Mechanical Hysteresis in Single Crystal Shape Memory Alloys

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Fatigue 06

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Brief History of Shape Memory

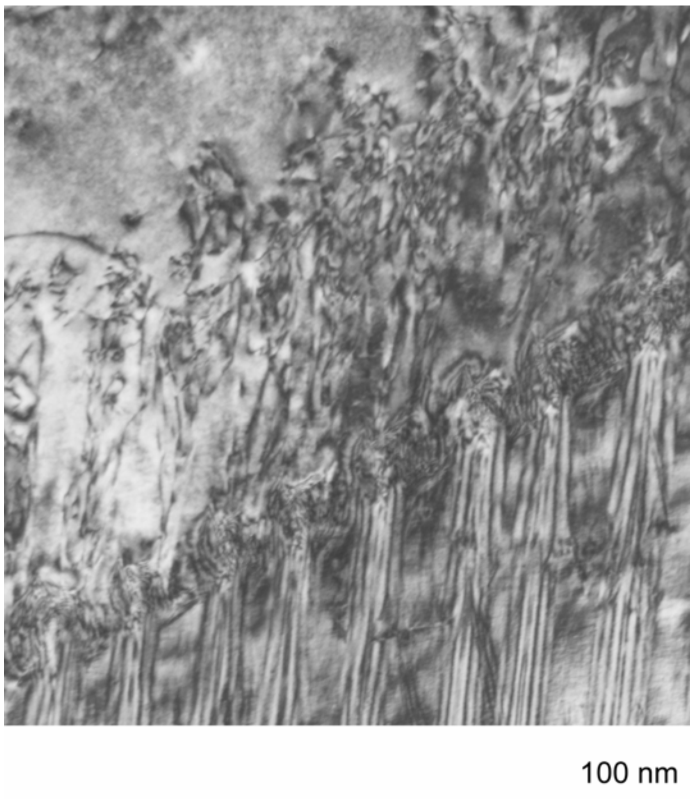
- Chang-Read discovered transformation reversibility in Au-Cd crystals (1950).
- Buehler (1960) discovered NiTi alloys –max. strains near 6% in polycrystals, 8% in single crystals. Fatigue performance is a concern.
- Cu- based alloys followed.
- NiTi found application in stents, and other biomedical applications. Some niche applications were developed as an actuator.
- A new generation of SMA are now studied with NiFeGa, CoNiAl type compositions. These materials have unprecedented fatigue resistance.

Background

[R. F. Hamilton, H. Sehitoglu, Y. Chumlyakov, H. J. Maier Acta Mat. 52 (2004)]

- **NiTi**
  - The hysteresis is a strong function of composition in NiTi alloys.
    - » Increases with Stress for low Ni alloys
    - » Decreases with Stress for high Ni alloys
  - The increase in hysteresis (in low nickel NiTi alloys) is linked to plastic relaxation of the internal stress in martensite variants.

Dislocations at martensite (internal twin) parent junctions

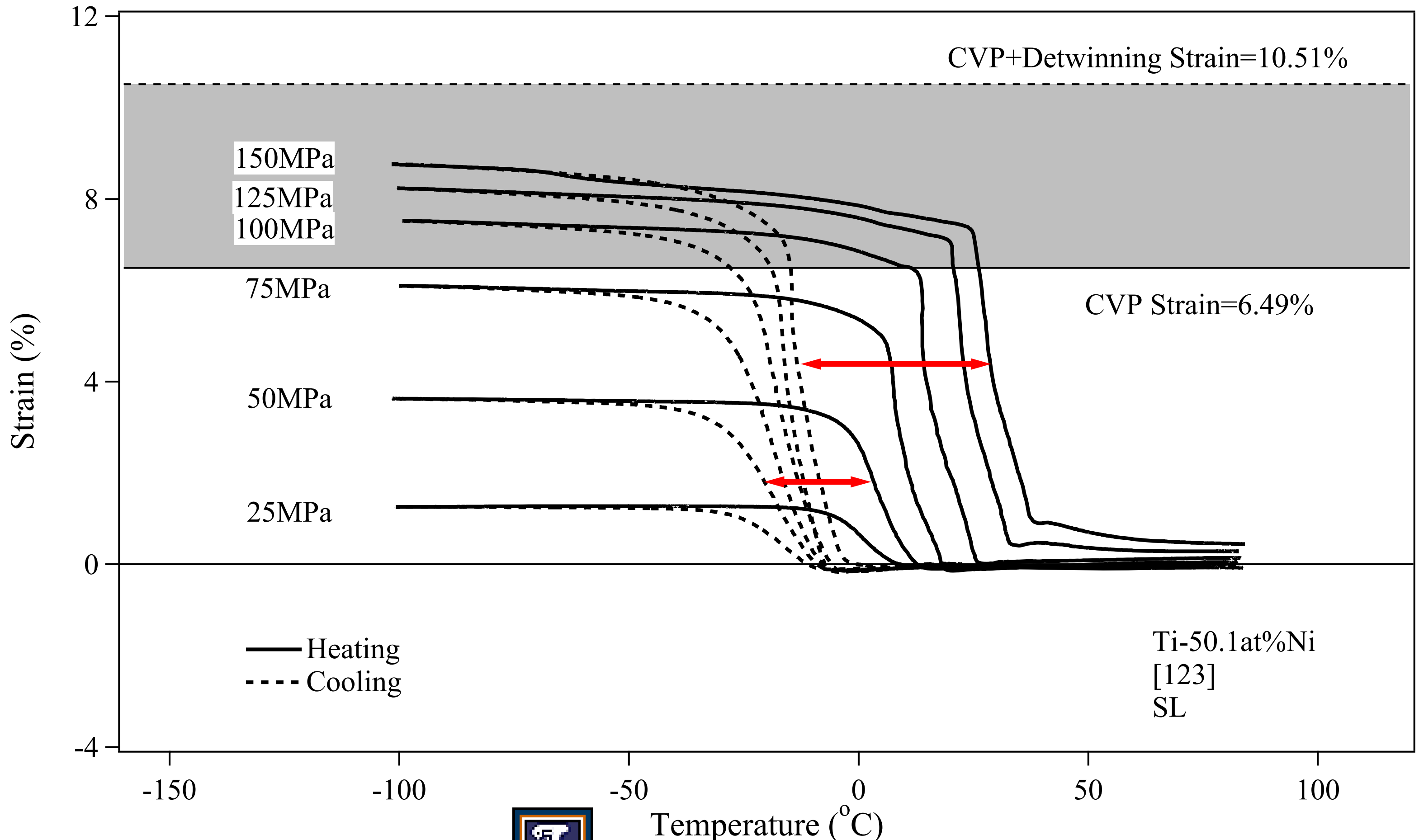


50.1 %Ni [111]

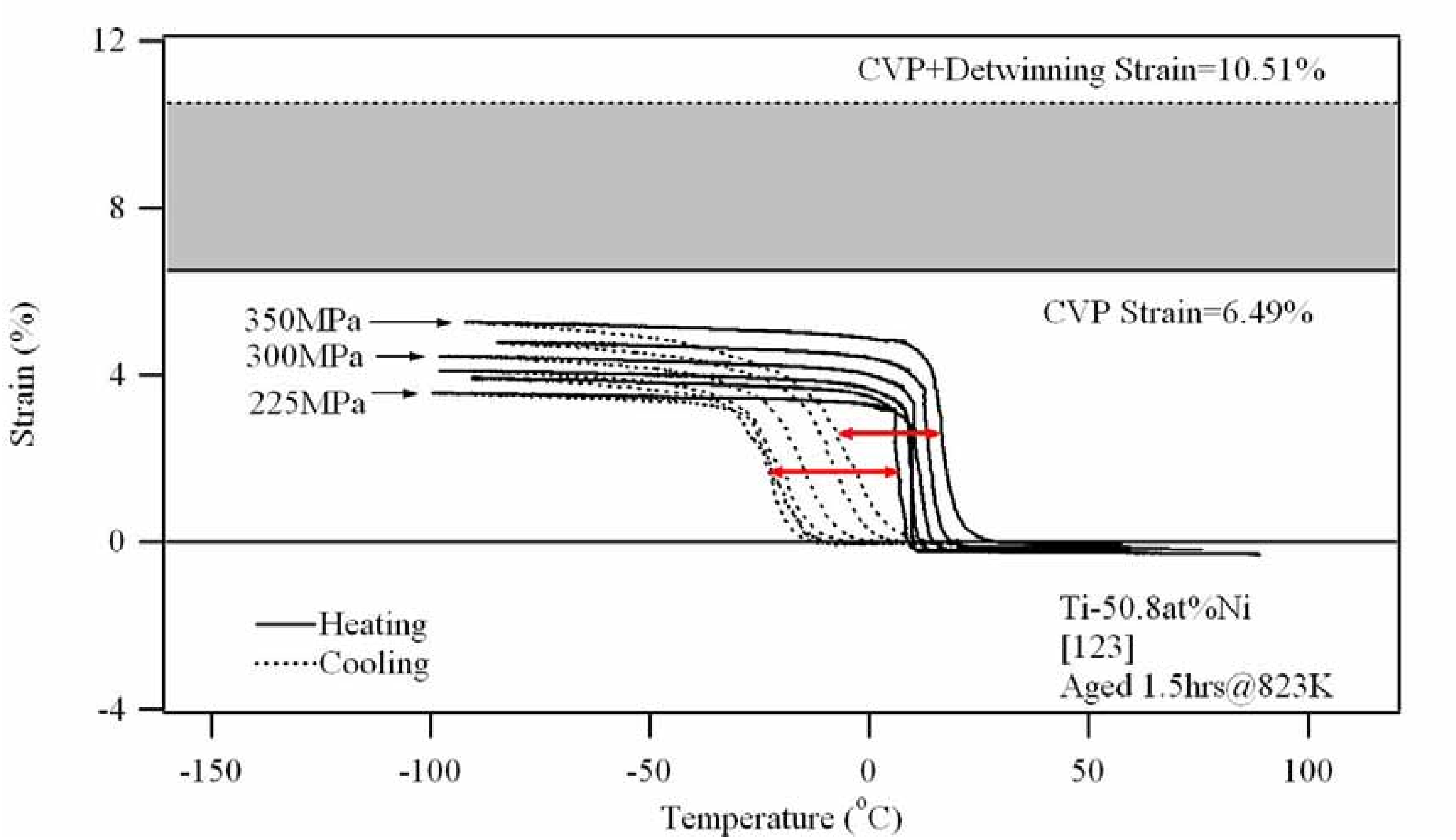
Dislocation Activity in the Parent Phase

