Numerical Approach to Modeling Shape Memory Alloys: Application to Tri-Linear Two-Phase Material

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Contents

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1. Motivation and Overview

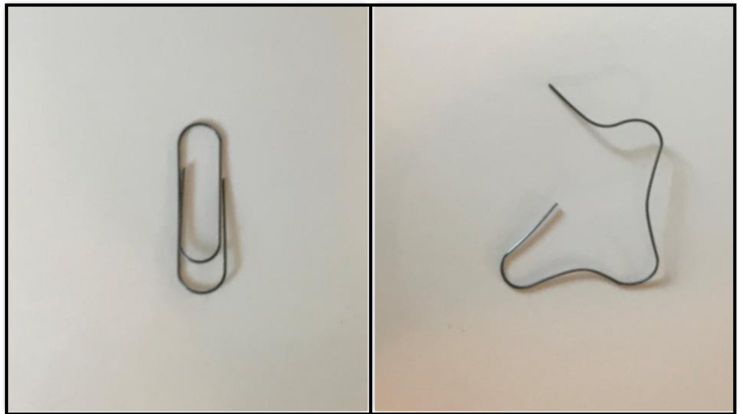
Applications of Shape Memory Alloys (SMAs)

SMAs have found many applications in medicine engineering, military and aerospace industry:

- Bendable eyeglasses, which recover their shape slowly to original form.
- Orthodontic braces, which support to align teeth in dentistry.
- Fuselages, which can be automatically returned back to the original shape after being damaged by bullets.
- Foldable spacecrafts, which can unfold again to the original shapes after being launched into space.

1. Motivation and Overview

Experiment of Shape Memory Alloy



Reference (left) and deformation (right) config. of SMA paper-clip at room temperature

Water at about 45^oC

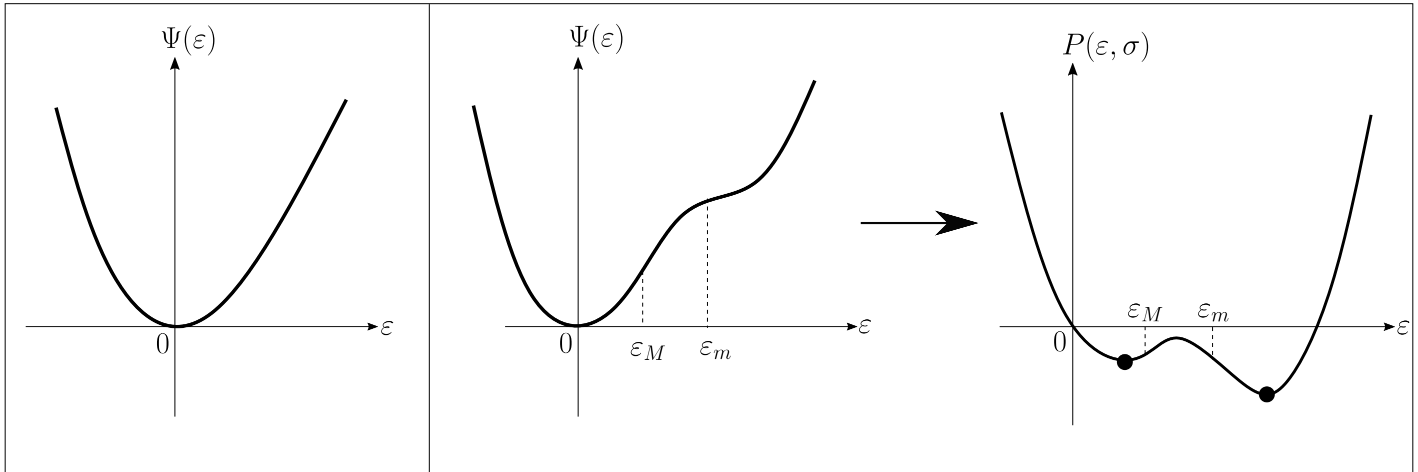
Background and overview:

- Evolution of Phase Transitions: A continuum theory; *Rohan Abeyaratne*, *James K. Knowles [2005].*
- Phase boundary propagation in heterogeneous bodies; *K. Bhattacharya [1999].*

Goals:

- A **thermodynamically-consistent** formulation of tri-linear two-phase material.
- Representation of hysteresis loops of the tri-linear material in 1D: **full** transition and **partial** transition.
- Description of **load-rise** and **load-drop** in two-phase loading.

