Towards effective simulation of effective elastoplastic evolution

Carsten Carstensen and Robert Huth

Humboldt Universität zu Berlin, Unter den Linden 6, Berlin Germany
cc@mathematik.hu-berlin.de or huth@mathematik.hu-berlin.de

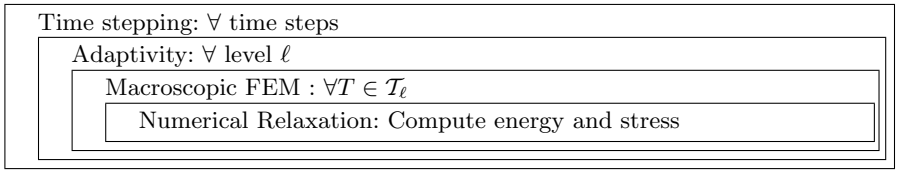
Summary. This paper summarises the general strategy for time evolving finite elastoplasticity and outlines encountered computational challenges in form of numerical benchmarks. Each time-step of some natural implicit time-discretisation is eventually recast into a possibly non-convex minimisation problem. Finite plasticity seems to imply the lack of lower semicontinuity of the energy functional and so leads to enforced fine strain oscillations called microstructures with required generalised solution concepts. The adaptive spacial discretisation is possible for convexified formulations from the relaxation finite element method (RFEM). For single-slip finite plasticity, one requires to relax numerically with laminates or semiconvexity notions.

Acknowledgement. The authors thank: S.Conti, A.Mielke and A.Orlando for stimulating discussions and collaborations and the DFG for support via the FG797

1 Introduction

The outcome of RFEM is the macroscopic behaviour of the highly nonlinear microscopic material also called effective behaviour and models the macroscopic energy and the macroscopic stress fields. The numerical simulation is equally important and difficult in many situations and the model example of our choice is the single-slip model. The numerical relaxation is performed via successive layers of fine microstructures and leads to approximations of the quasiconvex hull.

The numerical simulation of elastoplastic evolutions experiences severe difficulty in the interplay of adaptive timespace discretisation and numerical relaxation. The overall algorithm is depicted on the subsequent box.



The construction of effective algorithms and the erroranalysis in space as well as in time is even more challenging due to the unknown relaxation error. Since the numerical relaxation is in the deepest loop, time consumption is also a crucial factor.

The remainder of this paper is organised as follows. Section 2 recalls the generalised rate independent material and the notion of quasiconvexity. Its failure leads to nonexistence of solutions and the observation of microstructures in finite plasticity. Section 3 introduces the single-slip elastoplasticity without a closed form relaxation and so motivates the necessity of numerical relaxation. Section 4 is devoted to the introduction of the relaxation finite element Method (RFEM). Section 5 outlines the benchmark of computtaional micostructures [7] with closed form relaxation. Section 6 outlines adaptive mesh-refining algorithms. In Section 7 we list numerical relaxation schemes and shortly discuss their advantages and shortcomings. The hysteresis benchmark of Section 8 outlines the incremental problem with closed form condensed relaxation and spatial error control but without accumulated time discretisation errors.

2 Rate-Independent Materials

2.1 Standard Generalised Materials

Let $\varphi(\cdot,t)$ represent the deformation of a material body $\mathcal{B}$ from a reference configuration $\Omega_0 \subset \mathbb{R}^n$ to the current configuration $\varphi(\Omega_0,t)=\Omega_t$ and let $z(\cdot,t):\Omega_0\to\mathbb{R}^m$ denote internal variable like hardening or softening at the time t. Given the free Helmholtz energy $W(E,z)$ and the dissipation potential $\Delta(z,\dot z)$, in terms of the deformation gradient E and the internal variable z plus its rate $\dot z$, we consider the outer energy F from applied forces and define [13, 18]

$$\text{Gibb's energy}\qquad \mathcal{E}(t,\varphi,z)=\int_\Omega W(D\varphi(x,t),z(x,t))\,\mathrm{d}x - F(t,\varphi(\cdot,t)),$$

$$\text{Dissipation distance}\qquad \mathrm{d}(z_0,z_1)=\inf_{\substack{z\in C^1([0,1];\mathbb{R}^m)\\ z(0)=z_0,z(1)=z_1}}\int_0^1 \Delta(z(s),\dot z(s))\mathrm{d}s.$$

The dissipation distance is then the amount of energy which must at least be dissipated in a smooth transition from state z_0 to state z_1.