51.5%Ni [123]

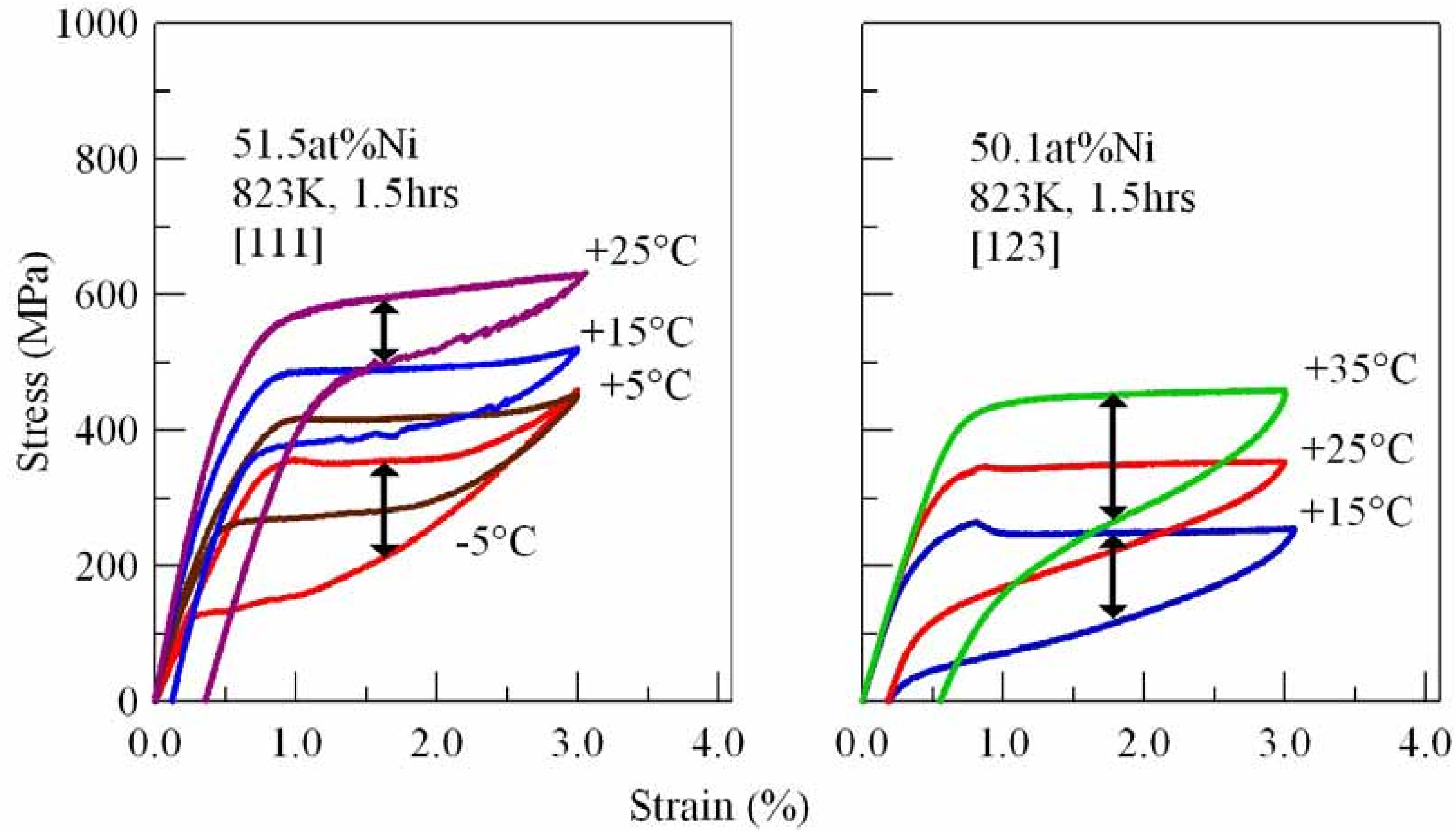
Strain-temperature Behavior under Constant Stress 50.1 at%Ni [123] (Shape Memory Response)



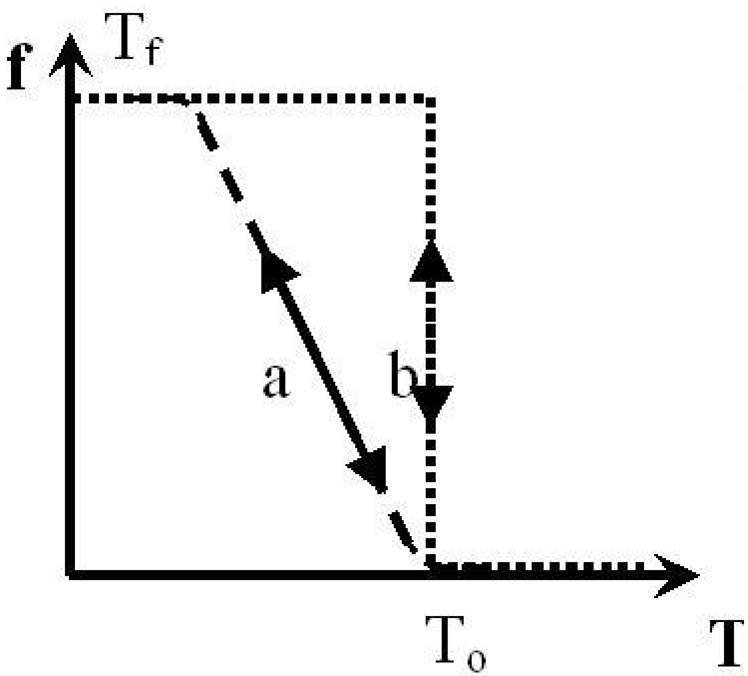
50.8 at%Ni [123]


CVP+Detwinning Strain=10.51%
CVP Strain=6.49%
350MPa
300MPa
225MPa
Heating
Cooling
Ti-50.8at%Ni
[123]
Aged 1.5hrs@823K
Strain (%)
Temperature (°C)
12
8
4
0
-4
-150
-100
-50
0
50
100

NiTi: Pseudoelastic Response



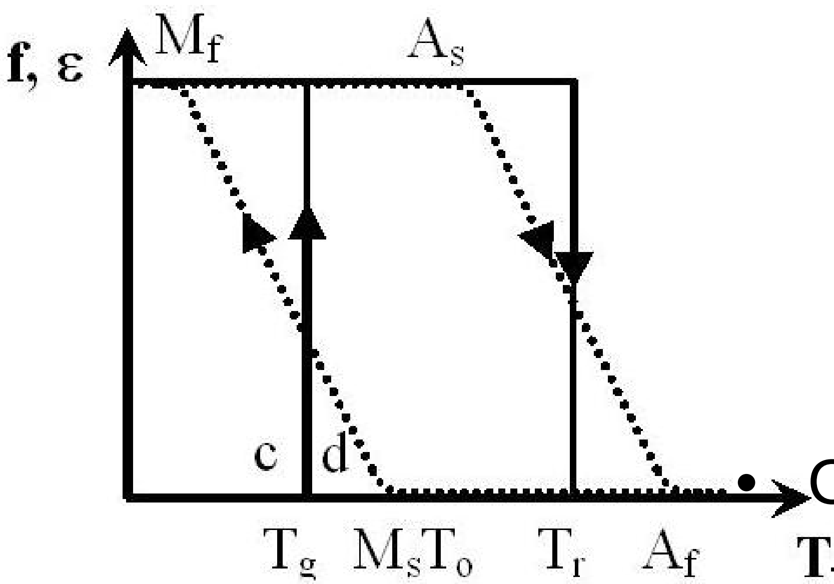
Elastic Strain Energy Without Energy Dissipation



- Curve a
  - Non-chemical free energy consists only of reversible elastic strain energy so the forward and reverse transformations follow the same thermal path without a hysteresis.
  - Elastic strain energy opposes forward transformation, facilitating additional under-cooling (cooling below To) and the austenite to martensite transformation is completed at Tf.

