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Multiphase Equations of State for Materials with Solid-Solid and Solid-Liquid Phase Transitions

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Many materials undergo a solid-solid phase transition where the crystal structure changes with a change in pressure or temperature. In addition materials melt, which is another phase transition. Across a phase boundary there are discontinuities in density and internal energy (latent heat). Although the volume change is small, even a small volume change may cause significant effects. For example under shock loading a phase transition may cause the shock to split into two distinct shocks. The equation of state (EoS) of a material with a phase transition may be modelled by determining the EoS for each individual phase separately. The phase that exists at any pressure and temperature is the phase with the lowest Gibb's free energy. Then the phase boundaries between phases are the loci of points in the pressure/temperature plane where two phases have the same Gibb's free energy. Along a phase boundary the EoS may be determined by assuming that the material consists of a mixture of two phases. Then the EoS in the mixed-phase region is completely determined by the EoS of the single phases. It can be shown that the bulk sound speed always falls when passing from a single-phase region into a mixed-phase region. Therefore, under isentropic compression through a phase boundary a shock will form. When implementing the EoS into hydrocodes an iterative method may be used to determine the solution to the equations: An initial guess is made of which phases exist at the required specific volume and internal energy and then the pressure, temperature and mass fractions are calculated. If the chosen phases have the lowest Gibb's free energy the solution has been found, otherwise another guess of the stable phases is made, and the iteration is repeated.