2.2 Continuous Formulation

The unknown deformation $\varphi:\Omega_0\times\mathbb{R}_+\to\mathbb{R}^n$ and internal variable $z:\Omega_0\times\mathbb{R}_+\to\mathbb{R}^m$ satisfy the following set of inequalities for all $0\le t\le T$ and $0\le t_1\le t_2\le T$ [18]

$$\mathcal{E}(t,\varphi(t),z(t))\le E(t,\hat\varphi,\hat z)+\int_\Omega \mathrm{d}(z(t),\hat z)\,\mathrm{d}x\quad\text{for all }(\hat\varphi,\hat z)\in V,$$

$$\mathcal{E}(t_1,\varphi(t_1),z(t_1))+\mathrm{Diss}(z;t_0,t_1)\le\mathcal{E}(t_0,\varphi(t_0),z(t_0))-\int_{t_0}^{t_1}F_t(s,\varphi(s))\,\mathrm{d}s,$$

$$\text{with}\quad \mathrm{Diss}(z;t_0,t_1)=\sup_{\substack{N\in\mathbb{N}\\ t_0\le\tau_0<\ldots<\tau_N\le t_1}}\sum_{j=1}^N\int_\Omega \mathrm{d}(z(\tau_{j-1}),z(\tau_j))\mathrm{d}x.$$

2.3 Incremental Formulation

The time discretisation of the continuous problem results in the incremental problem, where for each time step t_j, (φ_j, z_j) approximates $(\varphi(\cdot, t_j), z(\cdot, t_j))$ and minimises the functional $E(t_j, \varphi, z) + \int_\Omega \mathrm{d}(z_{j-1}, z)\,\mathrm{d}x$.

The partial minimisation with respect to z can be solved separately for each material point and gives rise to the condensed energy [19, 6]

$$W_{cond}(z_{j-1}; D\varphi) := \min_z \big(W(D\varphi, z) + \mathrm{d}(z_{j-1}, z)\big),$$
$$E_{cond}(\varphi) := \int_\Omega W_{cond}(z_{j-1}; D\varphi)\,\mathrm{d}x - F(\varphi).$$

The incremental problem is equivalently recast into the minimisation of E_{cond} among all admissible deformations. In practice, the condensed energy density W_{cond} has to be computed by analytical manipulations or some extra inner loop.

In the calculus of variations, the existence of minimisers of E_{cond} follows with its direct method, in the situation where W_{cond} is quasiconvex. In a typical finite plasticity problem, however, this is not the case and enforced microstructures are observed.

2.4 Generalised Notions of Convexity

The state-of-the-art calculus of variations [10] for the minimisation of the energy

$$E(v) = \int_\Omega W(x, v(x), Dv(x))\mathrm{d}x \quad \text{for all } v \in V \tag{M}$$

is concerned with semiconvexity of $W(x, v(x), \cdot)$. Besides growth and continuity conditions on the energy E, a sufficient condition for the existence of a minimiser of E is sequential lower weak semicontinuity equivalent to the quasiconvexity of W.