Non-convex strain energy density $\Psi(\varepsilon)$ and the associated two-well potential energy density $P(\varepsilon, \sigma)$, where $P(\varepsilon, \sigma) = \Psi(\varepsilon) - \sigma\varepsilon$, are schematized:

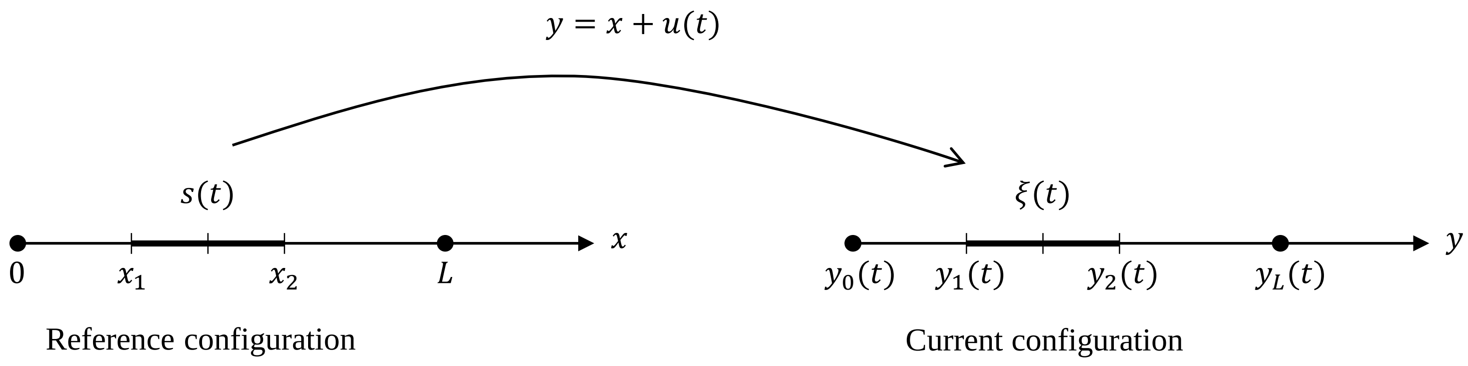


(a) Convex (b) Non-convex

Remarks:

- Shape Memory Alloy, e.g. NiTi, shows the transition of two phases identified by a distinct crystal structure.
- NiTi has a high-temperature **cubic** phase and low-temperature **monoclinic** phase.
- Material science convention: low-temperature phase (martensite) and high-temperature phase (austenite).
- **Non-convex two-well potential** has **two minima**, which is characteristic for two-phase material.

Reference and **current** configuration of a bar



Balance momentum of the sub-bar $[x_1, x_2]$ in the absence of body force requires that

$$\sigma(x_2, t) - \sigma(x_1, t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho v(x, t) dx$$

Field equation and its smoothness requirement yield:

$$\boxed{\begin{aligned} \sigma_{,x} &= \rho \ddot{x} \\ v_{,x} &= \dot{\varepsilon} \end{aligned}}$$

Displacement is assumed to be continuous, with piecewise continuous first and second derivative w.r.t. spatial and time coordinates. Hence, **jump conditions** require:

$$\boxed{\begin{aligned} [\![\sigma]\!] &= -\rho \dot{s} [\![v]\!] \\ [\![v]\!] &= -\dot{s} [\![\varepsilon]\!] \end{aligned}}$$

2. Preliminaries of Mathematical Modeling of Shape Memory Alloys

Dissipation rate obtained from **field equations** and **jump conditions** yields:

$$D(t) = \sigma v\Big|_{x_1}^{x_2} - \frac{d}{dt}\int_{x_1}^{x_2}\left(\frac{1}{2}\rho v^2 + W(\varepsilon)\right)dx$$

