

## Interactions of Phase Transformation and Crack Propagation in Anisotropic Microstructures

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The world's escalating energy demand for cooling has triggered the development of advanced materials and technology for energy conversion, with special consideration for the mitigation of greenhouse gas emissions. Recent research in this field has been concentrated on solid-state refrigeration utilizing the elasto, electro, or magnetocaloric effect, which is governed by a displacive and diffusionless mechanism known as martensitic phase transformation (MPT). MPT between the parent phase (austenite) and the product phase (martensite), commonly observed in various steels, shape memory alloys (SMAs), and ceramics, is accompanied by formation and evolution of microstructure. When it comes to design and application of these materials in multiphysics environments, a crucial attention should be paid to interactions between fracture and MPT, which are a highly important problem in the material science and engineering.

In this work, a coupled problem of crack initiation and propagation and two-variant MPT in anisotropic microstructures is developed based on a phase field approach [1]. The model established includes a coupled system of three time-dependent Ginzburg-Landau (TDGL) equations [2], which describes the evolution of damage variable, two martensite variants, and the quasi-static equilibrium equation, respectively. Therefore, it is able to characterize evolution of the distribution of austenite and two martensitic variants as well as crack growth in terms of corresponding order parameters. This work accounts for the positive dilatational component of the transformation strain, which accompanies the MPT from austenite to martensite phase, leads to an eigenstrain within the martensitic phase. Since the eigenstrain results in both tensile and compressive parts, the model considers the sign of the dilatational

component. The model is established based on a coupled system of the TDGL equations and the equilibrium elasticity equation, and it explains the evolution of distributions of austenite and different martensitic variants in terms of corresponding order parameters. To this end, two-variant martensitic microstructure consists of austenite and two martensitic variants and is represented in terms of the distribution of two order parameters. Transformation strain transforms crystal lattice of austenite into crystal lattice of martensitic variant. In addition, a constraint for the order parameters describing transformation strain is imposed. This can be done by constructing a Landau-type polynomial energy function to characterize the transformation among different martensitic variants.

The results obtained show the crack propagation does not start until MPT has grown through the microstructure to some extent. Moreover, load-displacement curve of microstructure specimen with isotropic and anisotropic elastic constants with different crystal lattice orientation have been discussed. Last but not least, two polycrystalline models have been built to study the coupled approach of fracture and phase transformation in polycrystalline microstructures.

### References

- [1] Borden, M. J., Hughes, T. J., Landis, C. M., & Verhoosel, C. V. (2014). *A higher-order phase-field model for brittle fracture: Formulation and analysis within the isogeometric analysis framework*. *Computer Methods in Applied Mechanics and Engineering*, 273, 100-118.
- [2] Khachaturyan, A. G. (2013). *Theory of structural transformations in solids*. Courier Corporation.