One calls function $W : \mathbb{R}^{m\times n} \to \mathbb{R}$ quasiconvex if for some open subset $\omega \subset \mathbb{R}^n$ and all $E \in \mathbb{R}^{m\times n}$;

$$W(E) = \inf_{\varphi \in C_c^\infty(\omega, \mathbb{R}^m)} \frac{1}{|\omega|} \int_\omega W(E + D\varphi)\mathrm{d}x$$

holds. The quasiconvex envelope W^{qc} is given

$$W^{qc}(E) = \sup\{W^*(E) : W^* \le W \text{ and } W^* \text{is quasiconvex}\}.$$

It is clear that W^{qc} is also quasiconvex. The quasiconvex energy

$$E^{qc}(v) = \int_\Omega W^{qc}(x, v(x), Dv(x))\,\mathrm{d}x \quad \text{for all } v \in V \tag{Q}$$

models relevant macroscopic properties like the displacement- or stress-field. However the notion of quasiconvexity is a difficult concept. A related concept is the notion of rank-one convexity: A function W is called rank-one convex, if for all matrices E and all rank-one matrices $a \otimes b$ the function $f : \mathbb{R} \to \mathbb{R}$ with $f(t) = W(E + ta \otimes b)$ is convex. The conjecture that all rank-one convex functions are quasiconvex has been an open problem for decades, before Sverak [20] found a counterexample based on

the function $\varphi(A) = xyz$ for all 3×2 matrix $A^T = (diag(x, y), [z, z])$. Even these days it remains an open question whether or not rank-one convexity is equivalent to quasiconvexity on $\mathbb{R}^{2\times 2}$.

Another related semiconvexity notion is polyconvexity: A function W is polaconvex if is is a convex function of a vector of all Minors. Similar to the quasiconvex envelope one defines the convex, polyconvex and the rank-one convex envelope W^{**}, W^{pc}, W^{rc} for which it is known that $W^{**} \leq W^{pc} \leq W^{qc} \leq W^{rc}$.

3 Single-Slip Finite Plasticity

In this example the resulting energy is not quasiconvex and the formation of microstructures are expected. The relaxation can not be done analytically and therefore numerical relaxation schemes have to be employed. The local deformation E is supposed to consist of an elastic deformation superimposing a plastic deformation,

$$E = D\varphi = E_e E_p \ .$$

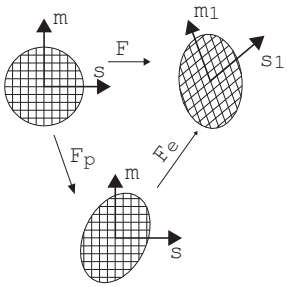


Fig. 1. Split of plastic and elastic deformation

Based on the givenslip directions s and $m \in \mathbb{R}^n$ with $|m| = 1 = |s|$, the plastic deformation

$$E_p = I + \gamma s \otimes m$$

depends only one the real shear parameter γ. With material parameters h, μ, the critical shear stress τ_{cr} and a neo Hookean energy U, the free energy reads [6]

$$W(E, z) = U(\det E_e) + \frac{\mu}{2}\mathrm{tr}(E_e^T E_e) + \frac{h}{2}p^2 \ .$$

The dissipation potential Δ and dissipation distance d are defined as

$$\Delta = \begin{cases} \tau_{cr}|\dot\gamma| \text{ if } |\dot\gamma| + \dot p \leq 0, \\ \infty \quad \text{otherwise,} \end{cases}$$

$$\mathrm{d}(\gamma_0, \gamma_1) = \begin{cases} \tau_{cr}|\gamma_1 - \gamma_0| \text{ if } |\gamma_1 - \gamma_0| \leq p_0 - p_1, \\ \infty \quad \text{otherwise.} \end{cases}$$

The resulting condensed energy E_{cond} from Subsection 2.3 utilises [19, 6]

$$W_{\mathrm{cond}}(E) = U(E) + \frac{\mu}{2}(|E|^2 - 2) - \frac{1}{2}\frac{(max(0, \mu|\boldsymbol{C}\boldsymbol{s}\cdot\boldsymbol{m}| - \tau_{cr}))^2}{\mu\boldsymbol{C}\boldsymbol{s}\cdot\boldsymbol{s} + h}.$$

Since W_{cond} is not quasiconvex its unknown quasiconvex envelope has to be computed as a benchmark for numerical relaxation algorithms. which is unknown. For a special case of U and $\tau_{cr} = 0$ the quasiconvex envelope is known [9].