Thermodynamically consistency requires:

$$\boxed{D(t) = f(t)\dot{s}(t) \geq 0}$$

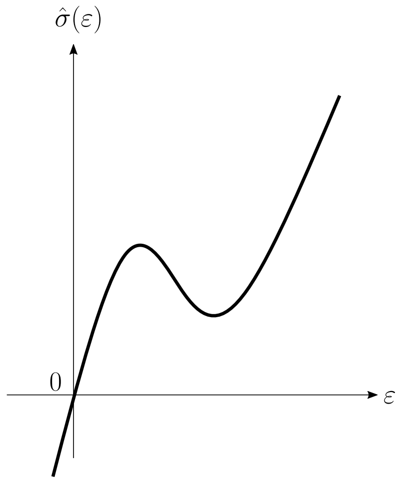
where driving force $f(t)$ is defined as

$$\begin{aligned} f = \hat{f}(\varepsilon^+, \varepsilon^-) &= [\![W(\varepsilon)]\!] - \frac{1}{2}(\hat{\sigma}(\varepsilon^+) + \hat{\sigma}(\varepsilon^-))[\![\varepsilon]\!] \\ &= \int_{\varepsilon^-}^{\varepsilon^+} \hat{\sigma}(\varepsilon)d\varepsilon - \frac{1}{2}(\hat{\sigma}(\varepsilon^+) + \hat{\sigma}(\varepsilon^-))(\varepsilon^+ - \varepsilon^-) \end{aligned}$$

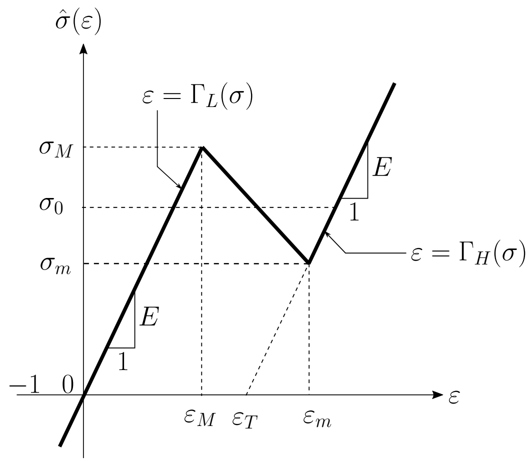
Single quasilinear equation:

$$[\hat{\sigma}'(\varepsilon)\varepsilon_{,x}]_{,x} = \rho\ddot{\varepsilon}$$

3. Tri-linear two-phase elastic material in 1D



(a) A general two-phase material.



(b) Tri-linear two-phase material.

Tri-linear two-phase material: all three branches of the stress-strain curve are straigh lines, with the two rising branches given by:

$$\sigma = \hat{\sigma}(\varepsilon) = \begin{cases} E\varepsilon, & -1 < \varepsilon \leq \varepsilon_M, \\ E(\varepsilon - \varepsilon_T), & \varepsilon \geq \varepsilon_m, \end{cases}$$

It follows that

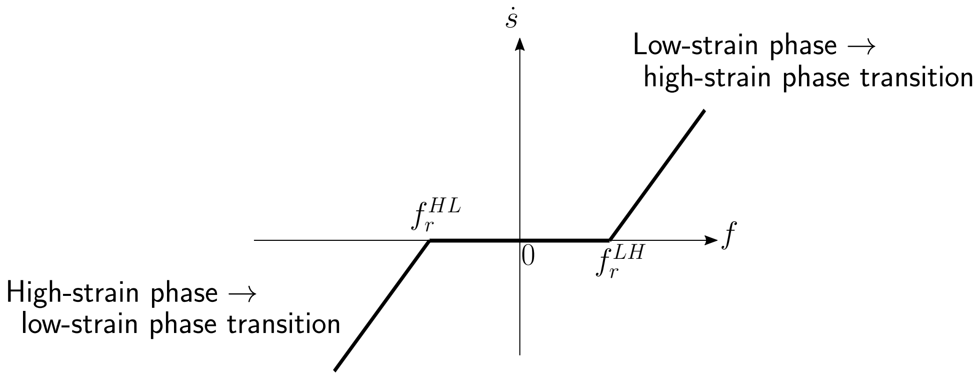
$$\boxed{\begin{aligned} \Gamma_L(\sigma) &= \sigma/E \\ \Gamma_H(\sigma) &= \varepsilon_T + \sigma/E \\ \sigma_0 &= (\sigma_M + \sigma_m)/2 \\ f &= (\sigma - \sigma_0)\varepsilon_T \end{aligned}}$$

