MODELLING OF MICROSTRUCTURE FORMATION BY MINIMIZATION OF INCREMENTAL ENERGY SUPPLY

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1. Microstructures and material instability

It is well documented experimentally that microstructures can form in initially homogeneous solids during plastic deformation or phase transition. This paper is concerned with the modelling of this phenomenon in rate-independent inelastic solids under quasi-static loading, with particular reference to plasticity of metal crystals and polycrystals and to martensitic phase transformation in shape memory alloys. Formation of dislocation cells, cell blocks, deformation bands and shear bands within single grains of plastically deformed metals and alloys, of networks of macroscopic shear bands in metal polycrystals, and of twinned martensite and austenite-martensite laminates in shape memory alloys, are viewed as basic examples. A unifying feature of these seemingly distinct microstructures is that non-uniformity of deformation associated with the microstructure formation in not enforced by external conditions but is due to intrinsic instability in the deformed material.

In elastic or pseudo-elastic solids, the well-known notions of ellipticity, rank-one convexity and quasi-convexity of a nonlinear elastic energy function are related to material stability whose loss leads to formation of fine microstructures. When the evolution of a microstructure is associated with intrinsic dissipation, the stability analysis becomes more complex. An extended condition of thermodynamic stability is developed which in general is less restrictive than the classical one on account of a rate-independent dissipation term in the respective Lyapunov functional. To describe microstructure formation, the total incremental energy supplied to a material element is minimized according to the energy criterion of stability of deformation paths [1, 2].

2. Minimization of incremental energy supply

This may be regarded as an extension of the standard approach based on minimization of the elastic or free energy to inelastic materials with rate-independent dissipation. The variational approach to determining microstructure formation in a homogeneous and uniformly strained inelastic material follows the basic rule:

(1) $\Delta E \rightarrow \min$ subject to kinematical constraints

where ΔE is the increment in energy to be supplied from external sources to the thermodynamic system under consideration to produce a virtual deformation increment. The analysis is restricted to isothermal quasi-static transformations. The prefix Δ denotes a virtual increment from a given state, corresponding to an increment of an external control parameter. ΔE is generally split into the sum $\Delta E = \Delta W + \Delta\Omega$ of the deformation work increment ΔW and the increment $\Delta\Omega$ in the potential energy of external loads. If the (virtual) dissipation $\mathcal{D}$ associated with a local deformation increment is defined then the further split $\Delta W = \Delta\bar{\phi} + \Delta\bar{\mathcal{D}}$ can be used involving the averaged increments $\Delta\bar{\phi}$ in the Helmholtz free energy and $\Delta\bar{\mathcal{D}}$ in the dissipated energy.

In applications, the energy functional in the minimization rule (1) is evaluated at least to the second-order terms since its first-order representation leaves the incremental deformation indeterminate. Accordingly, a symmetry restriction is imposed on the incremental stiffness moduli [1, 2] and dissipation function [3].

3. Examples

The microstructure formation is calculated by repetitive solving the incremental energy minimization problem (1) along a deformation path. This is illustrated below by the example of finite-element simulations of the post-critical plastic deformation of a homogeneous incrementally nonlinear material. The overall plane strain compression under periodic boundary conditions is applied, with a small amount of shearing superimposed starting from 29% compression. The deformation pattern shown in Fig. 1 emerges through a sequence of bifurcations. The advantage of using rule (1) is in automatic selection of the post-critical deformation path which is otherwise indeterminate. The rule (1) has also been applied to overcome the long-standing difficulty of non-uniqueness in crystal plasticity and to simulate the formation of banded microstructures in metal crystals.

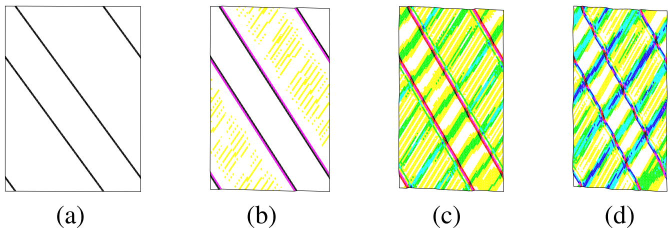

Figure 1. Calculated plane strain pattern at (a) 30% (b) 35% (c) 40% (d) 44% compression (with a small amount of shear) of a polycrystalline metal obeying the two-surface corner theory of plasticity [4].

Another area of applicability of (1) is the simulation of stress-induced martensitic microstructures in crystals of shape memory alloys, as shown schematically in Fig.2.

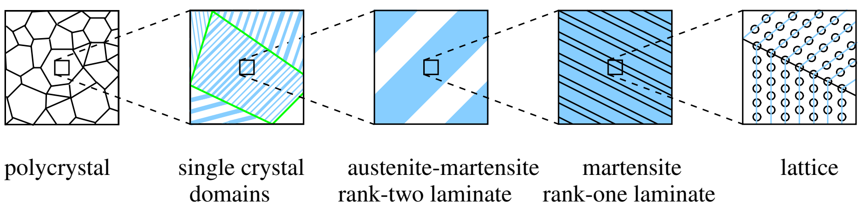

Figure 2. Schematic view of stress-induced martensitic microstructures in crystals of shape memory alloys.

4. References

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