4 Relaxation Finite Element Method (RFEM)

The piecewise constant strain can not develop any microstructures on each element and hence oscillations are mesh dependent as seen in Figure 2. To improve the

element ansatz functions further, the RFEM allows an arbitrary ansatz function on each element subject to the elementwise affine boundary conditions. The resulting RFEM minimises the energy

$$E_\ell(v_\ell) = \sum_{T\in\mathcal{T}_\ell} \left(\inf_{w\in C_c^\infty(\mathbb{R}^n,\mathbb{R}^m)} \int_T W(x, v_\ell(x), Dv_\ell(x) + Dw(x))\mathrm{d}x \right) - F(v_\ell).$$

The infimum on each triangle is the relaxation and allows the direct simulation of the macroscopic displacement field. For linear FE functions the infimum is the integral of the quasiconvex envelope of W,

$$E_\ell(v_\ell) = \sum_{T\in\mathcal{T}_\ell} \left(\int_T W^{qc}(x, v_\ell(x), Dv_\ell(x))\mathrm{d}x \right) - F(v_\ell).$$

The numerical outcome of for the computational microstructures benchmark is shown in Figure 2 [7].

5 Computational Microstructures Benchmark

This model is a typical example which is in its original formulation not quasiconvex and therefore oscillations and meshdenpendance of numerical solutions are observed. The relaxation in closed form for this example yields meshindependent solutions.

In this example we are looking for $\varphi : \mathbb{R}^2 \to \mathbb{R}$ and define the energy density

$$W(E) = |E - E_1|^2 |E - E_2|^2$$

for two different wells $E_1 = -E_2 = -(3,2)/\sqrt{13} \in \mathbb{R}^2$. The energy reads

$$E(v) = \int_\Omega \left(W(Dv) + |v - f|^2 \right) \mathrm{d}x \quad \text{for all } v \in V,$$

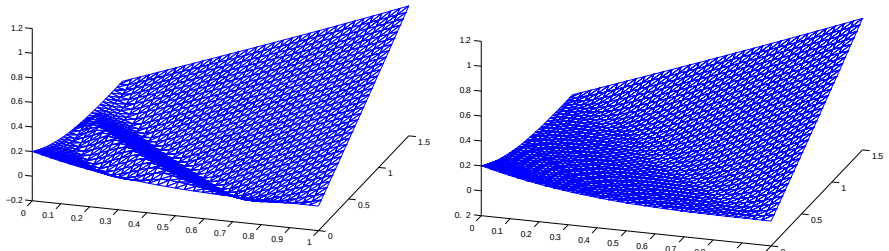
for a function given $f(x,y) = -3t^5/128 - t^3/3 \in C^1(\Omega); t = (3(x-1)+2y)/\sqrt{13}$. The quasiconvex envelope of W coinsides with the convex envelope $W^{**}(E) = W^{qc}(E) = \left((|E|^2-1)_+\right)^2 + 4|E|^2 - \left(((3,2)\cdot E)^2/13\right)$ [7]. The original problem faces severe difficulties in its numerical treatment and mesh dependent microstructures are observed.