3. Tri-linear two-phase elastic material in 1D

Next, consider a **particular kinetic relation**:

$$\dot{s} = \bar{\Phi}(f) = \begin{cases} M\varepsilon_T(f - f_r) & \text{if } \ f > f_r, \\ 0 & \text{if } \ -f_r \leq f \leq f_r, \\ M\varepsilon_T(f + f_r) & \text{if } \ f < -f_r. \end{cases}$$

where $M > 0$ is the phase boundary *mobility*.



which can be recast into:

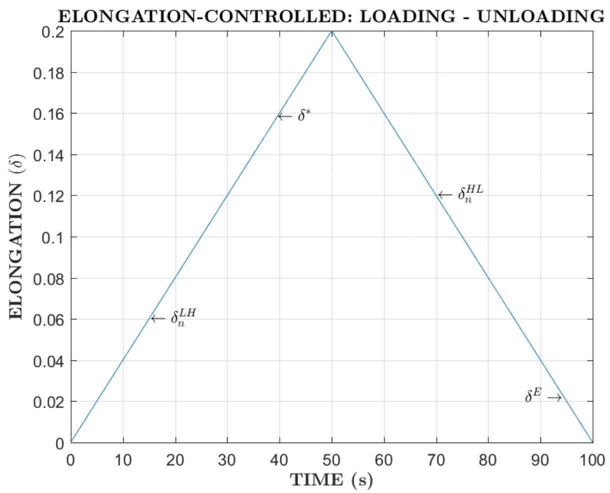
$$\dot{s} = {\color{red}\bar{\Phi}(\sigma)} = \begin{cases} M\varepsilon_T(\sigma - \sigma_r^{LH}) & \text{if } \ \sigma > \sigma_r^{LH}, \\ 0 & \text{if } \ \sigma_r^{HL} \leq \sigma \leq \sigma_r^{LH}, \\ M\varepsilon_T(\sigma - \sigma_r^{HL}) & \text{if } \ \sigma < \sigma_r^{HL}. \end{cases}$$

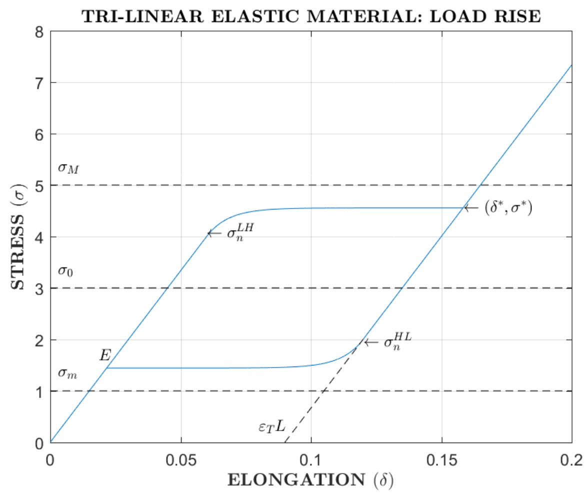
Finally, **master differential equation** is obtained:

$$\left[p(\sigma) - \varepsilon_T'(\sigma)\frac{\delta}{L} \right] \dot{\sigma} + \varepsilon_T(\sigma)\frac{\dot{\sigma}}{L} = \varepsilon_T^2(\sigma){\color{red}\bar{\Phi}(\sigma)}L$$

$$p(\sigma) = \Gamma_L(\sigma)\Gamma_H'(\sigma) - \Gamma_L'(\sigma)\Gamma_H(\sigma)$$

