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Title: Boettger-Wallace Phase Transition Model Revisited

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Boettger-Wallace Phase Transition Model Revisited

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The Boettger-Wallace phase transition model is reviewed. The nuts and bolts of implementing the metastability and kinetics models in a simulation code are described in detail. The limitations of the BW model are discussed.

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Motivation

Why talk about work that was completed more than 10 years ago?

The nuts and bolts of implementing the Boettger-Wallace phase transition model (**metastability** and **kinetics**) in a numerical simulation code never has been presented in a comprehensive form.

Metastability Model

Assumptions

- There are two phases, a low P phase (1) and a high P phase (2).
- The equations of state (**EOSs**) for both phases are known.
- LTE is maintained during transition; $P = P_1 = P_2$ and $T = T_1 = T_2$.
- The instantaneous mass fraction of the 2 phase is denoted by λ.
- The metastable mass fraction of the 2 phase is denoted by λ_m.
- The metastable state is **long-lived** compared to the duration of the experiment.

Metastability Under Loading

Incremental load increase → incremental ($\Delta G = G_2 - G_1$) increase **$d\Delta G$** → incremental λ_m increase **$d\lambda_m$**. Material transformed also should be proportional to (**$1 - \lambda_m$**). Try

$$B\, d\lambda_m = (1 - \lambda_m)\, d\Delta G.$$

Integrating yields the **metastability equation**.

$$\lambda_m = 1 - \exp\left[1 - \exp(A - \Delta G / B)\right]$$

A = (+) energy barrier or (-) shear stress enhancement
B = energy width of the transition.

An equivalent expression can be deduced for the reverse transition.

Solving for P, T, and λ_m Given V and E in a Cell

1. **Estimate P, T, and λ_m** – Taken from previous time step.
2. **Determine P and T with λ_m fixed** – Solve four equations in four unknowns (V_1, V_2, E_1, E_2) **iteratively** using Newton's method

$$0 = (1 - \lambda_m) V_1 + \lambda_m V_2 - V$$
$$0 = (1 - \lambda_m) E_1 + \lambda_m E_2 - E$$
$$0 = P_1 (V_1,E_1) - P_2 (V_2,E_2)$$
$$0 = T_1 (V_1,E_1) - T_2 (V_2,E_2)$$

3. **Determine λ_m with P and T fixed** – Solve metastability equation.

Problem – **Nested do loops** for each cell and time step. Outer loop over λ_m is unstable unless damped and then has **slow convergence**.

Step 2: Solving the set of 4 equations

Write equations in matrix form as

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} (1-\lambda)V_1 + \lambda V_2 - V \\ (1-\lambda)E_1 + \lambda E_2 - E \\ P_1 - P_2 \\ T_1 - T_2 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} V_1 \\ E_1 \\ V_2 \\ E_2 \end{bmatrix}$$

Make an initial guess for unknowns, $\mathbf{x_0}$, and expand $\mathbf{F(x)}$ about $\mathbf{x_0}$.

$$\mathbf{F}(\mathbf{x}) = \mathbf{F}(\mathbf{x_0}) + \mathbf{A} \cdot (\mathbf{x}-\mathbf{x_0})$$

Step 2: Solving the set of 4 equations

$$\mathbf{A}(\mathbf{x}) = \begin{bmatrix} (1-\lambda) & 0 & \lambda & 0 \\ 0 & (1-\lambda) & 0 & \lambda \\ \frac{\partial P_1}{\partial V_1} & \frac{\partial P_1}{\partial E_1} & -\frac{\partial P_2}{\partial V_2} & -\frac{\partial P_2}{\partial E_2} \\ \frac{\partial T_1}{\partial V_1} & \frac{\partial T_1}{\partial E_1} & -\frac{\partial T_2}{\partial V_2} & -\frac{\partial T_2}{\partial E_2} \end{bmatrix}$$

Slow for tabular EOS

Solve for **X**.

$$\mathbf{x} = \mathbf{x_0} - \mathbf{A}^{-1} \cdot \mathbf{F}(\mathbf{x_0}).$$

Now replace $\mathbf{X_0}$ with **X** and iterate to convergence.

Step 2 is slow but the outer do loop over λ can be accelerated.

Accelerating the Outer Loop Over λ_m

Use an iterative procedure similar to Newton's method

1. Input $\lambda_{i1} = \lambda_m$ from last time step (or 0) $\rightarrow$ output = λ_{o1}.
2. Input $\lambda_{i2} = 0.5\ (\lambda_{i1} + \lambda_{o1})$ $\rightarrow$ output = λ_{o2}.
3. Assume $\lambda_o = \alpha + \beta\ \lambda_i$, with α and β from last two iterations. Input λ_{i3} from intercept with $\lambda_o = \lambda_i$ $\rightarrow$ output = λ_{o3}.
4. Now iterate to convergence, $\Delta\lambda < 0.01$.