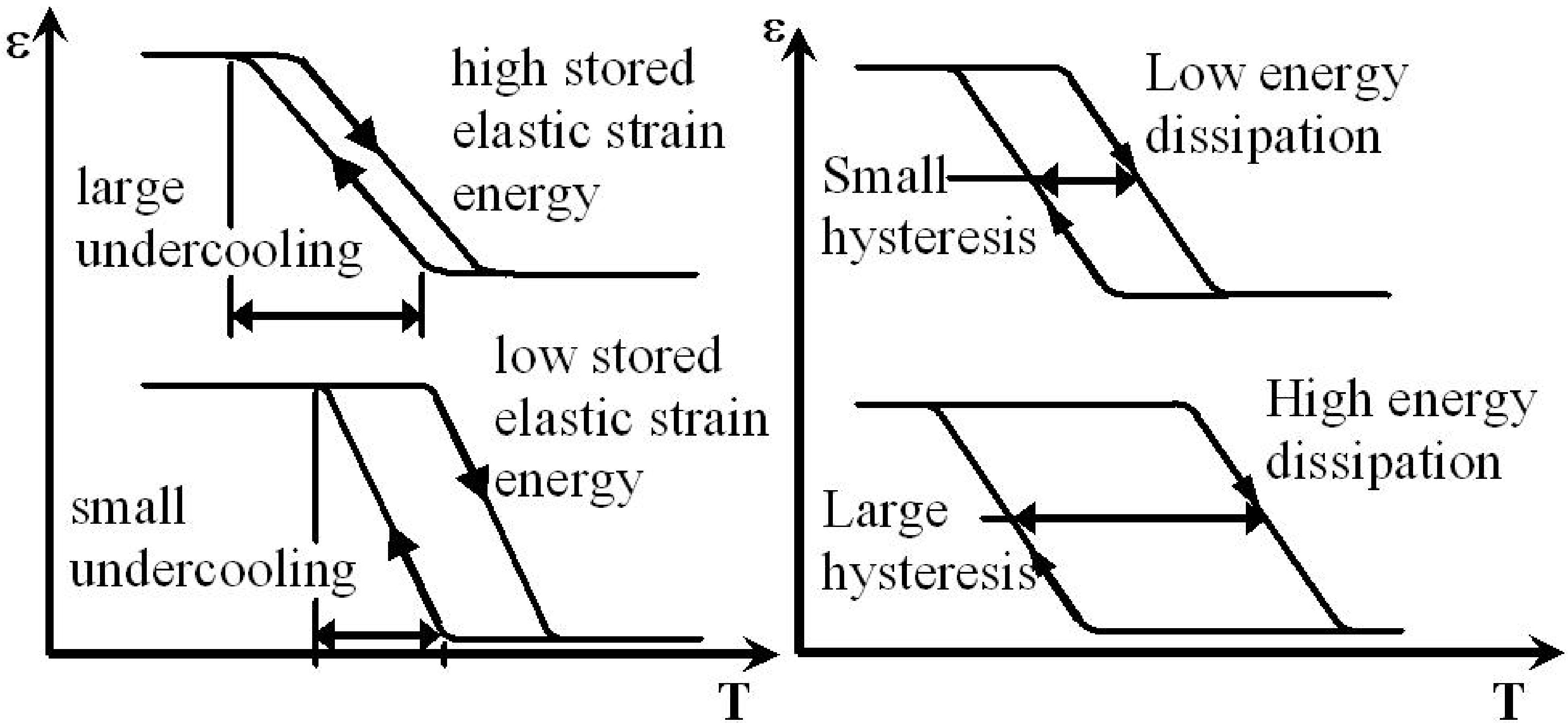
Curve b
  - Ideally reversible because non-chemical contributions are not considered; therefore, the forward and reverse transformations occur at the phase equilibrium temperature, To.
  - Note that the under-cooling, facilitated by accruing elastic strain energy, inclines curve in a compared to b.

Frictional and Elastic Strain Energy Dissipation



- Curve c
  - Ignoring stored elastic strain energy considering constant frictional resistance during the transformation, the forward and reverse, which requires additional undercooling and overheating, transformations start and finish at the constant temperatures T_g and T_r respectively.
- Curve d
  - Schematic stress-strain curve exhibiting the evolution of stored elastic strain energy and variable frictional dissipation give rise to the slope of the curve.

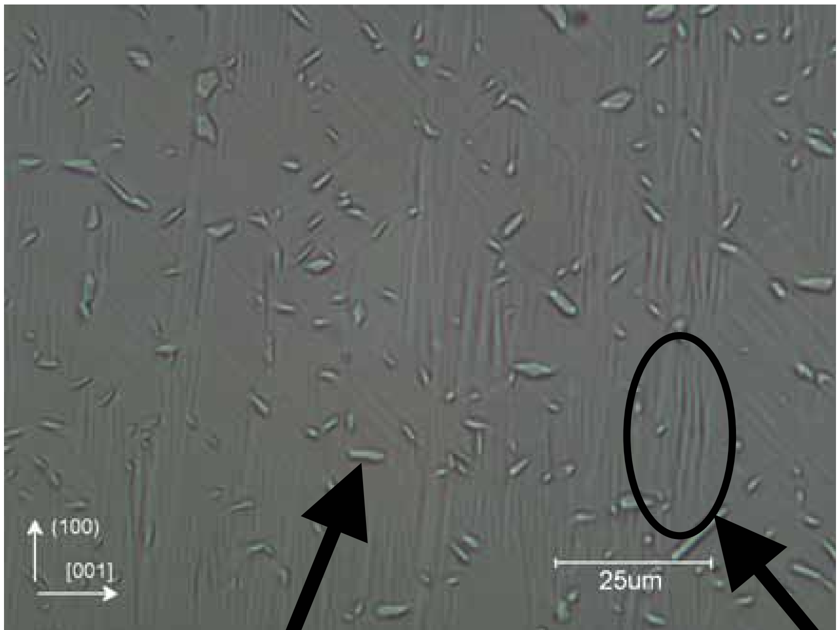
Effect of Elastic Strain Energy and Energy Dissipation on Hysteresis



Transition to New Materials-NiFeGa Single Crystals

- Atomic order of parent phase changes during cooling from high temperature B2 phase to higher ordered $L2_1$ structure
- The $L2_1$ austenite transforms to the final tetragonal $L1_0$ martensite via intermediate transitions to layered (modulated) structures (e.g. 5-layered or 7-layered)
- Pseudoelastic and shape memory response
- Excellent recoverability
- Narrow hysteresis
- Tailor response via heat treatment
- Room temperature cyclic behavior

