.