ISSN: 0973-3469, Vol.17, (Special Issue) 2020, Pg. 03-06

Material Science Research India

www.materialsciencejournal.org

Evolution of Martensitic Nanostructure in NiAl Alloys: Tip splitting and Bending

ARUNABHA M. ROY*

University of Michigan, Aerospace Engineering Department, Ann Arbor, MI 48109, U.S.A.

Abstract

A phase-field (PF) model for the phase transformation (PT) between austenite and martensite and twinning between two martensite is presented where PT is described by a single order parameter. Such a description helps us to obtain the analytical solution of interface energetics and kinetics. PF-elasticity problems are solved for cubic-to-tetragonal PT in NiAl. The stress and temperature-induced PT and corresponding twinning and growth of the martensitic phase inside a nanocrystal are simulated. It reproduces nontrivial experimentally observed nanostructure such as splitting and bending of martensitic nanostructure as well as twins crossing. The evolution and morphology of such interesting nanostructures are discussed.

Article History

Received: 23 July 2020
Accepted: 30 July 2020

Keywords:
Ginzburg-Landau (G-L) Equation;
Phase-Field Approach;
Phase Transition In Martensite.

Short Communication

Phase-field (PF) method is a powerful technique to simulate different types of PTs. One of the main applications of this method can be found in PT in solid phases such as martensitic PT.[1-8] Martensitic PT plays an important role for overall material response by altering nanostructure in such materials. Different shape memory alloys exhibit martensitic PTs and form different interesting and non-trivial nanostructure during PT due to stress and temperature.[9-14] For stress-induced martensitic PT, the material interface experiences biaxial tension of magnitude of the surface energy. However, it is difficult to characterize such interface as material parameters in general at the interface are unknown for heterogonous nature of the interface. Hence it is challenging to formulate and incorporate constitutive equations that can capture the strong heterogonous properties and complex stress-strain fields in the interface. This problem has been solved by formulating a constitutive equation which successfully introduces interfacial stress in the martensitic interface.[15-18] Such interface stress has also been introduced in multiphase PF theory for generalized n phases[19-21] as well as martensitic PTs.[15-18] The PF theory in,[11-14] formulated in polar coordinate system, requires single order parameter to capture martensite-martensite PT and twinning.

CONTACT Arunabha M. Roy arunabhr@umich.edu University of Michigan, Aerospace Engineering Department, Ann Arbor, MI 48109, U.S.A.

Doi: http://dx.doi.org/10.13005/msri.17.special-issue1.02

Such a description allows us to get the analytical solution of interface profile, energy, and width as well as interfacial stress. This interfacial stress is thermodynamically consistent even for sharp interface limit. In general, martensite possess sharp tips with thickness of the order of 1nm. Hence, the interface stress plays a significant role for the evolution of different non-trivial nanostructures which were observed in the experiments. In this work, the stress and temperature-induced PT and corresponding twinning and growth of the martensitic phase inside a nanocrystal are simulated with a proper implementation of interface tension in the interface. The combined A↔T and T_1↔T_2 PTs and corresponding microstructure evolution similar to experimentally observed microstructures of NiAl alloy[22, 23] are discussed. The novelty of this work is that this model able to capture the nontrivial experimentally observed microstructures in our simulations both qualitatively and quantatively. It includes tip splitting and bending, and twins crossing. In this model,[11-14] austenite A and two martensitic variants, T_1 and T_2 are considered. The radial order parameter Υ describes A↔T_1 and A↔T_2 PTs. The angular order parameter ϑ describes T_1↔T_2 (variant-variant) transformations. It is bounded by $0 \le \vartheta \le 1$. The Cauchy stress tensor has the following form[11-14]

$$\sigma = \frac{\rho}{\rho_0} V.\frac{\partial \psi}{\partial B}.V - \frac{\rho}{\rho_0}(\nabla\Upsilon \otimes \frac{\partial \psi}{\partial \nabla\Upsilon}) - \sum_{i=1}^{n-1} \frac{\rho}{\rho_0}(\nabla\vartheta_i \otimes \frac{\partial \psi}{\partial \nabla\vartheta_i})$$

The stress tensor can be split into two part, $\sigma = \sigma_e + \sigma_{st}$. The dissipative part and the surface tension contribution are obtained by decomposing σ. The non-mechanical type of stress

$$\sigma_{st} = (\psi^{\nabla} + \psi^{\vartheta})I - \beta_{\Upsilon}\nabla\Upsilon \otimes \nabla\Upsilon - q(\Upsilon)\beta_{\vartheta}\nabla\vartheta \otimes \nabla\vartheta$$

is called "surface tension". It is localized at the interface.