3.1 Tri-linear two-phase elastic material in 1D: full transition - load rise





Loading: low-strain phase $\quad \sigma = \dfrac{\delta E}{L}$

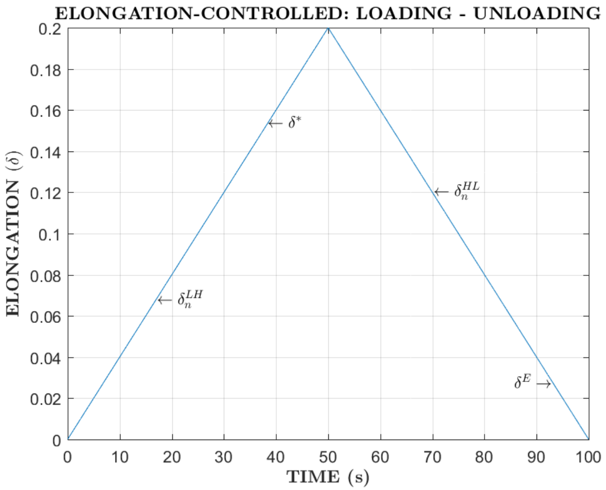
Loading: two-phase $\quad \sigma = \sigma_n^{LH} + E\nu + (\sigma_n^{LH} - \sigma_r^{LH} - E\nu)\exp\left(-\dfrac{\delta - \delta_n^{LH}}{\nu L}\right)$

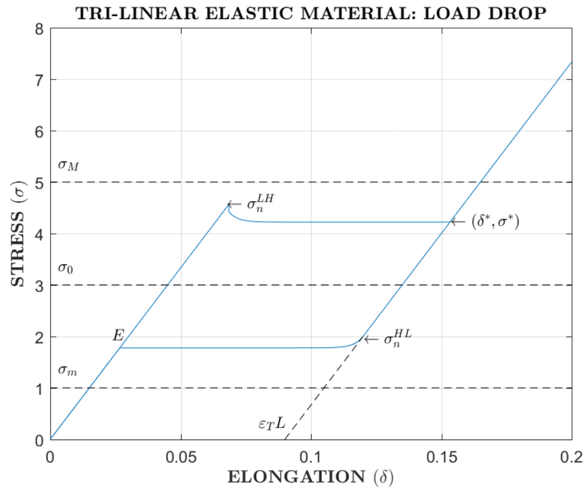
Loading: high-strain phase $\quad \sigma = \dfrac{\delta E}{L} - E\varepsilon_T$

Unloading: two-phase $\quad \sigma = \sigma_n^{LH} - E\nu + (\sigma_n^{LH} - \sigma_r^{LH} + E\nu)\exp\left(\dfrac{\delta - \delta_n^{LH}}{\nu L}\right)$

Unloading: low-strain phase $\quad \sigma = \dfrac{\delta E}{L}$; where $\nu = \dfrac{\dot{\delta}}{EM\varepsilon_T^2}$; with $\boxed{\dot{\delta} > \varepsilon_T \bar{\Phi}(\sigma_n^{LH})}$

3.2 Tri-linear two-phase elastic material in 1D: full transition - load drop





Loading: low-strain phase $\sigma = \dfrac{\delta E}{L}$

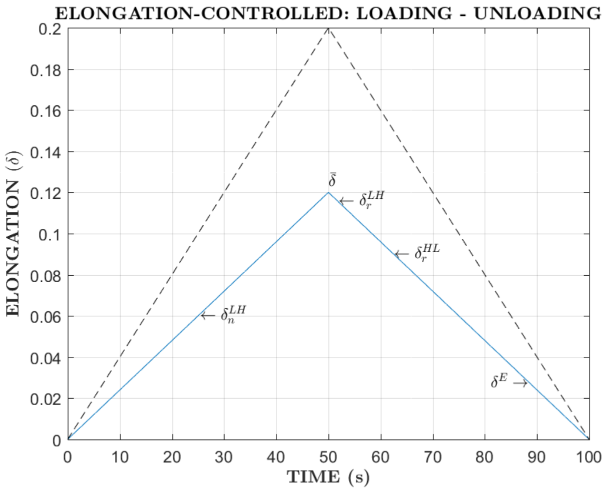
Loading: two-phase $\sigma = \sigma_n^{LH} + E\nu + (\sigma_n^{LH} - \sigma_r^{LH} - E\nu)\exp\left(-\dfrac{\delta - \delta_n^{LH}}{\nu L}\right)$

