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Supporting Information

Phase field approach for nanoscale interaction between crack propagation and phase transformation

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1. The total system of equations for interaction between crack propagation and phase transformation

We denote contractions between tensors $\boldsymbol{A}=\{A_{ij}\}$ and $\boldsymbol{B}=\{B_{ij}\}$ as $\boldsymbol{A}\cdot\boldsymbol{B}=\{A_{ij}B_{jk}\}$, $\boldsymbol{A}:\boldsymbol{B}=A_{ij}B_{ji}$, and $\boldsymbol{A}\otimes\boldsymbol{B}=A_{ij}B_{kl}$. The subscripts 0, d, A, and M are for the undamaged solid, fully-damaged solid, austenite, and martensite, respectively. The PT and damage are described by the order parameters η and ϕ, respectively; both vary between zero and unity. η is the order parameter which describes phase transformation; The austenite (A) corresponds to η=0 and martensite M to η=1. ϕ is the order parameter which describes damage; the undamaged state is described by ϕ=0 and fully damaged by ϕ=1. The crack surface with a narrow width in which the material is partially broken is described by $0<\phi<1$. Equations related to PTs, fracture, and surface-induced PTs alone are most close to those presented in the previous models[1-3], respectively.

The relationship between strain $\boldsymbol{\varepsilon}$, displacement $\boldsymbol{u}$, and decomposition of the strain into elastic $\boldsymbol{\varepsilon}_e$ and transformational $\boldsymbol{\varepsilon}_t f(\eta)$ parts are

$$\boldsymbol{\varepsilon} = 0.5\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T\right) = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_t f(\eta)\,; \qquad \text{(S1)}$$

$$f(\eta) = a\eta^2 + (4-2a)\eta^3 + (a-3)\eta^4\,. \qquad \text{(S2)}$$

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The interpolation function f is justified[1] and satisfies $f(0)=0$, $f(1)=1$, and $f'(0)=f'(1)=0$ and will be used for any material property. This allows one to ensure that η=0 and η=1 are the thermodynamic equilibrium values of η for any temperature and stresses. The Helmholtz *free energy* is

$$\psi=\psi^{e}+\psi^{f}+\psi^{PT};\quad \psi^{f}=\psi^{c}+\psi_{\phi}^{\nabla};\quad \psi^{PT}=\breve{\psi}+\tilde{\psi}+\psi_{\eta}^{\nabla}, \tag{S3}$$

where ψ^{f} and ψ^{PT} are the fracture and PT energy.

Elastic energy has the form

$$\psi^{e}=0.5(1-\phi)^{2}\boldsymbol{\varepsilon}_{e}:\boldsymbol{C}_{0}:\boldsymbol{\varepsilon}_{e};\quad \boldsymbol{C}_{0}=\boldsymbol{C}_{\mathrm{A}}+(\boldsymbol{C}_{\mathrm{M}}-\boldsymbol{C}_{\mathrm{A}})f(\eta), \tag{S4}$$

where $\boldsymbol{C}_0$ is the tensor of elastic moduli. Isotropic elasticity is used for simplicity, for which tensors $\boldsymbol{C}$ ($\boldsymbol{C}_{\mathrm{A}}$ and $\boldsymbol{C}_{\mathrm{M}}$) have the following structure

$$\boldsymbol{C}=(K_{0}-\frac{2}{3}G_{0})\boldsymbol{I}\otimes\boldsymbol{I}+2G_{0}\boldsymbol{I}_{4}, \tag{S5}$$

where G_0 and K_0 are shear and bulk moduli, $\boldsymbol{I}$ is the second-order identity tensor, and $\boldsymbol{I}_4$ is the symmetric fourth-order identity tensor.

