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Influence of interfacial stress on microstructural evolution in NiAl alloys

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Phase-field (PF) or Ginzburg–Landau (G-L) theory is used to capture various first-order solid-solid phase transformations (PTs) such as martensitic PT [1–4] which plays a crucial role in the evolution of unique microstructures in different materials such as shape memory alloys [5–11]. It is well known that the material interface experiences biaxial tension of magnitude of the surface energy [12]. However, most of the cases the material parameters for interfaces are unknown. Hence it is challenging to formalize simple constitutive equations that could capture the complex, strongly heterogeneous properties, strains, and stresses fields across an interface. This problem has been overcome in [13–16]. Such interface stress has also been introduced in multiphase PF theory for generalized n phases [17–19] as well as martensitic PTs [9, 11, 17]. The PF theory in [11], formulated in polar coordinate system, only requires one order parameter to describe variant-variant PT and twinning. Such a description allows us to get the analytical solution of interface profile, energy, and width as well as interfacial stress which is consistent with the sharp interface limit. The thickness of the martensitic variant is of the order of 1 nm and they possess sharp tips. Hence, the interface stress plays a significant role in different interesting twinning microstructures [11, 17, 19]. In this work, the effect of the interface tension and the stress and temperature-induced growth of the martensitic phase inside austenite, and twining are simulated. Some of the nontrivial experimentally observed microstructures which were reproduced in the simulations [9, 11] are discussed in detail.

In this model [9, 11], austenite A and two martensitic variants, T_1 and T_2 are considered. The radial order parameter Υ describes $\mathsf{A}\leftrightarrow\mathsf{T}_1$ and $\mathsf{A}\leftrightarrow\mathsf{T}_2$ PTs. The angular order parameter ϑ, bounded by $0 \le \vartheta \le 1$ describes $\mathsf{T}_1 \leftrightarrow \mathsf{T}_2$ (variant-variant) transformations. The Cauchy stress tensor has the following form [9, 11]: $\boldsymbol{\sigma} = \frac{\rho}{\rho_0}\mathbf{V} \cdot \frac{\partial\psi^h}{\partial\mathbf{B}}\cdot\mathbf{V} - \frac{\rho}{\rho_0}\left(\boldsymbol{\nabla}\Upsilon\otimes\frac{\partial\psi^h}{\partial\boldsymbol{\nabla}\Upsilon}\right)_s - \sum_{i=1}^{n-1}\frac{\rho}{\rho_0}\left(\boldsymbol{\nabla}\vartheta_i\otimes\frac{\partial\psi^h}{\partial\boldsymbol{\nabla}\vartheta_i}\right)_s$. The stress tensor $\boldsymbol{\sigma}$ can be splitted into two parts, $\boldsymbol{\sigma} = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}_{st}$. The dissipative part and the surface tension contribution are obtained by decomposing the $\boldsymbol{\sigma}$. The term $\boldsymbol{\sigma}_{st} = (\psi^{\nabla} + \breve{\psi}_\theta)\mathbf{I} - \beta_\Upsilon\boldsymbol{\nabla}\Upsilon\otimes\boldsymbol{\nabla}\Upsilon - q(\Upsilon)\,\beta_\vartheta\boldsymbol{\nabla}\vartheta\otimes\boldsymbol{\nabla}\vartheta$ is defined as a non-mechanical type of stress called "surface tension" which is localized at the interface and equal to zero in the bulk. The combined $\mathsf{A}\leftrightarrow\mathsf{T}$ and $\mathsf{T}_1 \leftrightarrow \mathsf{T}_2$ PTs and corresponding microstructure evolution similar to experimentally observed microstructures of NiAl alloy [20, 21] are discussed. Material parameters are taken from [11]. In the final microstructure, bending and splitting of martensitic tips are observed in Fig. 1c, e, similar to experiments [20, 21]. Since, between T_1 and T_2 there is invariant plane interface, it requires mutual rotation of these variants by the angle $\beta = 12.1°$. Here the angle between horizontal and vertical variants T_2 is $1.5\beta = 18.15°$, which is in good agreement with our simulations. The narrowing and bending of the tips of one T_2 horizontal plates due to the reduction of the boundary area, caused by a reduction in the internal stresses at this boundary [20]. For intermediate stage of the evolution, one twin penetrates in to region of another twin, results in crossed twins type microstructure as shown in Fig. 1e. They were also observed in experiments [21]. Moreover, most of the cases the twin planes are visibly bending or reorienting in areas close to the interface and the small microtwin variants penetrating into the other varients. In these zones, the formation of a needle like microtwin occurs which usually tapered to the microtwin boundary, and the penetrating microtwin variant tends to disappear.

Summarizing, a PF approach is applied to multivariant martensitic phase transformations and twinning within these variants. Different types of nontrivial experimentally observed microstructures which were reproduced in the simulations [9, 11] are discussed. It is found that the interfacial stress is an important factor, influencing the stress distribution at interfaces and the PF solution significantly.

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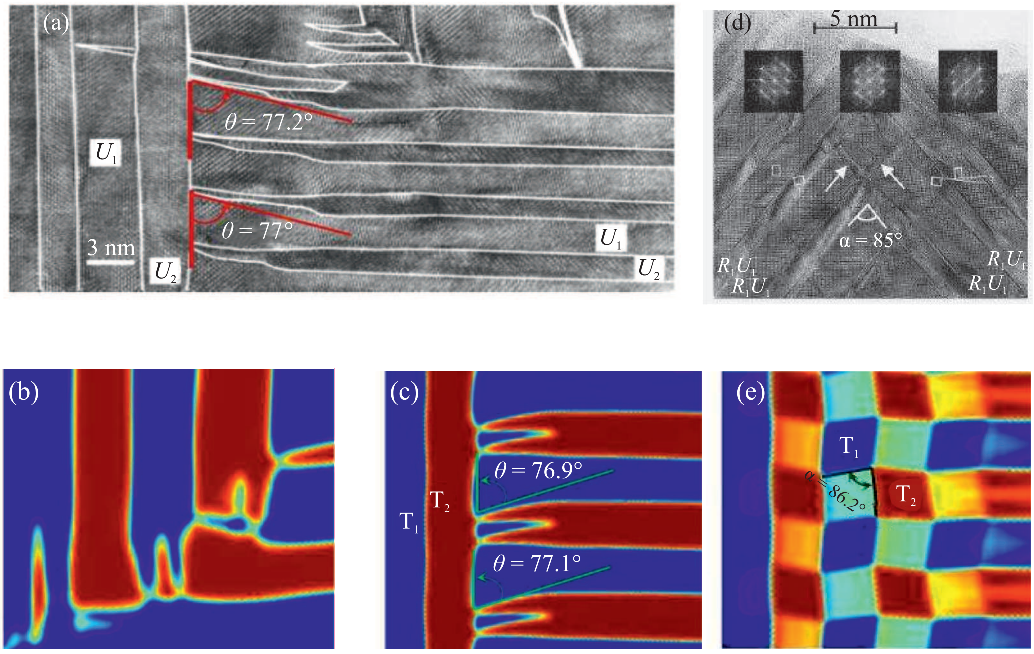

Fig. 1. (Color online) Comparison of simulation result with TEM image of NiAl alloy [20]. (a), (d) – TEM microscopy image of NiAl alloy [20]. (b) – Simulation results showing L shaped twin microstructure. (c), (e) – Simulation results from [11] showing tip splitting, bending, and crossed martensite twins. A is represented as green. Blue and red are for T_1 and T_2, respectively

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