In most cases this procedure converges after 3 iterations.

The overall metastability calculation is still very slow.

Metastability Model

Some observations

- Must track whether each cell is **loading or unloading**. I tracked V using a tolerance of ΔV = 0.00005 to avoid spurious switching due to ringing or numerical noise; i.e., reversal by less than ΔV is ignored.
- Calculations are much faster for analytic EOS than for tabular EOS, but are still **slow** compared to single phase EOS look-up.

Metastability Model

Could make metastability tractable with tabular EOS

- **Pre-calculate $\lambda_m(V,E)$, $P_m(E,V)$, and $T_m(E,V)$ for loading and unloading on a dense mesh, then interpolate using standard tabular EOS software.**

Phase Transition Kinetics

Characteristic assumptions of BW model

- System drives toward **metastable** state not equilibrium state.
- The transition rate is **linear** in distance from metastable state.
- Driving force is ΔG(P,T) → distance measured at **fixed (P,T)**.

This gives the **kinetics equation**.

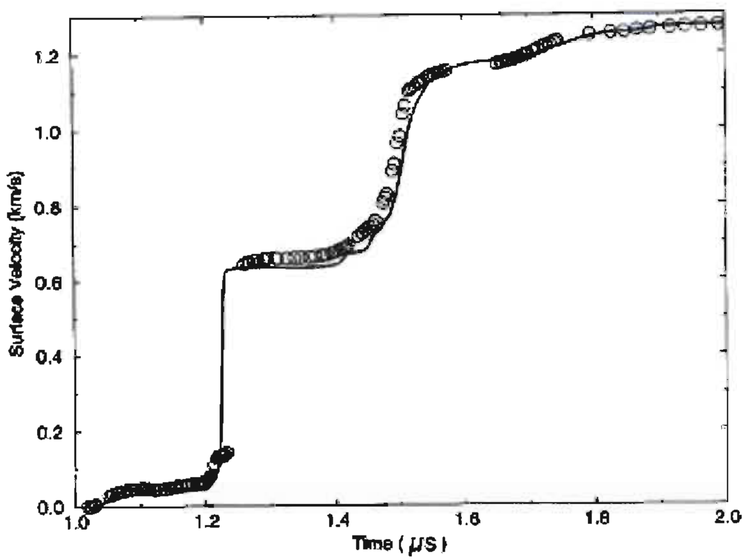
$$\frac{d\lambda}{dt} = \frac{\lambda_m(P,T) - \lambda(P,T)}{\tau}$$

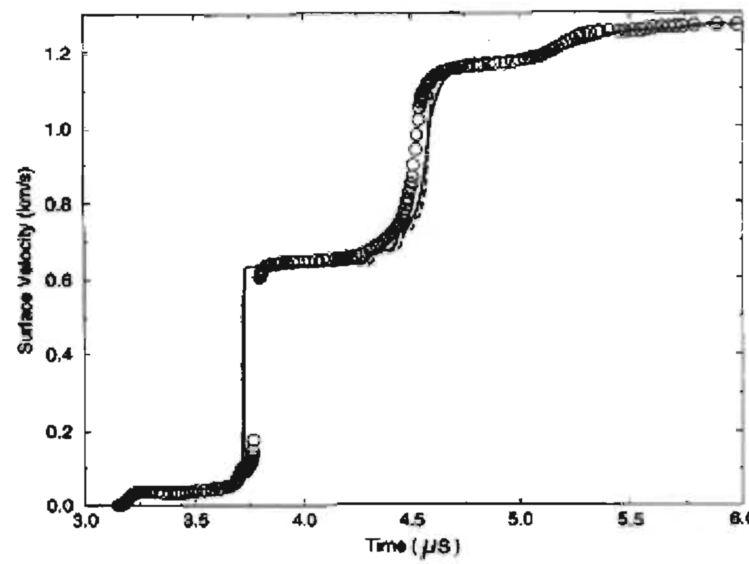
Phase transition kinetics

Some observations

- The maximum amount of material transformed in a given time step Δt is calculated as **$\Delta\lambda = (d\lambda/dt)_{avg}\,\Delta t$**, where $(d\lambda/dt)_{avg}$ is an average of rates calculated before and after the time step.
- Adding kinetics to the metastability model **does not slow down** the simulations.
- The kinetics model is however **fundamentally flawed**.

Application to Fe free surface experiments





Peak stress 23.6 GPa, sample thickness 6.370 mm – Best fit with τ = **30 ns**.

Peak stress 23.7 GPa, sample thickness 19.14 mm – Best fit with τ = **50 ns**.

Phase transition kinetics

A major problem with the kinetics equation

- For Fe, the relaxation time τ appears to depend on **peak stress** and **sample thickness**, and has to be fitted for each experiment.
- τ is not a constant as in BW model or a thermodynamic function $\tau(P,T)$ as in some other models.
- τ is a **constitutive property** that depends on microstructure and strain rate.