6 Adaptive Finite Element Method (AFEM)

An adaptive mesh refining algorithm consists of a successive loop of

$$solve \Rightarrow estimate \Rightarrow mark \Rightarrow refine\ .$$

The refinement indicator $\eta_E = h_E^{1/p'} \| [\sigma_\ell]\, \nu_E \|_{L^{p'}(E)}$ from subroutine *estimate* is monitored in *mark* for possible refinement of the edge E. Figure 3 shows admissible refinements of a triangle up to rotation. The error estimator through the sum over all η_E suffers from a reliability/efficiency gap [7]. This does not prevent a convergence proof for the AFEM in [4]. Moreover, optimal complexity is visible in numerical experiments for the microstructures benchmark [7].



oscillations and mesh sensitivity

no oscillations for RFEM

Fig. 2. Microstructures for the 2 well benchmark [7].

7 Numerical relaxation

Since direct approaches to approximate the quasiconvex envelope of a given function $W : \mathbb{R}^{n\times n} \to \mathbb{R}$, are of the same complexity as findig the solution of the original problem, numerical relaxation algorithms fall back to the notion of polyconvexity and rank-one convexity, which gives upper and lower bounds for the quasiconvex envelope and may even coinside with the latter.

7.1 Polyconvexification

A reliable and efficient computation of the polyconvex envelope

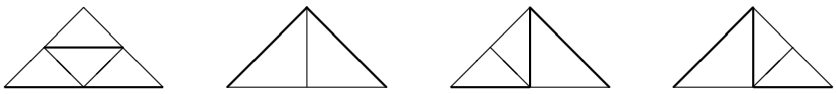
$$W^{pc}(E) = \inf\left\{\sum_{\ell=1}^{\tau+1}\lambda_\ell W(A_\ell) | A_\ell \in \mathbb{R}^{n\times n}, \lambda_\ell \geq 0, \sum_{\ell=1}^{\tau+1}\lambda_\ell T(A_\ell) = T(E)\right\}$$

in terms of a vector of all minors $T(A) \in \mathbb{R}^\tau$ of matrices $A \in \mathbb{R}^{n\times n}$ is studied in [1, 12].

7.2 Lamination

The approximation of the rank-one convex envelope by successive lamination [10, 2, 11, 14, 15, 16, 19] results in an upper bound for the rank-one convex envelope and quasiconvex envelope.

On the other hand, in finite lamination, one approximates W^{rc} by a laminate of second order, which are in practice sufficient approximations. The lamination is parametrised and a difficult nonlinear optimisation problem arises [3].



red(T) green(T) blue_{left} blue_{right}

Fig. 3. Refinement rules for the red-green-blue strategy

A combined numerical and analytical relaxation exploits the special structure of the single-slip plasticity analytically in [5]. This leads to initial guesses for a local minimisation algorithm to compute layers within layers and a dramatic reduction in the numerical effort.

7.3 Numerical Relaxation Benchmark

Figure 4 displays a comparison of several numerical relaxation methods for the single-slip plasticity benchmark. Therein $W^{\mathrm{opt}}_{\mathrm{BCHH}}$ denotes the outcome of finite lamination and $W^{\mathrm{pc}}_{\mathrm{BCHH}}$ of polyconvexification as an upper and lower bound for the quasiconvex envelope [3]. The new lamination solution W^{opt} as an upper bound and the approximated lower bound $\ell + m$ are taken from [5]. W^{ana} is an analytical relaxation obtained for a simplification of the underlying model [5].

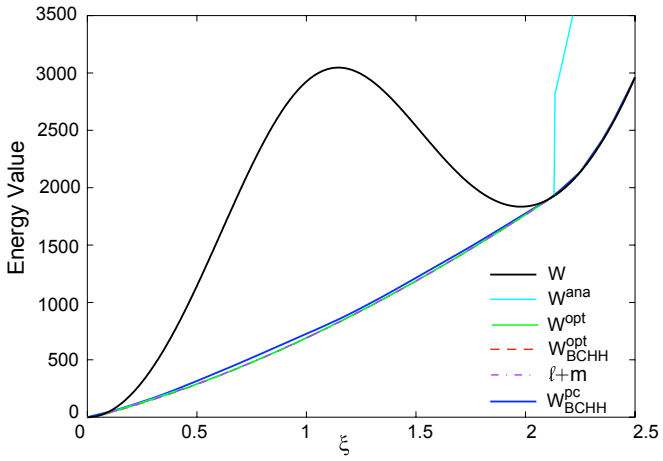


Fig. 4. Comparison of various relaxation methods along some rank-one line [5].