Cohesion energy is

$$\psi^{c}=\frac{2\gamma(\eta)}{l(\eta)}f(\phi);\quad \gamma(\eta)=\gamma_{\mathrm{A}}+(\gamma_{\mathrm{M}}-\gamma_{\mathrm{A}})f(\eta);$$
$$l(\eta)=l_{\mathrm{A}}+(l_{\mathrm{M}}-l_{\mathrm{A}})f(\eta);\ l_{\mathrm{M}}-l_{\mathrm{A}}=\boldsymbol{n}\cdot\boldsymbol{\varepsilon}_{t}\cdot\boldsymbol{n}l_{\mathrm{A}}, \tag{S6}$$

where $\gamma(\eta)$ is the specific isotropic surface energy, l is the initial distance between two planes forming crack surfaces, and $\boldsymbol{n}=\nabla\phi/|\nabla\phi|$ is normal to this plane. Change in surface energy during the PT from its value for A γ_{A} to that for M γ_{M} is explicitly included in the formulation. This integrates our PFA to fracture and PTs with PFA to surface-induced PTs and pretransformations[4, 5], which was not previously applied to fracture. We use the advanced expression for $\gamma(\eta)$[6], which, in contrast to the other models[4, 5], allows for the non-contradictory description of the equilibrium states at the surface.

Gradient energies for crack ψ_{ϕ}^{∇} and PT ψ_{η}^{∇} are

$$\psi_{\phi}^{\nabla}=0.5\beta_{\phi}(\eta)|\nabla\phi|^{2};\quad \beta_{\phi}(\eta)=0.612\gamma(\eta)l(\eta); \tag{S7}$$

$$\psi_\eta^\nabla = 0.5\beta_\eta(\phi)\left|\nabla\eta\right|^2; \quad \beta_\eta(\phi) = \beta_0 + (\beta_d - \beta_0)\,f(\phi),$$

where the expression for $\beta_\phi(\eta)$ is taken from [2].

The *double-well barrier* function for PT is

$$\breve{\psi} = \bar{A}\eta^2(1-\eta)^2; \quad \bar{A} = A(\theta-\theta^c); \\ A = A_0 + (A_d - A_0)\,f(\phi);\ \theta^c = \theta_0^c + (\theta_d^c - \theta_0^c)\,f(\phi), \tag{S8}$$

where θ^c is the critical temperature at which stress-free A loses its thermodynamic stability, $\bar{A}$ is the barrier for transformation between A and M and A is material parameter.

Chemical part of the free energy $\tilde{\psi}$ is

$$\tilde{\psi} = \Delta G^\theta f(\eta),\ \Delta G^\theta = -\Delta s^e(\theta-\theta^e); \\ \Delta s^e = \Delta s_0^e + (\Delta s_d^e - \Delta s_0^e)\,f(\phi);\ \theta^e = \theta_0^e + (\theta_d^e - \theta_0^e)\,f(\phi), \tag{S9}$$

where θ^e is the thermodynamic equilibrium temperature for stress-free A and M and Δs^e is the jump in specific entropy at θ^e. Analyzing analytical solutions for the A-M interface[7] and the crack surface [2], we accept for a specific model:

$$A_d = 0;\ \theta^c = \theta_0^c = \theta_d^c;\ \beta_d = 0;\ \Delta s^e = \Delta s_0^e = \Delta s_d^e, \\ \text{and}\ \theta^e = \theta_0^e = \theta_d^0;\ l(\eta) = l_{\mathrm{A}} := l. \tag{S10}$$

These assumptions, in particular, imply that the A-M interface energy vanishes during damage. We also assume a=0 for interpolation of $\tilde{\psi}$ [1] and a=3 for ψ^c [2] and all other parameters.