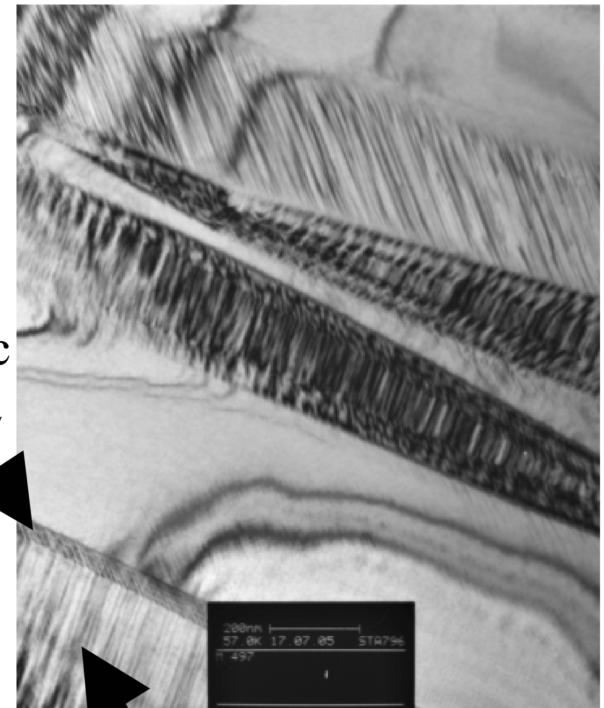
NiFeGa Microscopy



Second-phase

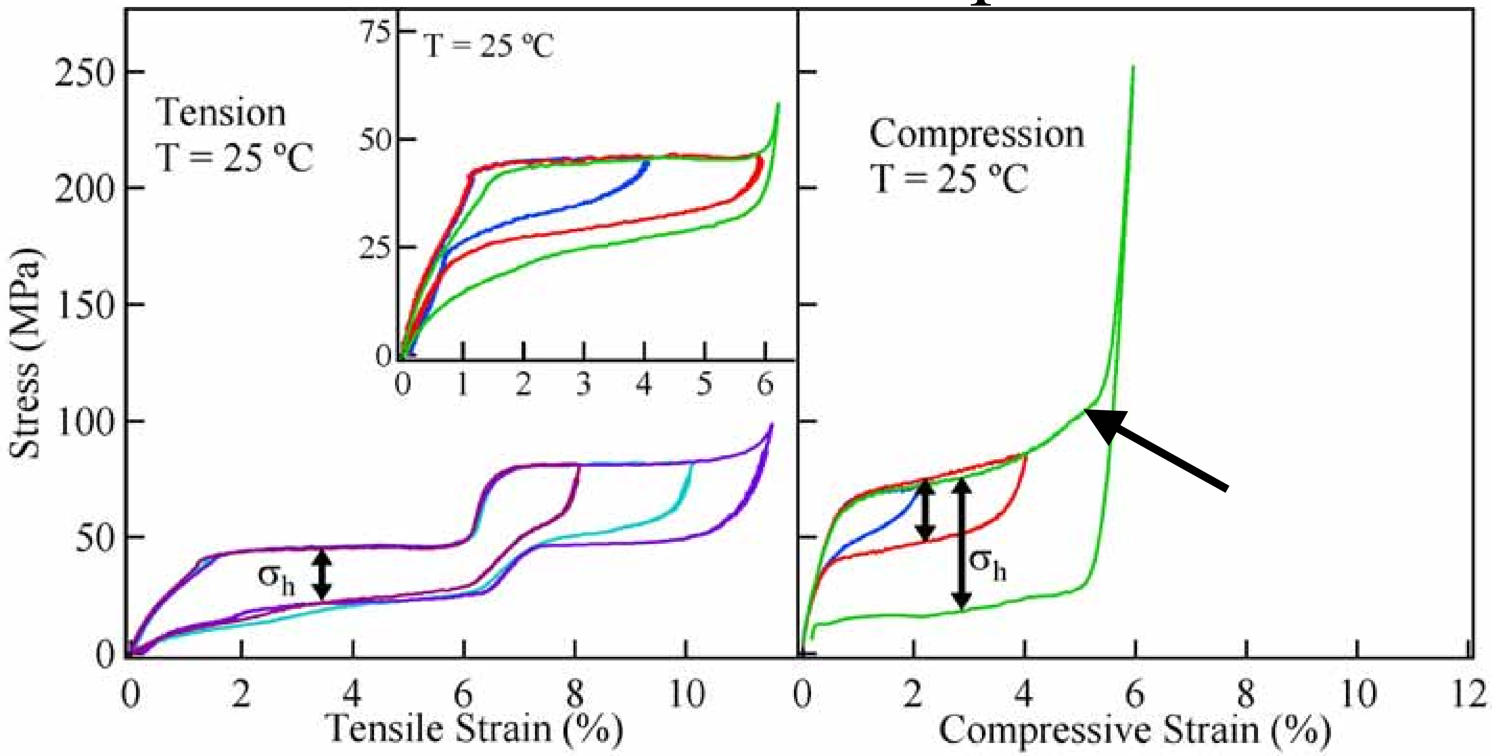
Martensite

Inter-Martensitic Structure 2



Inter-Martensite Structure 1

Pseudoelastic Response

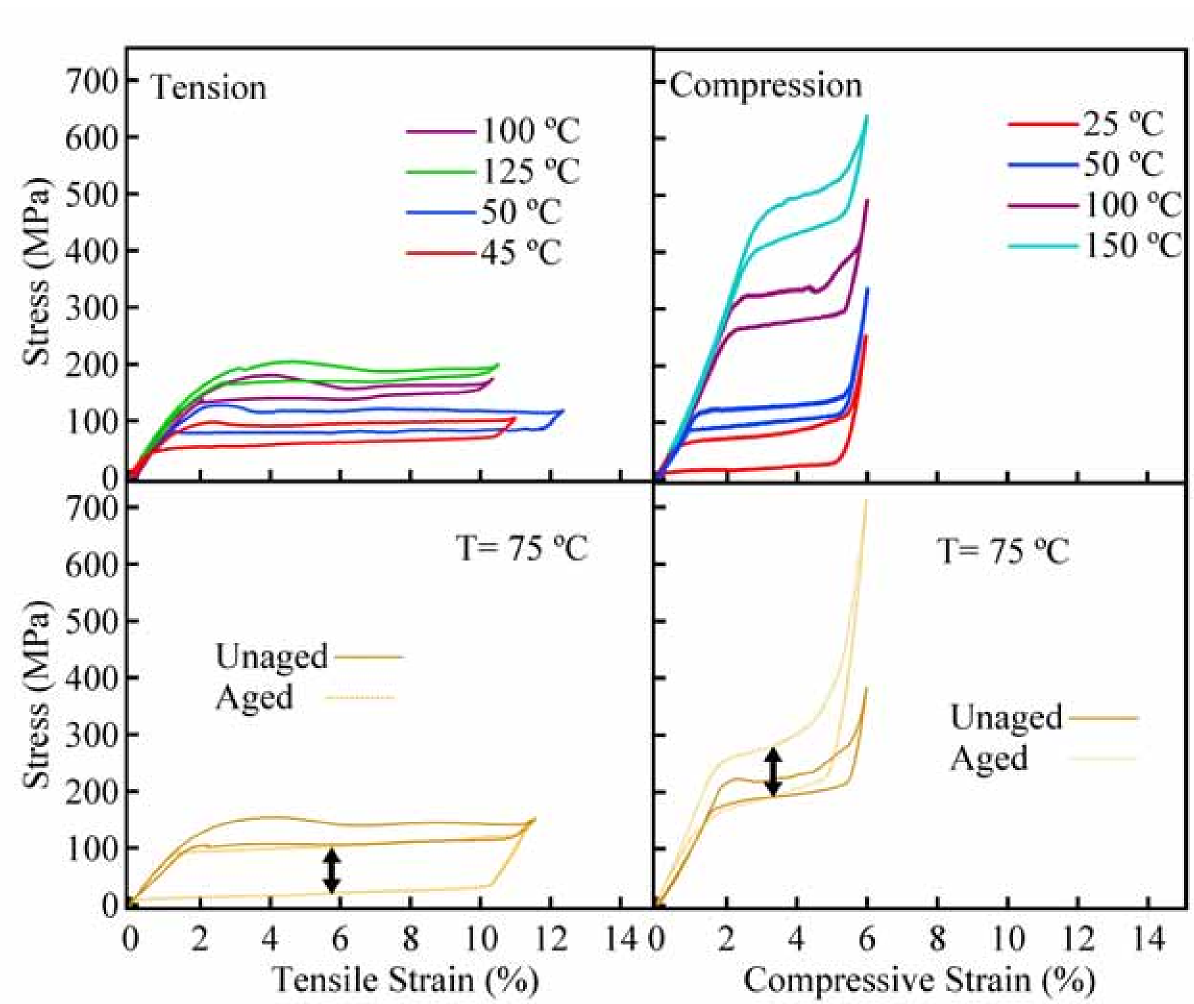


Tension: Intermediate MTs causes two stress plateaus

σ_h = stress hysteresis

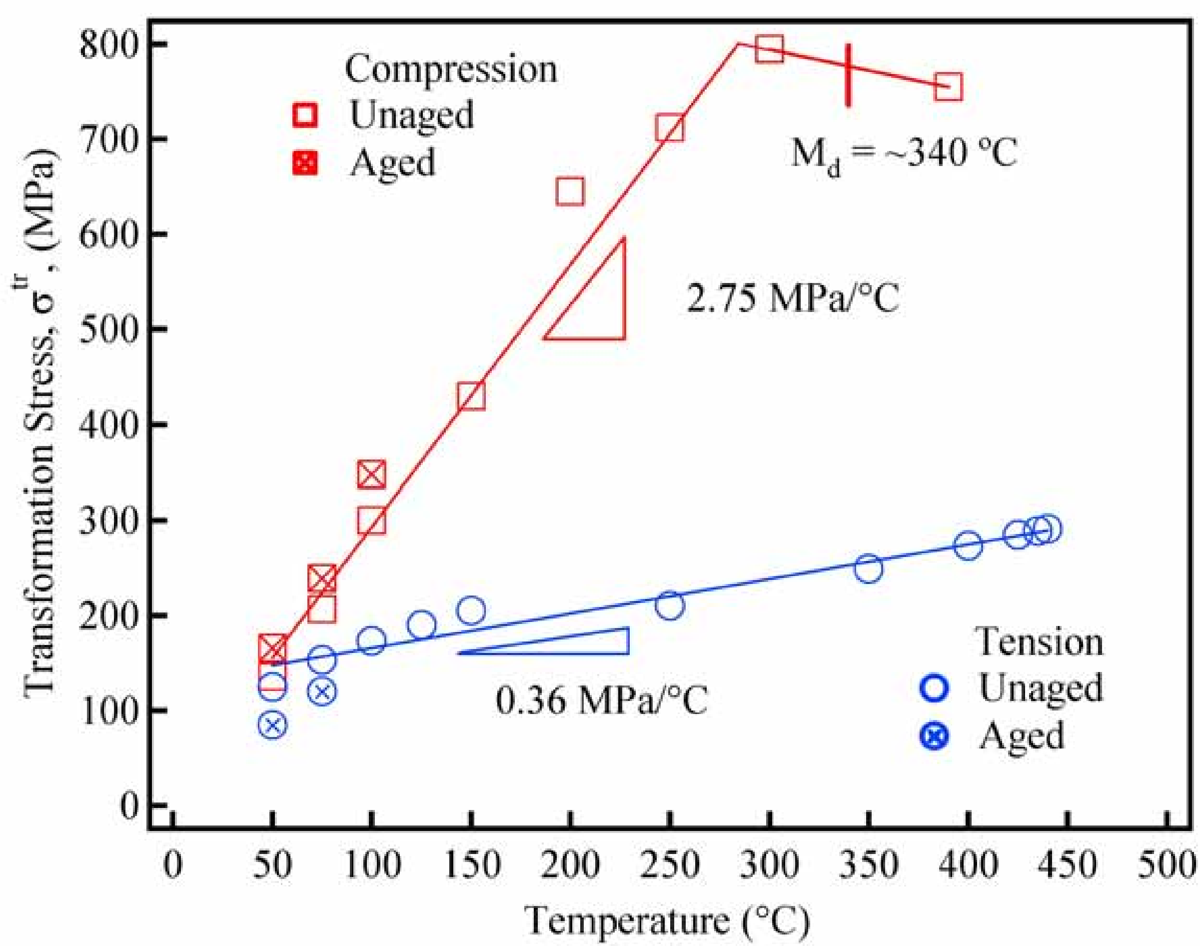
Intermediate MTs causes gradual upturn prior to elastic deformation of martensite and results in large increase in σ_h