The overall impression of the numerical outcome of Figure 4 displays roughly the same energy. It is less clear whether or not they coinside.

8 Shape-Memory Alloys Benchmark

A rate independent hysteresis of phase transitions in shape memory alloys is modelled by a mixture $\chi^{(1)} = 1 - \chi^{(2)}$ of two materials, with given material constants $\kappa, W_{0,1}, W_{0,2} \in \mathbb{R}$ and $E_1, E_2 \in \mathbb{R}^2$, and resulting free energy

$$E(t,\chi) = \inf_{v \in V} \int_\Omega \sum_{i=1}^{2} \chi^{(j)} W_j(\varepsilon(v))\,\mathrm{d}x - F(t,v),$$

$$W_j(E) = \frac{1}{2}\left(E - E_j, \mathbb{C}\,(E - E_j)\right)_{\mathbb{R}^{n\times n}} + W_{0,j}\ ,$$

and the dissipation for re-arrangement of a phase mixture $\zeta \to \chi$,

$$\mathrm{d}(\chi,\zeta) = \int_\Omega \kappa|\chi-\zeta|\,\mathrm{d}x.$$

The incremental problem formulation allows a condensed form, which requires a quasiconvexification [17]. The effective model reads: for fixed time t_j compute the minimiser $\varphi_j \in V$ of

$$E_{\chi_{n-1}}(v) = \int_\Omega \Big(W_2(\varepsilon(v)) + 2\gamma H(\chi^{(1)}_{n-1}, \ell(\varepsilon(v))\Big)\,\mathrm{d}x - F(t_j, v)$$

and thereafter compute the update $\chi^{(1)}_j = M(\chi^{(1)}_{j-1}, \ell(\varepsilon(u_j)))$ with the definition $\gamma = \gamma(E_1, E_2, \mathbb{C})$, [17, 8] and

$$\ell(E) = \frac{1}{2\gamma}\,(W_2(E) - W_1(E)) + \frac{1}{2},$$

$$H(r,s) = \begin{cases} \frac{\kappa}{2\gamma}\,r & \text{if } s \le -\frac{\kappa}{2\gamma}, \\ \frac{\kappa}{2\gamma}\,r - \frac{1}{2}(s+\frac{\kappa}{2\gamma})^2 & \text{if } -\frac{\kappa}{2\gamma} \le s \le r - \frac{\kappa}{2\gamma}, \\ \frac{1}{2}\,r^2 - rs & \text{if } r - \frac{\kappa}{2\gamma} \le s \le r + \frac{\kappa}{2\gamma}, \\ -\frac{\kappa}{2\gamma}\,r - \frac{1}{2}(s-\frac{\kappa}{2\gamma})^2 & \text{if } r + \frac{\kappa}{2\gamma} \le s \le 1 + \frac{\kappa}{2\gamma}, \\ \frac{\kappa}{2\gamma}\,(1-r) + \frac{1}{2} - s & \text{if } s \ge 1 + \frac{\kappa}{2\gamma}, \end{cases}$$

$$M(r,s) = \begin{cases} 0 & \text{if } s \le -\frac{\kappa}{2\gamma}, \\ s + \frac{\kappa}{2\gamma} & \text{if } -\frac{\kappa}{2\gamma} \le s \le r - \frac{\kappa}{2\gamma}, \\ r & \text{if } r - \frac{\kappa}{2\gamma} \le s \le r + \frac{\kappa}{2\gamma}, \\ s - \frac{\kappa}{2\gamma} & \text{if } r + \frac{\kappa}{2\gamma} \le s \le 1 + \frac{\kappa}{2\gamma}, \\ 1 & \text{if } s \ge 1 + \frac{\kappa}{2\gamma}. \end{cases}$$

The algorithms are derived in [8] where spatial a priori and a posteriori error analysis is developed for one time step only. It remained as an open problem to control the error accumulated over various time steps.