Stress tensor is defined by the *Hooke's law*:

$$\boldsymbol{\sigma} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} = (1-\phi)^2\boldsymbol{C}_0 : \boldsymbol{\varepsilon}_e. \tag{S11}$$

Ginzburg-Landau equations are

$$\frac{1}{L_\eta}\frac{\partial\eta}{\partial t} = -\frac{\partial\psi}{\partial\eta}\Big|_{\boldsymbol{\varepsilon}} + \nabla\cdot\frac{\partial\psi}{\partial\nabla\eta} = \\ 6\eta(1-\eta)\boldsymbol{\sigma}:\boldsymbol{\varepsilon}_t - 3\eta(1-\eta)(1-\phi)^2\boldsymbol{\varepsilon}_e:(\boldsymbol{C}_{\mathrm{M}}-\boldsymbol{C}_{\mathrm{A}}):\boldsymbol{\varepsilon}_e - \\ 12\eta^2(1-\eta)\Delta G^\theta - 2(1-3\phi^2+2\phi^3)\eta(1-\eta)\times(1-2\eta)A_0(\theta-\theta^c) - \\ 3\eta(1-\eta)\left[\frac{4(\gamma_{\mathrm{M}}-\gamma_{\mathrm{A}})}{l}(3\phi^2-2\phi^3) + (\beta_{\mathrm{M}}-\beta_{\mathrm{A}})\left|\nabla\phi\right|^2\right] + \nabla\cdot\left[\beta_0(1-3\phi^2+2\phi^3)\nabla\eta\right]; \tag{S12}$$

$$\begin{aligned}&\frac{1}{L_\phi}\frac{\partial\phi}{\partial t}=-\frac{\partial\psi}{\partial\phi}\Big|_{\boldsymbol{\varepsilon}}+\nabla\cdot\frac{\partial\psi}{\partial\nabla\phi}=\\&(1-\phi)\boldsymbol{\varepsilon}_e:\boldsymbol{C}_0:\boldsymbol{\varepsilon}_e+3\phi(1-\phi)\left[2A_0(\theta-\theta^c)\eta^2(1-\eta)^2+\beta_0\left|\nabla\eta\right|^2\right]-\\&\frac{12}{l}\phi(1-\phi)\left[\gamma_\text{A}+(\gamma_\text{M}-\gamma_\text{A})(3\eta^2-2\eta^3)\right]+\nabla\cdot\left\{\left[\beta_\text{A}+(\beta_\text{M}-\beta_\text{A})(3\eta^2-2\eta^3)\right]\nabla\phi\right\},\end{aligned}\tag{S13}$$

where L_ϕ and L_η are the kinetic coefficients; $L_\phi=0$ when the crack is under closing compressive stresses[2]. In such a way we exclude crack propagation under closing stresses. This is a stricter approach[2] than to exclude some parts of elastic energy, which are related to the compressive stresses/strains, from the driving force for crack propagation[8].

Coupled system of Eqs. (1)-(13) (some of them are included in the extended version of Eqs. (12)-(13)) along with equilibrium equations $\nabla\cdot\boldsymbol{\sigma}=\boldsymbol{0}$ and boundary conditions for the order parameters, $\boldsymbol{n}\cdot\partial\psi/\partial\nabla\eta=0$ and $\boldsymbol{n}\cdot\partial\psi/\partial\nabla\phi=0$, are solved using the finite-element method and COMSOL code. A flow chart for the problem formulation and solution is presented in Fig. S1.