Asymmetric Pseudoelastic Response



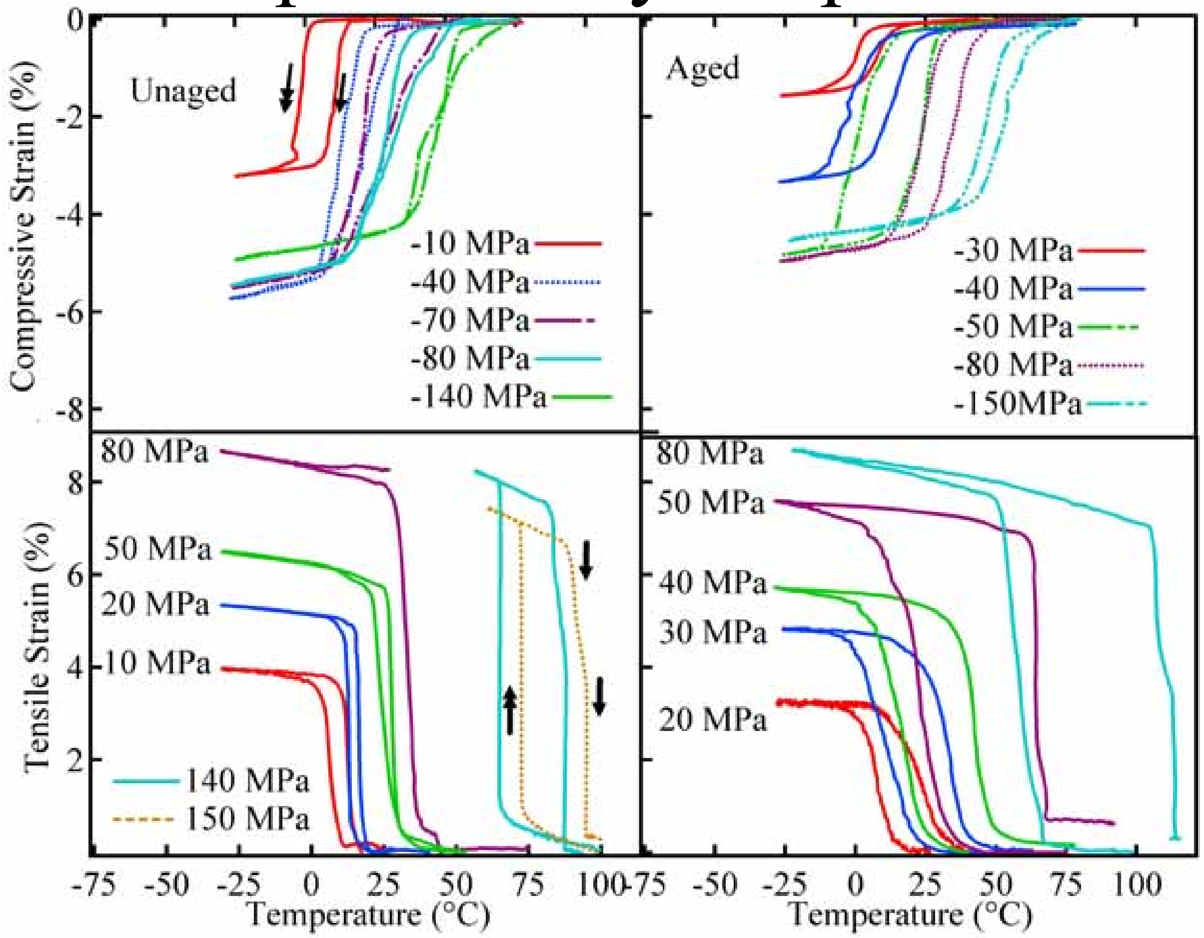
- •Tension: Inter-martensitic transitions prior to stress plateau gives rise to stress drop
- •T= 50 °C provides optimum pseudoelastic response, i.e. large transformation strains and small hysteresis.
- •The stress hysteresis widens after the heat treatment yet transformation strains are comparable

Critical Stress vs. Temperature



- Large pseudoelastic temperature range
- Distinct asymmetry of C-C slope
- Tension: Inter-martensitic transitions overlap within barrier.

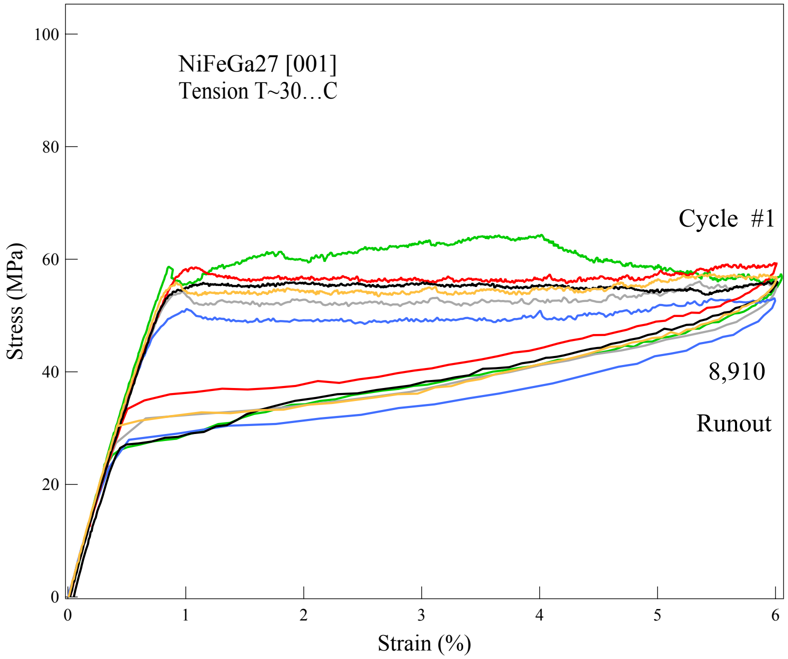
Shape Memory Response



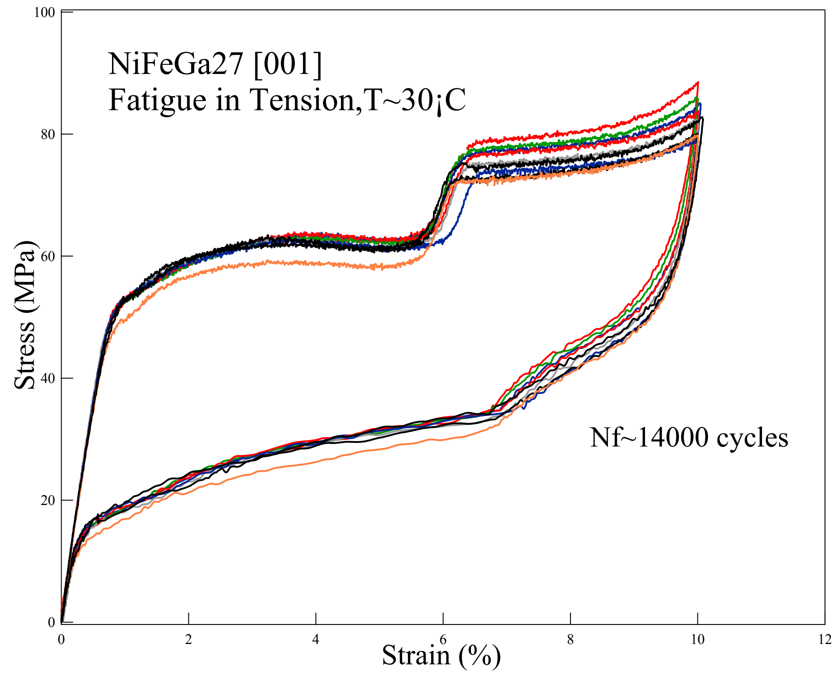
- •Intermediate transitions cause shrinkage of the hysteresis.
- •In tension, high stress forward intermediate conversions occur in burst fashion, similar to pseudoelastic behavior at high temperatures, and hysteresis grows.
- •Aging produces larger thermal hysteresis.