References

1. S. Bartels (2003) Reliable and efficient approximation of polyconvex envelopes. SIAM J. Numer. Anal. 43 No. 1, 363-385
2. S. Bartels (2003) Linear convergence in the approximation of rank.one convex envelopes. ESAIM M2AN. 38 No. 5, 811-820
3. S. Bartels, C. Carstensen, K. Hackl and U. Hoppe (2003) Effective relaxation for microstructure simulations: algorithms and applications. Comput. Meth. Appl. Mech. Engng: 193, 5143-5175
4. C. Carstensen (2007) Convergence of an adaptive FEM for a class of degenerate convex minimization problems IMA Journal of Numerical Analysis, published online
5. C. Carstensen, S. Conti, A. Orlando (2008) Mixed analytical-numerical relaxation in finite single-slip crystal plasticity. submitted

6. C. Carstensen, K. Hackl, and A. Mielke (2002) Non-convex potentials and microstructures in finite-strain plasticity. Proc. Royal Soc. London, Ser. A, 458: 299-317
7. C. Carstensen and K. Jochimsen (2003) Adaptive finite element methods for miocrostructures? Numerical experiments for a 2-well benchmark. computing: 71, 175-204
8. Carstensen, C. and Plechac, P. (2001) Numerical Analysis of a Relaxed Variational Model of Hysteresis in Two-Phase Solids. M2AN, 35, 865-878
9. Conti, S. (2006) Relaxation of single-slip single-crystal plasticity with linear hardening. Multiscale Materials Modeling, Fraunhofer IRB, 2006, 30-35
10. Dacorogna, B. (2007) Direct Methods in the Calculus of Variations. Applied Mathematical Sciences 78, Springer New York
11. G. Dolzmann (1999) Numerical computation of rank.one convex envelopes. SIAM J. Numer. Anal. 26, 1621-1635
12. G. Dolzmann (2003) Variational Methods for Crystalline Microstructure - Analysis and Computation. Lecture Notes in Mathematics 1803/2004, Springer Berlin / Heidelberg
13. B. Halphen and Q.S. Nguyen (1975) Sur les materiaux standards generalizes, J Mech 14 , 39-63
14. C. Miehe (2002) Strain-Driven Homogenization of Inelastic Microstructures and Composites Based on an Incremental Variational Formulation. International Journal for Numerical Methods in Engineering 55 Issue 11, 1285-1322
15. C. Miehe and M. Lambrecht (2003) A two-scale finite element relaxation analysis of shear bands in non-convex inelastic solids: small-strain theory for standard dissipative materials. Comput. Methods Appl. Mech. Engrg. 192, 473-508
16. C. Miehe, J. Schotte and M. Lambrecht (2002) Homogenization of Inelastic Solid Materials at Finite Strains based on Incremental Minimization Principles. Journal of the Mechanics and Physics of Solids 50 (2002), 2123-2167
17. Mielke, A. and Theil, F (1999) A mathematical Model for rate-independant phase transformations with Hysteresis. Workshop of Continuum Mechanics in Analysis and Engineering, Aachen, 117-129
18. A. Mielke (2003) Energetic formulation of multiplicative elasto-plasticity using dissipation distances. Cont. Mech. Thermodynamics, 15: 351-382
19. Ortiz, M. and Repetto, E. A. (1999) Non-convex energy minimization and dislocation structures in ductile single crystals. J. Mech. Phys. Solids 47, 397-462
20. Sverak, V. (1992) Rank-one convexity does not imply quasiconvexity. Proc. Roy. Soc. Edinb. 120A, 185-189