In this work, an initial random distribution of austenite nuclei are considered in 50nm ×50nm sample and homogeneous biaxial strain is applied at the surfaces of the sample. For detail description, readers are suggested to look.[11-14] In the final microstructure, bending and splitting of martensitic tips are observed in Fig. 1-(c, e), similar to experiments.[22, 23] In Fig. 1-(c), martensitic variant T_2 is at an angle θ =76.9°.Since, there is an invariant plane interface in-between T_1 and T_2, it requires mutual rotation of these variants by the angle β = 12.1°. Here the angle between horizontal and vertical variants T_2 is 1.5β = 18.15°. As shown in In Fig. 1, our simulation result is in good agreement with the experimental micrograph.[22, 23]

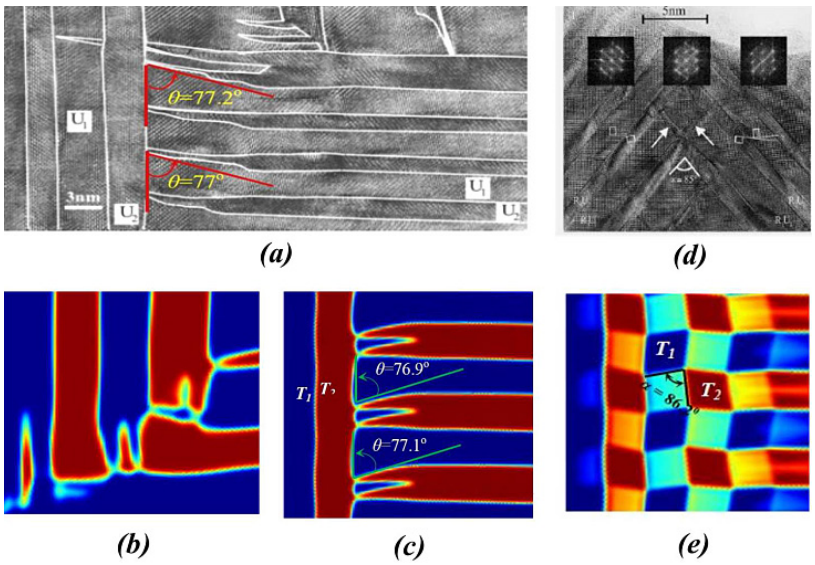

Fig. 1: Comparison of simulation result with TEM image of NiAl alloy.[21] (a,d) TEM microscopy image of NiAl alloy[21]; (b) simulation results showing L shaped twin microstructure; (c,e) simulation results from[11] showing tip splitting, bending, and crossed martensite twins. A is represented as green. Blue and red are for T_1 and T_2, respectively.

Due to reduction in the interface energy at invariant plane interface, narrowing and bending of the tips of T_2 horizontal plates occurs. For intermediate stage of the evolution, one twin penetrates into the region of another twin as shown in Fig. 1-(e). This results in crossed twins type microstructure. Such microstructure was also observed in experiments.[22] 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 variants. 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.

Conclusion

Summarizing, a PF approach is applied to multivariant martensitic phase transformations and twinning within these variants. The stress and temperature-induced PT and corresponding twinning and growth of the martensitic phase inside a nanocrystal are simulated. It reproduces nontrivial experimentally observed nanostructure such as splitting and bending of martensitic nanostructure as well as twins crossing. The evolution and morphology of such interesting nanostructures are discussed. It is found that interfacial stress significantly influences the nanostructure evolution of martensitic PT in NiAl alloys.

Acknowledgement

The help of Dr. V.I. Levitas from Iowa State University is gratefully acknowledged.

Funding

Los Alamos National Lab (Contract No. 104321) and National Science Foundation (Grant No. CMMI-0969143)

Conflict of Interest

The authors do not have any conflict of interest.

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