CHALMERS

Calibration of the Bergström-Boyce model: Explicit expressions

HÅKAN JOHANSSON, KENNETH RUNESSON

Department of Applied Mechanics
Division Material & Computational Mechanics
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg 2005

Research report 2005:02

Calibration of the Bergström-Boyce model: Explicit expressions

Håkan Johansson, Kenneth Runesson

Department of Applied Mechanics
Division Material & Computational Mechanics
CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden, 2005

Calibration of the Bergström-Boyce model: Explicit expressions
HÅKAN JOHANSSON, KENNETH RUNESSON

Research report 2005:02
ISSN 1652-8557

Department of Applied Mechanics
Division Material & Computational Mechanics
Chalmers University of Technology
SE-412 96 Göteborg
Sweden
Telephone +46 (0)31 772 1000

CALIBRATION OF THE BERGSTRÖM-BOYCE MODEL: EXPLICIT EXPRESSIONS

Håkan Johansson* **and Kenneth Runesson**†

Department of Applied Mechanics
Chalmers University of Technology
* e-mail: hakan.johansson@sem.chalmers.se
† e-mail: kenneth.runesson@sem.chalmers.se

Key words: Calibration; parameter identification; viscoelasticity; Bergström-Boyce model

Abstract. *In this report we derive the explicit expressions associated with the calibration of the Bergström-Boyce model of nonlinear viscoelasticity. These expressions are intended for practical use in a computational algorithm.*

1 Introduction

Computational calibration of constitutive models are based on the solution of an optimization problem, where a set of parameter values are to be determined such that the discrepancy between the predicted (simulated) response and the experimentally observed response is minimized. A framework that is based on the formulation of an adjoint problem has been proposed [1],[2] for the solution of such optimization problems. For a specific realization of the general format, the derivatives are needed of the underlying constitutive relation, both with respect to the parameters to be calibrated, as well as with respect to the evolution (internal) variables. In this report, those relations pertinent to the Bergström-Boyce model are derived. These relations are later to be used for carrying out numerical simulations, to appear in [3].

The Bergström-Boyce model was proposed in [4] to describe the mechanical response for rate-dependent materials which exhibit hysteresis upon cyclic loading, often denoted as the Mullins effect. Typical materials of this type are rubber elastomers, in particular those with carbon black particle fillers, although unfilled elastomers also display hysteresis [5].

This report is organized as follows. First, the Bergström-Boyce model is described in finite strain kinematics, as can be found in several publications, e.g. [4], [5], [6], and the restriction to uniaxial stress state is made and the assumption of incompressibility is adopted. Thereafter, the explicit derivatives with respect to parameters and state variables are derived. Finally, explicit expressions for derivatives of the objective function associated with the optimization problem are shown.

2 Bergström-Boyce model

First, we give a short description of the Bergström-Boyce model, as described in detail in [6] in a finite strain setting. We then proceed with the simplification to the 1D uniaxial stress state and incompressible material. The corresponding rheological model, depicted in Figure 1, consists of two networks (A) and (B) connected in parallel. Network (A) is a hyperelastic spring while (B) is a hyperelstic spring serially connected to a viscous dashpot. The total deformation is $\boldsymbol{F} = \boldsymbol{F}^{(\mathrm{A})} = \boldsymbol{F}^{(\mathrm{B})}$. The stress acting on Network A is given via the 8-chain hyperelastic model proposed by [7] and reformulated in [6] as

$$\boldsymbol{\sigma}^{(\mathrm{A})} = \frac{\mu^{(\mathrm{A})}}{Jj(\boldsymbol{B}^*)} \frac{\mathcal{A}^{-1}(j(\boldsymbol{B}^*)/j_{\mathrm{lock}}^{(\mathrm{A})})}{\mathcal{A}^{-1}(1/j_{\mathrm{lock}}^{(\mathrm{A})})} \boldsymbol{B}_{\mathrm{dev}}^* + \kappa[J-1]\mathbf{1} \tag{1}$$

