NUMERICAL SIMULATION OF EVOLVING MICROSTRUCTURE AT MARTENSITIC PHASE TRANSITIONS

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Two finite element approaches are suggested for the modeling of multivariant martensitic phase transitions (PT) in elastic materials at different length scales. The first one is developed for the description of PT at nanoscale and based on the Landau theory with a new thermodynamic potential that captures the main features of macroscopic stress-strain curves. Distributions of different martensitic variants are the result of the solution of the corresponding boundary value problem for order parameters. It is shown that the simulation of evolving microstructure during PT can be reduced to the solution of the coupled heat transfer and elastic problems with the replacement of temperature by different order parameters. The numerical algorithm consists of the following elements. The observation time is subdivided into 'm' small time increments. For each time increment, a split operator is suggested that allows the solution of uncoupled heat transfer and elastic problems within a time increment. Then the following procedure is used for each time increment. First 'n' heat transfer problems are solved for the determination of evolution of 'n' order parameters (the order parameter is equivalent to temperature in the heat transfer equation, 'n' is the number of martensitic variants). Stresses during the solution of heat transfer problems are assumed fixed and known from the previous time increment. Then the elastic problem with a given transformation strain (the transformation strain changes for each time increment due to the change of order parameters) is solved for the calculation of stresses. Such an algorithm is implemented into the finite element program 'FEAP'. A numerical example of modeling of evolving microstructure during multivariant martensitic PT in an austenitic plate is given and analyzed.

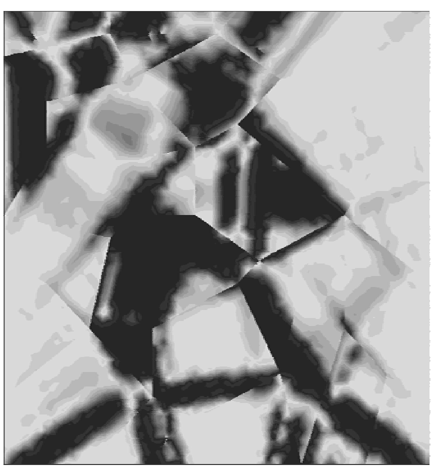

Fig.1 Calculated martensitic microstructure in polycrystal (white color - austenite, black color - martensite)

The second approach is designed for the modeling of PT at a large length scale including mesoscale. It is based on the thermomechanical phenomenological model for PT that represents strain softening during PT. In contrast to the known publications on PT, which apply the standard elastoplastic models with strain softening, our model is related to multivariant martensitic PT. Rate dependent constitutive equations used in the model facilitate avoidance of the mesh sensitivity at the numerical implementation of the approach. Due to strain softening a microstructure containing pure martensitic and austenitic domains with the small transition zones can be obtained as the solution of the corresponding boundary value problem. A finite element algorithm for the second approach is developed and implemented into the software ABAQUS. Several two dimensional problems for martensitic PT in single crystal and polycrystal elastic materials are solved and analyzed. One of these results is shown in Fig. 1.