NiFeGa- Fatigue

6% runout



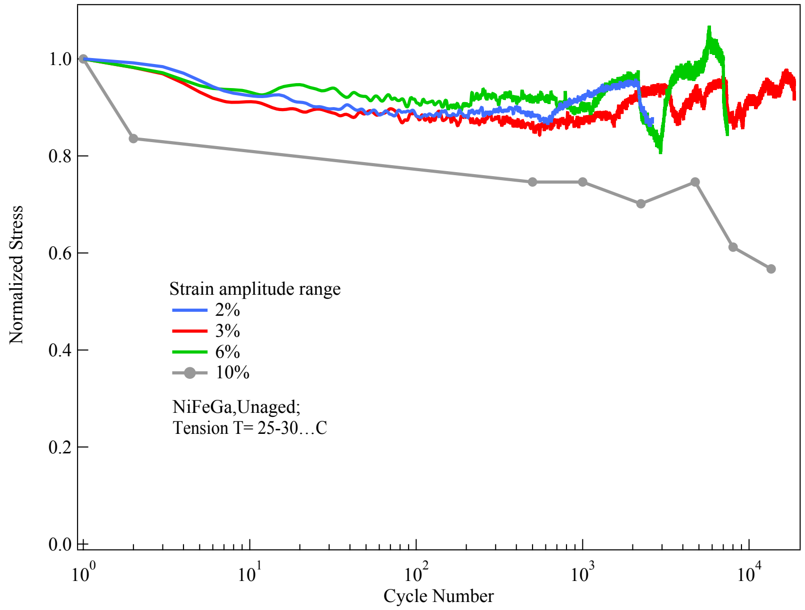
10%; 13,578 cycles

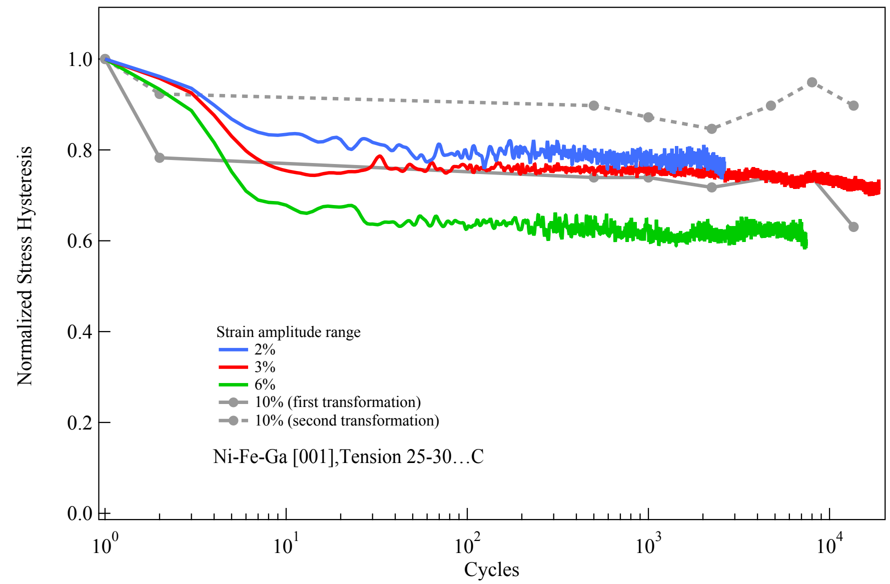


- Cyclically stable stress-strain behavior when loaded to a 3% to 6% strain amplitude

- A two stage transformation is observed at large applied strains.

NiFeGa- Fatigue

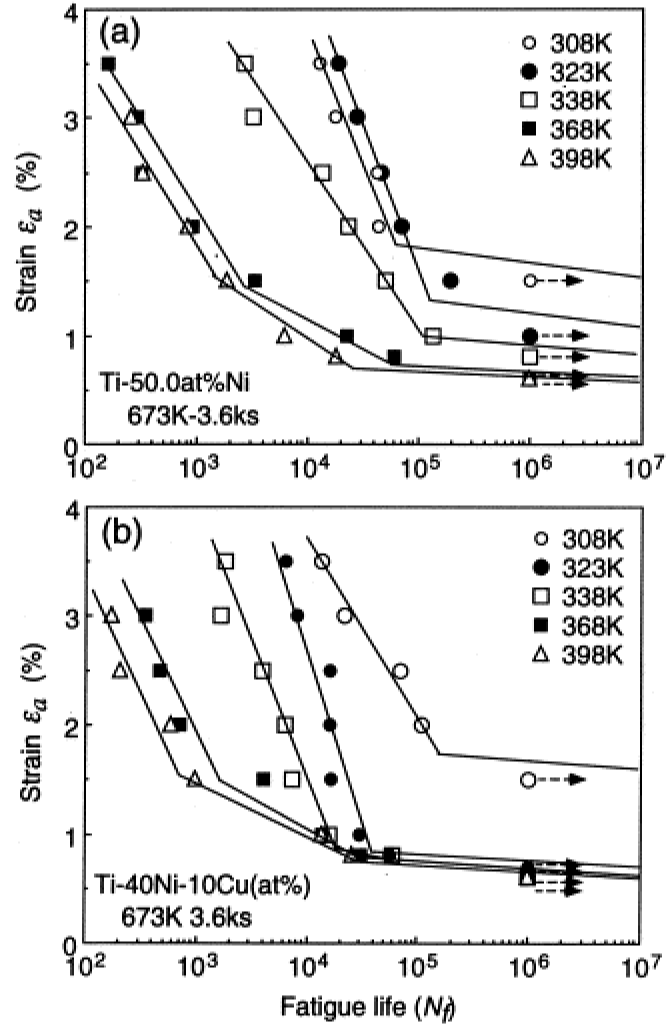




Negligible decrease in critical stress when compared to other SMA's

- The decrease in stress hysteresis stabilizes rapidly to approximately 20%.

Rotating Bending Fatigue Results on NiTi and NiTiCu, Miyazaki et al (1999)



Constitutive Equations

Patoor et al. J. de Physique (1995); Gall-Sehitoglu et al. IJP (2000), Hamilton-Sehitoglu et al. Acta Mat. 52 (2004); Hamilton-Sehitoglu et al. Acta Mat. 54 (2006)

- Complimentary free energy

$$\Psi(\Sigma_{ij},T,f^n)=B(T_o-T)\sum_n f^n+\frac{1}{2}\Sigma_{ij}C_{ijkl}\Sigma_{kl}+\Sigma_{ij}\sum_n \varepsilon_{ij}^n f^n+\frac{1}{2V}\int_\Omega \sigma_{ij}^{dist}\varepsilon_{ij}^{dist-tr}dV$$

$$-\sum_{n,m}H^{nm}f^n f^m$$

Thermal Hysteresis

R. F. Hamilton, H. Sehitoglu, Y. Chumlyakov, H. J. Maier Acta Mat. 52 (2004)

- Plastic relaxation captured through modified transformation strain

$$\varepsilon_1^{\mathrm{n}} = \alpha \varepsilon^n$$

- New transformation criterion

Atomistic Calculations →

$$F^C = \Sigma_{ij}^F \varepsilon_{ij}^n - \sum_m H^{nm} f_m - B(T - T_o)$$

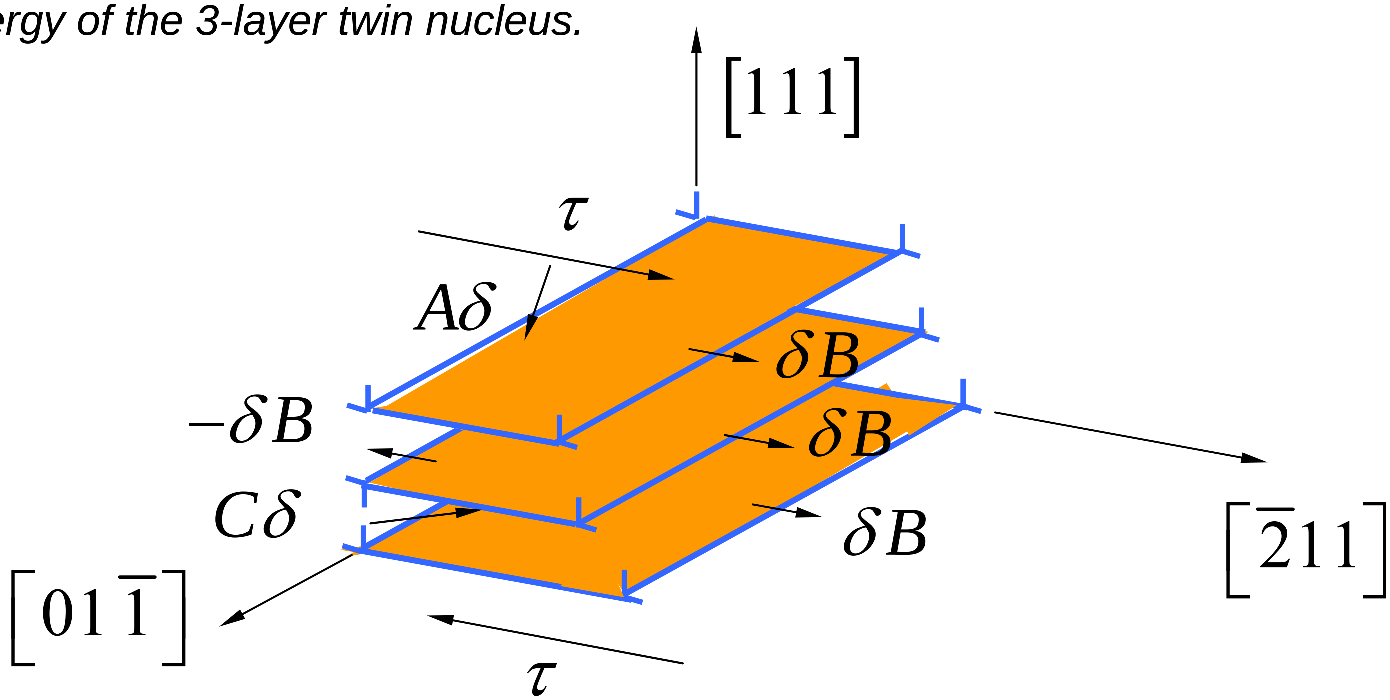
$$-F^C = \Sigma_{ij}^R \alpha \varepsilon_{ij}^n - \sum_m \alpha^2 H^{nm} f_m - B(T - T_o)$$

- Thermal hysteresis

$$\mathrm{H_m} = \mathrm{T_r} - \mathrm{T_f} = \tfrac{1}{\mathrm{B}}\left(\sum_{\mathrm{m}} \mathrm{H^{mn} f^m}(1-\alpha^2) - \Sigma_{ij} \varepsilon_{ij}^n (1-\alpha)\right)$$