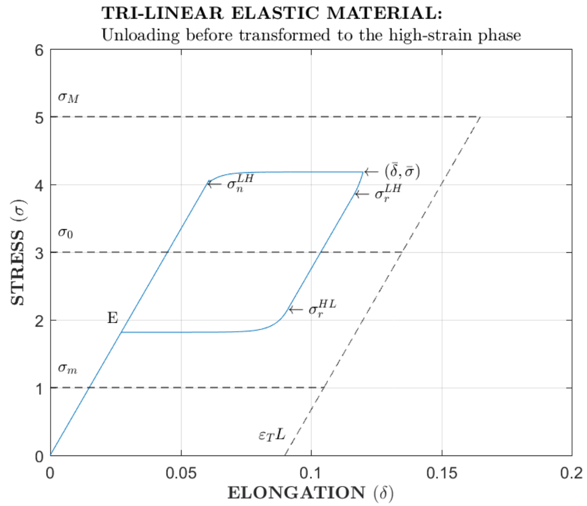
Loading: high-strain phase $\sigma = \dfrac{\delta E}{L} - E\varepsilon_T$

Unloading: two-phase $\sigma = \sigma_n^{LH} - E\nu + (\sigma_n^{LH} - \sigma_r^{LH} + E\nu)\exp\left(\dfrac{\delta - \delta_n^{LH}}{\nu L}\right)$

Unloading: low-strain phase $\sigma = \dfrac{\delta E}{L}$; where $\nu = \dfrac{\dot{\delta}}{EM\varepsilon_T^2}$; with $\boxed{\dot{\delta} < \varepsilon_T \bar{\Phi}(\sigma_n^{LH})}$

3.3 Tri-linear two-phase elastic material in 1D: partial transition





Loading: low-strain phase $\quad \sigma = \dfrac{\delta E}{L}$

Loading: two-phase $\quad \sigma = \sigma_n^{LH} + E\nu + (\sigma_n^{LH} - \sigma_r^{LH} - E\nu)\exp\left(-\dfrac{\delta - \delta_n^{LH}}{\nu L}\right)$

Unloading: Stage 1 $\quad \sigma = \sigma_r^{LH} - R\nu + (E\nu + \bar{\sigma} - \sigma_r^{LH})\exp\left(\dfrac{\delta - \bar{\delta}}{\nu L}\right)$

Unloading: Stage 2 $\quad \sigma = \sigma_r^{LH} + \dfrac{E}{L}(\delta - \delta_r^{LH})$

Unloading: Stage 3 $\quad \sigma = \sigma_r^{LH} + E\nu\left(\exp\left(\dfrac{\delta - \delta_r^{HL}}{\nu L}\right) - 1\right) \qquad$ where $\nu = \dfrac{\dot{\delta}}{EM\varepsilon_T^2}$

4. Extension to 3D problem of two-phase thermoelastic material

Starting point of 3D problem of two-phase thermoelastic material is the free energy function Ψ defined as

$$\boxed{\Psi = c_0(\Theta) + d(\Theta)\left[\frac{I_3}{p^3}\right] + e(\Theta)\left[\left(\frac{I_2}{p^2}\right)^2 - 3\frac{I_2}{p^2} + 9\frac{I_3}{p^3}\right]}$$

where $p = \frac{1}{2}(\eta_1^2 - 1)$, in which η_1 is the stretch, i.e. a ratio between 2 edges of 2 considered lattices, and I_2 and I_3 are invariants of Green strain $\mathbf{E} = \frac{1}{2}\left(\mathbf{U}^2 - \mathbf{I}\right)$, defined as

$$\begin{aligned} I_2 &= E_{11}E_{22} + E_{22}E_{33} + E_{33}E_{11} \\ I_3 &= E_{11}E_{22}E_{33} \end{aligned}$$

