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Title: Equations of State and Fluid Dynamics

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Equations of State and Fluid Dynamics

Ralph Menikoff

Course Description

An equation of state (EOS) describes the material properties needed for compressible fluid flow. Solids at high pressures, above the yield strength, behave like fluids. The focus of this course is on EOS that describe solids. General constraints on an EOS required by thermodynamic consistency and stability are reviewed. Additional constraints on an EOS, needed for fluid flow to have the experimentally observed properties of shock waves, are presented. Empirical fitting forms, used for solid EOS, are studied and analyzed.

Part I. Foundation

A. Thermodynamic framework

wk 1. Thermodynamics: basics

Themodynamic variables
Fundamental identity
  Phase space
  Local Thermodynamic Equilibrium
Key EOS parameters
Consistent units

wk 2. Fluid equations (1-D)

Conservation form
Euler equations
  Entroup equation
Characteristic form
  Relaxation phenomena
Incomplete EOS
  Extend to complete EOS

wk 3. Thermodynamics: advanced

Thermodynamic potentials
  Thermodynamic statability
  Legendre transfrom
Thermodynamic identities
Phase transition
  Phase diagrams

wk 4. Thermo-Elastic solid

Elastic models
Stress & strain tensors
Moduli
Acoustic waves
1-D uniaxial strain
Phase transitions

B. Shock waves

wk 5. Hugoniot locus

- Jump conditions
- Riemann problem
  - Graphical solution
- Shock change equations
- Numerical algorithms
  - Front tracking
  - Shock capturing
    - Numerical dissipation

wk 6. Shock stability

- 1-D stability
- 2-D stability
  - Constraint on EOS
- Digression
  - Shock polars & wave patterns
  - Whitham-Chisnell shock dynamics

wk 7. Hugoniot locus for phase transitions

- Equilibrium wave structure
  - (V, P)–plane
  - (u_p, u_s)–plane
  - (u, P)–plane
- Rate dependent transition
  - Elastic-plastic transition
  - Wave structure
    - Split wave
    - Partly dispersed wave
    - Fully dispersed wave

Part II. Empirical EOS models for solids

A. Experimental measurements

wk 8. Measurement of shock locus

Example data
- LASL shock Hugoniot data

Methods to generate shocks

Calibrate standard
- Principal Hugoniot locus
- EOS off principal locus

Impedance match experiments

wk 9. Experimental isotherm & isentrope

High pressure experiments
- Isotherms
- Isentropes

Case study
- HMX isotherm

wk 10. Mie-Grüneisen EOS

Incomplete EOS
- Fitting form

Complete EOS
- Grüneisen coefficient
- Temperature

Common solid EOS
- Linear u_p-u_s shock relation
- Domain of model EOS

Shock polar

B. Theory

wk 11. **Debye model**
Helmholtz free energy
  Additive decomposition
Debye approximation for acoustic modes
  Phonon density of states
  Grüneisen coefficient & specific heat
Optical modes

wk 12. **Statistical mechanics**
Configuration space
Statistical ensembles
Atomic potentials
Computational techniques
  Molecular dynamics
  Monte Carlo
Numerical experiments

C. Common fitting forms

wk 13. **Simple analytic forms**
Perfect gas
Stiffened gas EOS
Hayes EOS

wk 14. **Generalized Hayes EOS**
Hayes EOS
Thermal component
Reference isotherm

wk 15. **Semi-analytic EOS**
Porous materials
P-T equilibrium mixture
Chemical equilibrium
Two-phase EOS

Bibliography

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