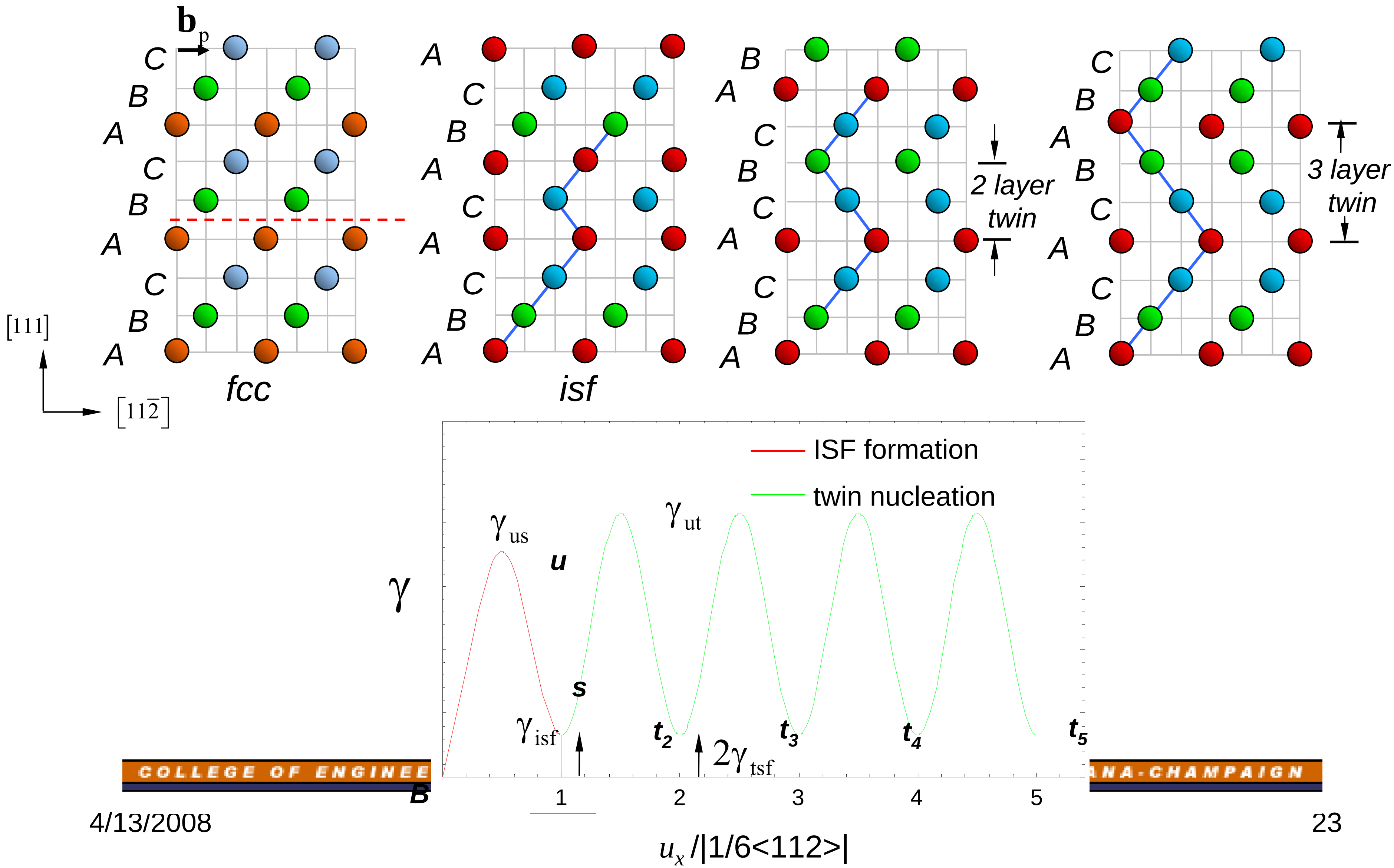
Mesoscale model for twin nucleation

To determine non-ideal twinning stress required to nucleate a twin, minimize the total energy of the 3-layer twin nucleus.



Only $A\delta$ *and* $C\delta$ *are mixed partial dislocations. All* δB *twinning partials are pure edge dislocations (Mahajan and Chin)*

Generalized planar fault energy (GPFE) curve



Energy calculation

Total energy of the twin:

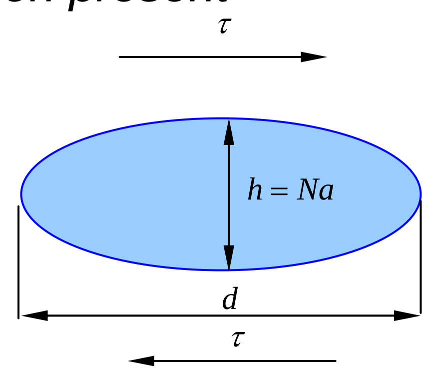
$$E_{total} = E_{edge} + E_{screw} + E_{\gamma\text{-}twin} - E_{\gamma\text{-}SF} - W_{\tau}$$

$$E_{total} = \frac{Gb_e^{\,2}d}{4\pi(1-\upsilon)}\left[N^2\left\{ln\left(\frac{d}{N}\right)+\frac{1}{2}\right\}-N\,ln\left(\frac{d}{r_0}\right)-\frac{1}{6}ln(N)\right]$$
$$+\frac{Gb_s^{\,2}}{9\pi}dN^2\left[ln\left(\frac{d}{N}\right)-\frac{1}{2}\right]$$
$$+(N-1)d\int_0^d \gamma_{twin}(\lambda(x))dx - d\int_0^d \gamma_{SF}(\lambda(x))dx - N\tau d^2 b_{twin}$$

Critical twin size and twinning stress can be determined by minimizing E_{total} relative to d and N.