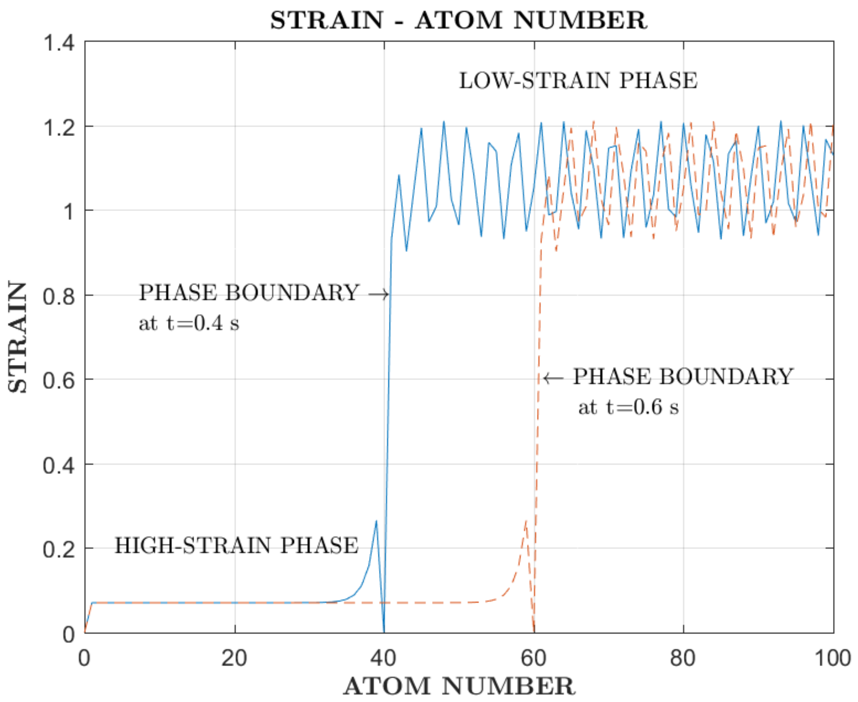
and coefficients $e(\Theta)$ and $d(\Theta)$ satisfy the following conditions

$$\begin{aligned} e(\Theta) &> 0, & 3e(\Theta) &> d(\Theta) > -3e(\Theta) \\ d'(\Theta) &> 0, & d(\Theta_T) &= 0 \end{aligned}$$

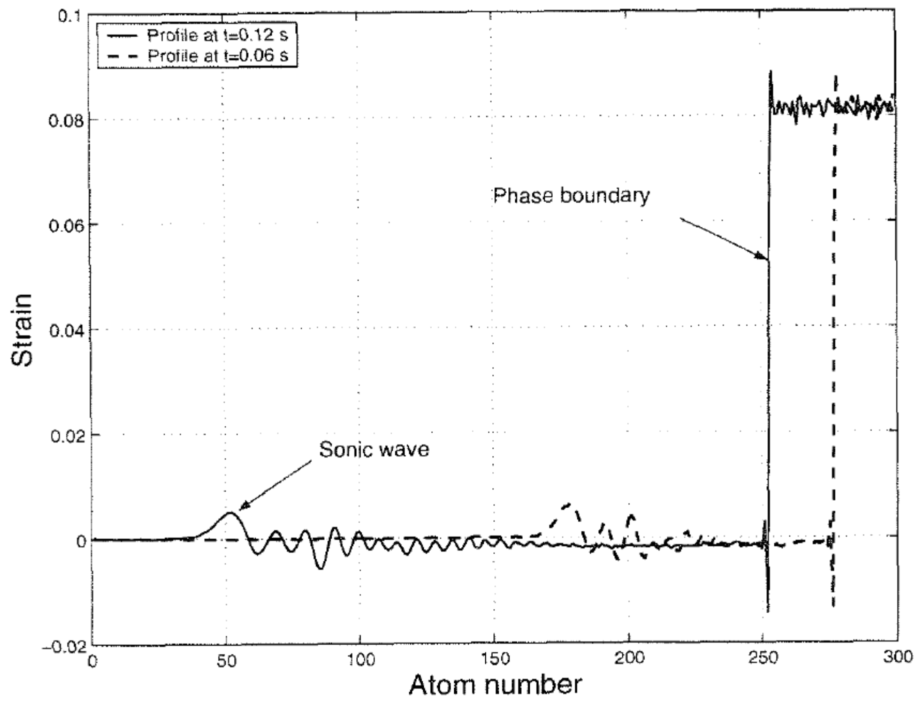
where Θ_T is "*Transformation temperature*".