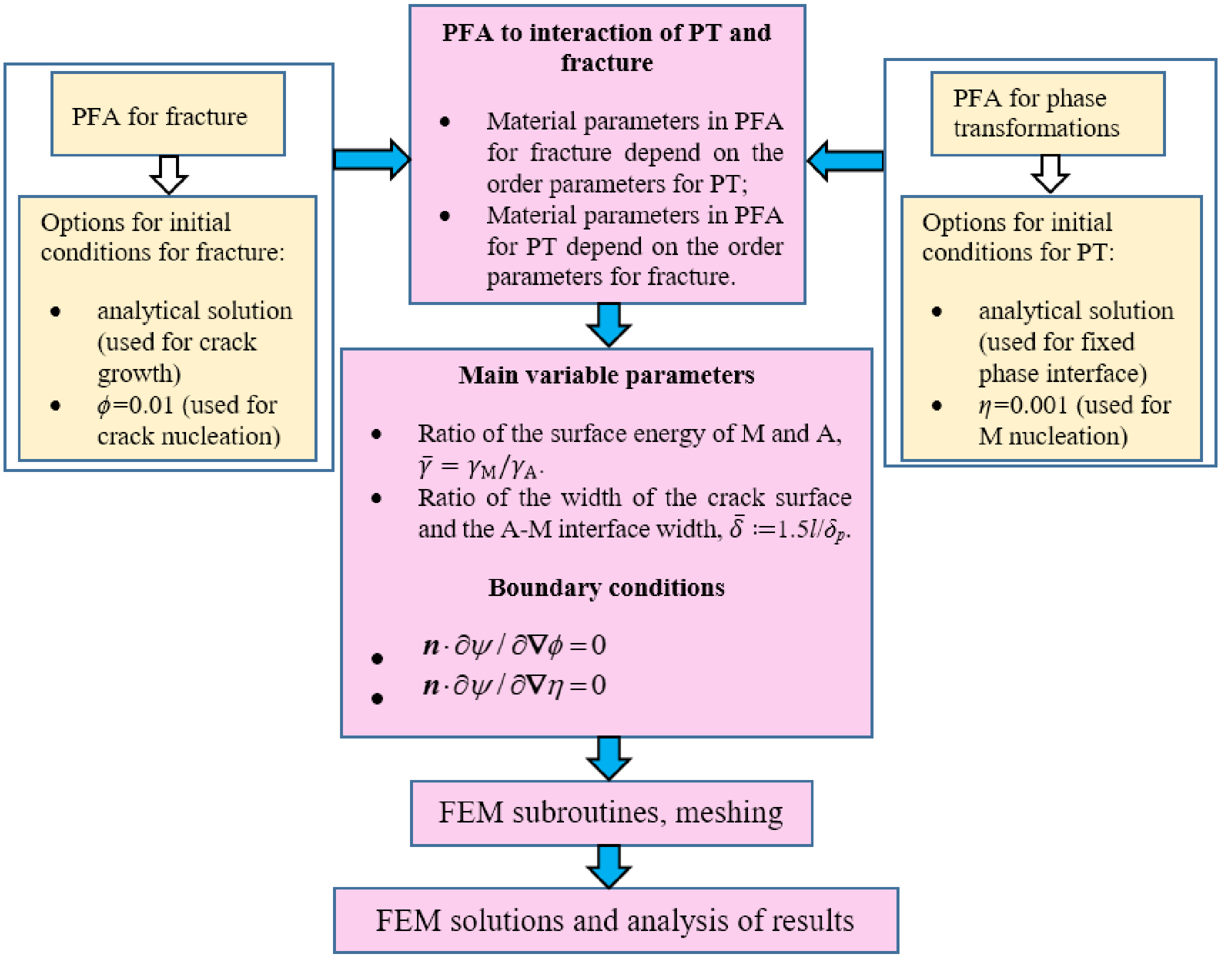

Figure S1. Flow chart of the methodology

2. Material Parameters

We consider phase transformation between cubic austenite and tetragonal martensite in NiAl associated with the transformation strain $\boldsymbol{\varepsilon}_t$. All material parameters are collected in Table S1.

Table S1. Material parameters and their physical meaning

Definition/physical meaning	Value from the literature [7] unless otherwise stated
Isotropic bulk modulus (the same for austenite and martensite)	K_0=112.62 GPa
Isotropic shear modulus (the same for austenite and martensite)	G_0=71.5 GPa
Transformation strain from cubic austenite to tetragonal martensite	$\boldsymbol{\varepsilon}_t$=(0.215,−0.078,−0.078)
Double well barrier parameter between the austenite and martensite	A_0=4.40 MPa/K
Gradient energy coefficient for the phase transformation	$\beta_0=5.18\times10^{-10}$ N
Phase equilibrium temperature for the stress-free austenite and martensite	θ^e=215 K
Critical temperature at which stress-free A loses its thermodynamic stability	θ^c=−183 K
Energy of phase interphase	E=0.2245 N/m
Kinetic coefficients for phase transformation	$L_\eta=2596.5\ (\mathrm{P\ a\cdot s})^{-1}$
Kinetic coefficients for fracture (assumed from the accepted range[2])	$L_\phi=1000(\mathrm{Pa\cdot s})^{-1}$