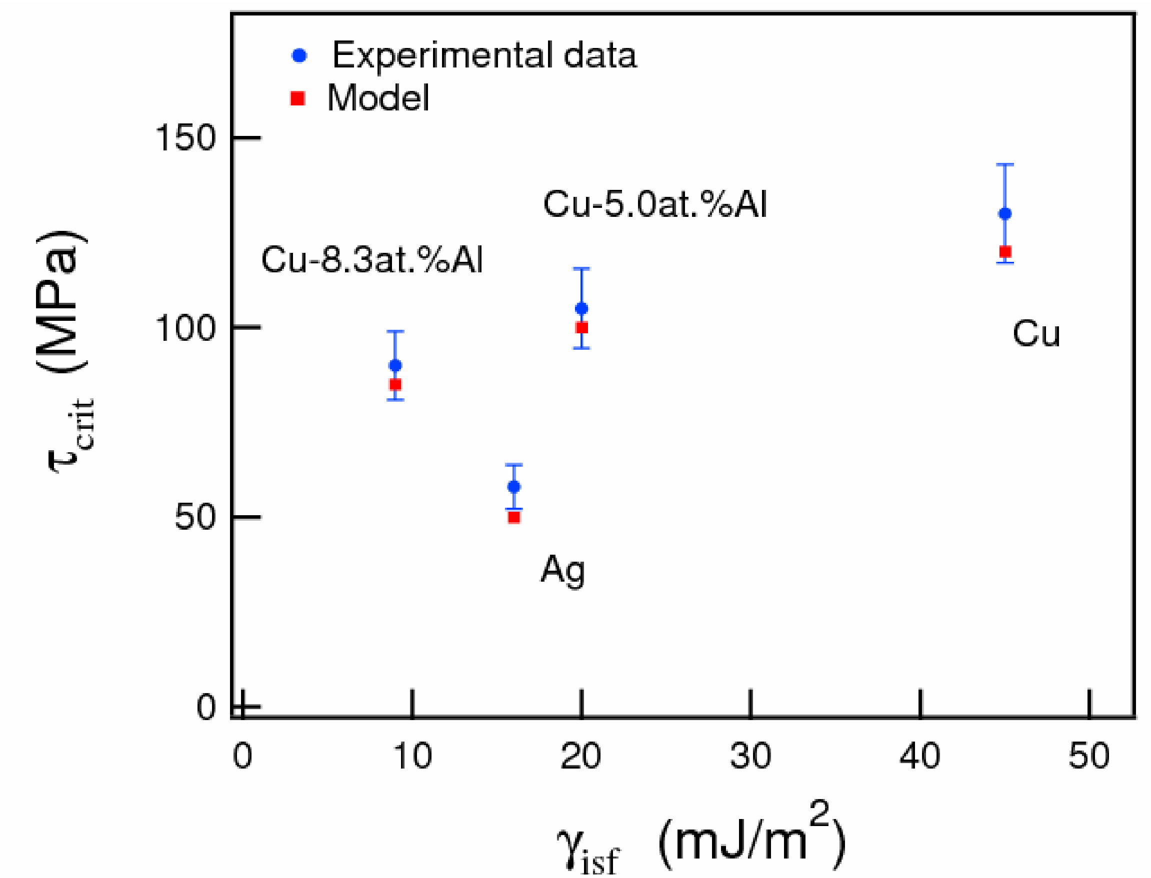
Twinning stress equation

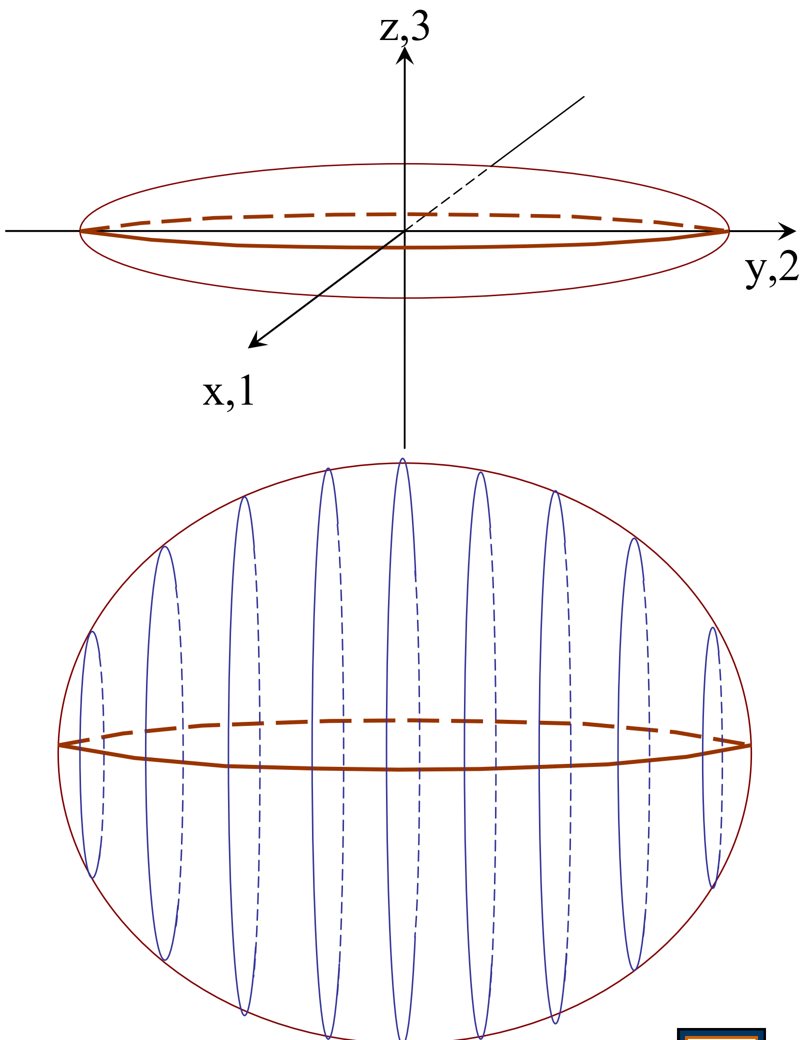
Relation between twin size and twinning stress based on present analysis:



$$
\begin{aligned}
\tau_{crit} = {} & \frac{GN}{\pi}\left[\frac{b_e^{2}}{(1-\upsilon)} + b_s^{2}\right] + \frac{2}{3N}\left(\frac{3N}{4}-1\right)\left[\gamma_{ut} + \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\frac{1}{b_{twin}} \\
& + \frac{1}{6b_{twin}}\left[\gamma_{ut} - \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right)\right] \\
& - \frac{(N-1)}{3N}\frac{1}{b_{twin}}\left[\gamma_{ut} - \frac{(\gamma_{tsf}+\gamma_{isf})}{2}\right]\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right) + \frac{d}{\sqrt{d^2+w^2}}\right] \\
& - \frac{2}{3N}\left(\frac{\gamma_{us}+\gamma_{isf}}{b_{twin}}\right) + \frac{1}{3N}\left(\frac{\gamma_{us}-\gamma_{isf}}{b_{twin}}\right)\left(\frac{w}{d}\right)\left[\ln\left(\frac{d+\sqrt{d^2+w^2}}{w}\right) + \frac{d}{\sqrt{d^2+w^2}}\right]
\end{aligned}
$$

Predicted twinning stress for fcc alloys





Large internal stresses develop near the interface due to misfit strains.

When the stresses exceed the critical stress, dislocations are generated at the interface.

The emission of dislocations from the interfaces lowers the elastic strain energy of the transforming martensite.

Assume that dislocations form in the interface as martensite thickens in z-direction.

- Contributions to stress arise from the external load (E), martensite particle (M), friction stress (F), and existing loops (L)

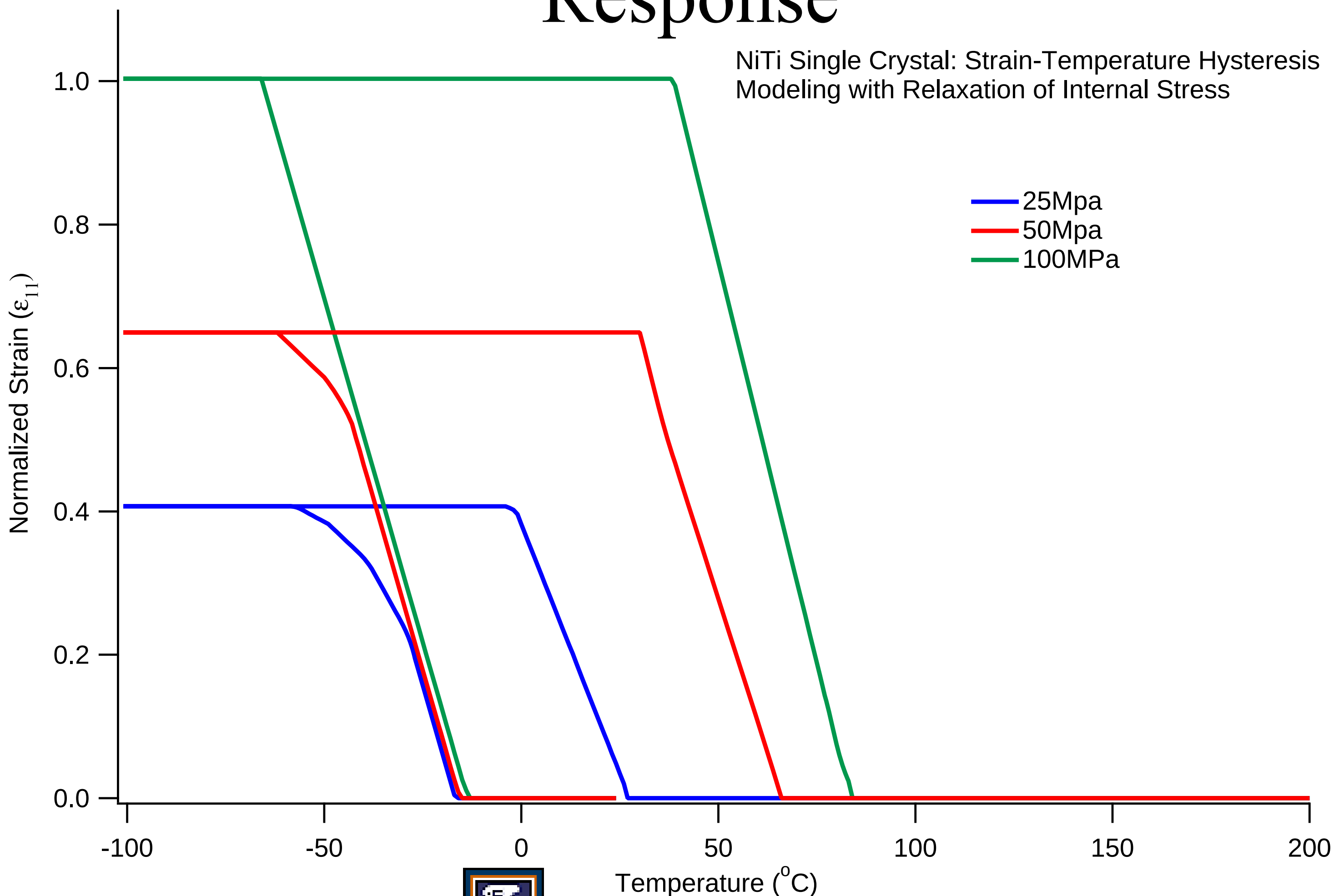
- Equilibrium condition is

$$[\sigma_{xx}^{M}(y_i)+\sigma_{xx}^{F}+\sigma_{xx}^{E}]b_e+[\tau_{xz}^{M}(y_i)+\tau_{xz}^{F}+\tau_{xz}^{E}]b_s$$

$$+\sum_{\substack{j=1\\ j\neq i}}^{N}[\sigma_{xx}^{L(j)}(y_i)b_e+\tau_{xz}^{L(j)}(y_i)b_s]=0$$

- Solve using Newton iteration method by increasing the value of N until the equilibrium condition is no longer satisfied

The Role of Plastic Relaxation on Hysteresis Response



Stress Hysteresis

R. F. Hamilton, H. Sehitoglu, C. Efstathiou, Y. Chumlyakov, H. J. Maier Acta Mat. 54 (2006)

$$\left(\Sigma^F - \Sigma^R\right)\varepsilon_o = F^c\left(1+\frac{1}{\alpha}\right) + \sum_m H^{nm} f_m\left(1-\alpha\right) - \varepsilon_o \frac{d\Sigma_{cr}}{dT}(T - T_o)\left(\frac{1}{\alpha} - 1\right)$$

- Three terms on the right hand side represent contributions to the stress hysteresis due to frictional resistance, variant interaction, and the temperature dependence of the critical (transformation) stress respectively.

Conclusions

- NiFeGa attains large transformation strains and exhibits remarkable recoverability
- The pseudoelastic temperature range is large and exceeds 300 °C.
- Aging allows for tailoring of the hysteresis without compromising transformation strains
- The fatigue resistance of NiFeGa with inter-martensitic transitions far exceeds other shape memory materials.
- Elastic strain energy is relaxed due to dislocation emission at the martensite/austenite interface. Atomistic calculations, in conjunction with realistic dislocation configurations, can help with establishing the constants in continuum formulations.
- The strain energy relaxation is incorporated in the governing thermo-mechanical formulation via the alpha term introduced in our works [Acta Mat. 52 (2004); Acta Mat. 54 (2006)] utilizing a dislocation model at the micro-scale.