Remarks:

- Ψ is a quartic polynomial $\rightarrow$ multiwell character is desired.
- Ψ shows the **austenitic** energy well at the origin $\mathbf{E} = \mathbf{0}$.
- Ψ shows three **martensitic** energy wells at $\mathbf{E} = \mathbf{E}_1$, $\mathbf{E}_2$, and $\mathbf{E}_3$.



(a) Figure deduced from R. Abeyaratne and J. Knowles [2005].



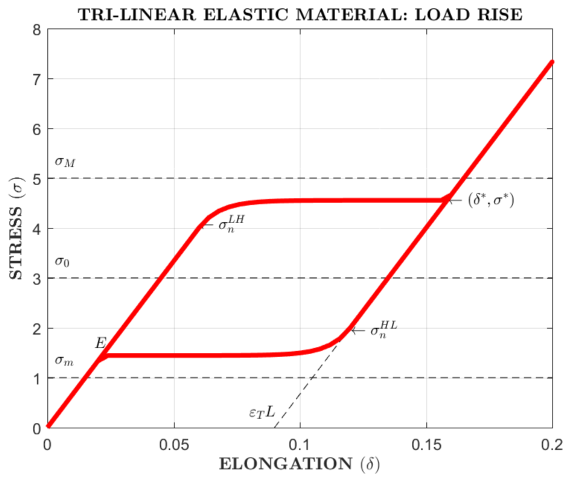
(b) Figure of Purohit dissertation [2002].

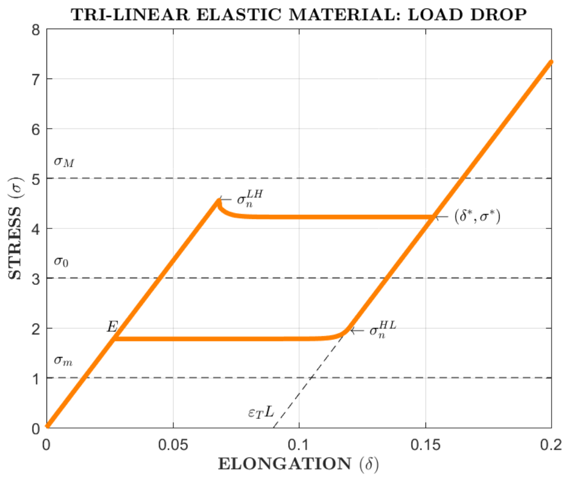
Idea:

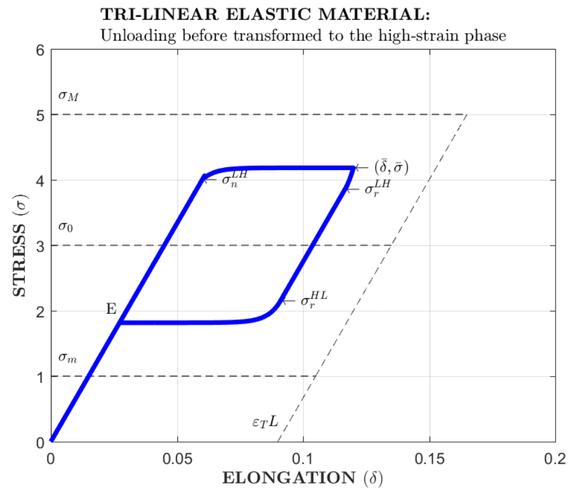
Atoms along the phase boundary are modeled by a **one-dimensional chain of particles**, each of **mass** m, connected by a linear spring of **stiffness** k and **natural length** d to describe the **jump** between low-strain phase and high-strain phase.

6. Summary and conclusions

Evolution of Phase Transitions of Tri-Linear Elastic Two-Phase Material:







Results obtained

- Mathematical modeling of one-dimensional tri-linear two-phase elastic material based on continuum theory.
- A thermodynamically consistent formulation is presented.
- Description of load drop behavior of tri-linear elastic material is shown.
- Description of partial transition of tri-linear elastic material is shown.

Future study possibilities

- Extension into three-dimension of tri-linear two-phase elastic material.
- Investigation into thermoelastic two-phase material.