3. Propagation of the interfacial crack

Here, the same problem is solved as in Figure 4 of the main text (i.e. evolution of the initial interfacial crack at $\theta=\theta^e$), with all the same material parameters, including $\bar{\gamma}=\gamma_{\mathrm{M}}/\gamma_{\mathrm{A}}$, but both γ_{A} and γ_{M} are decreased by a factor of two. Results are generally close to those in Figure 4, but nonzero damage spreads over a large region around a secondary crack outside the interface, which is unexpected. However, this is not contradictory, because as our analysis[2] shows, most phase field models for fracture, including the current one, allow stable damage below the ultimate strength, which causes deviation of the stress-strain curve from the straight line. In our case, large stresses at the crack tip and due to termination of the lattice misfit at the crack's free surfaces became close to the ultimate strength of martensite due to the small chosen γ_{M}=0.5 N/m. This does not happen at γ_{M}=1 N/m due to the larger ultimate strength of martensite. Due to the smaller ultimate strength of martensite, the crack moves faster in Figure S2 than in Figure 4. Also, crack propagation is not continuous. In Figure S2 (b), maximum damage in martensite is shifted from the crack tip in austenite due to smaller strength. After stress exceeds the ultimate strength of the martensite at this location, material instability starts and a new crack nucleates in Figure S2 (c). Next, both cracks coalesce and the resultant crack continues propagation in the martensite (Figure S2 (d)). Figure S2 (a) also shows the deviation of crack to martensite due to its smaller ultimate strength without new crack nucleation.

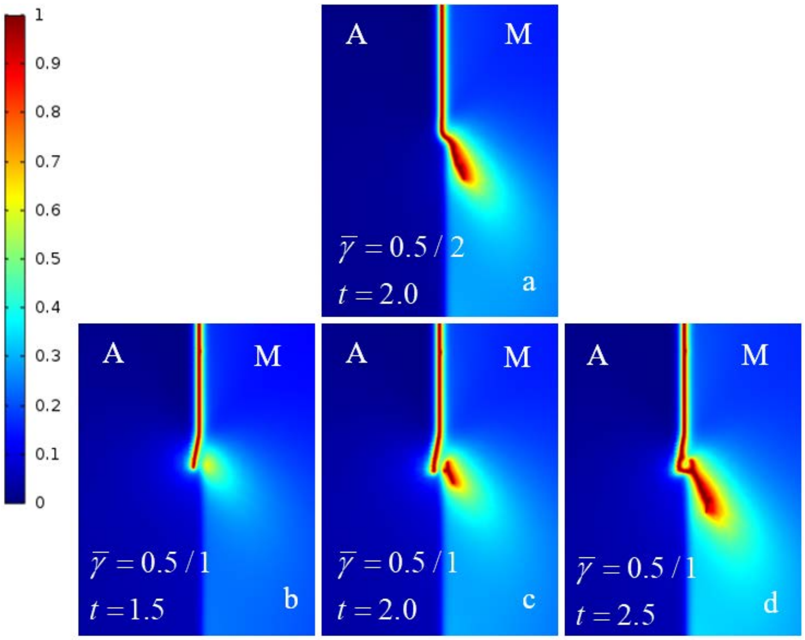

Figure S2. Damage distribution ϕ within and outside the phase interface shown in the region [*x*,*y*]=[(-10 10),(25 50)] for *l*=1 and different conditions. (a) Damage at time t=2 for $\bar{\gamma}=0.5/2$; (b) – (d) Damage evolution for times 1.5, 2.0, and 2.5 for $\bar{\gamma}=0.5/1$.

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