where $\boldsymbol{\sigma}^{(\mathrm{A})}$ is the Cauchy stress in network A, $J = \det[\boldsymbol{F}]$, $\boldsymbol{B}^* = J^{-\frac{2}{3}}\boldsymbol{F}\cdot\boldsymbol{F}^{\mathrm{T}}$ and $j(\boldsymbol{B}^*) = \sqrt{\mathrm{Tr}[\boldsymbol{B}^*]/3}$. Moreover, $\mathcal{A}^{-1}(x)$ is the inverse Langevin function given by

$$\mathcal{A}(x) = \coth(x) - \frac{1}{x} \tag{2}$$

In (1), $\mu^{(\mathrm{A})}$, $j_{\mathrm{lock}}^{(\mathrm{A})}$ and κ are material parameters.

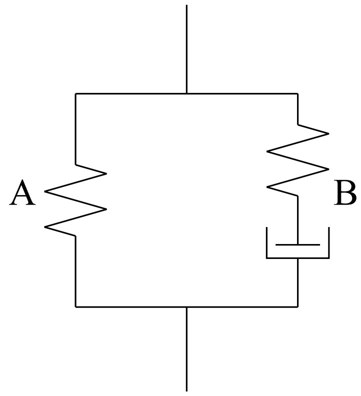

Figure 1: Rheological representation of the Bergström-Boyce constitutive model for rubber.

Since the ingredients in (1) are all directly computable from $\boldsymbol{F}$, it is convenient from a computational point to treat the stress as a function of $\boldsymbol{F}$, i.e.

$$\boldsymbol{\sigma}^{(\mathrm{A})} \overset{\mathrm{def}}{=} \boldsymbol{\sigma}^{(\mathrm{A})}(\boldsymbol{F}) \tag{3}$$

The stress in Network B is expressed like (1); however, in terms of the elastic portion, $\boldsymbol{F}^{\mathrm{e}}$, of the total deformation via a multiplicative split, $\boldsymbol{F} = \boldsymbol{F}^{\mathrm{e}}\boldsymbol{F}^{\mathrm{v}}$, with $\mu^{(\mathrm{B})}$, $j_{\mathrm{lock}}^{(\mathrm{B})}$ as parameters. The total stress is simply the sum of the two network contributions

$$\boldsymbol{\sigma}(\boldsymbol{F}) = \boldsymbol{\sigma}^{(\mathrm{A})}(\boldsymbol{F}) + \boldsymbol{\sigma}^{(\mathrm{B})}(\boldsymbol{F}^{\mathrm{e}}) \tag{4}$$

The evolution law is expressed in terms of the rate of deformation, $\boldsymbol{L} \overset{\mathrm{def}}{=} \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$ which can be split as $\boldsymbol{L} = \boldsymbol{L}^{\mathrm{e}} + \tilde{\boldsymbol{L}}^{\mathrm{v}}$ with $\tilde{\boldsymbol{L}}^{\mathrm{v}} \overset{\mathrm{def}}{=} \boldsymbol{F}^{\mathrm{e}}\boldsymbol{L}^{\mathrm{e}}(\boldsymbol{F}^{\mathrm{e}})^{-1}$. The evolution law is then chosen as

$$\tilde{\boldsymbol{L}}^{\mathrm{v}} = \dot{\gamma}\boldsymbol{N}^{(\mathrm{B})} \tag{5}$$

where

$$\dot{\gamma} = \gamma_0 \left(j(\boldsymbol{B}^{\mathrm{v}}) - 1\right)^C \tau_{(B)}^m \tag{6}$$

$$\boldsymbol{N}^{(\mathrm{B})} = \frac{\boldsymbol{\sigma}_{\mathrm{dev}}^{(\mathrm{B})}}{\tau_{(B)}} \tag{7}$$

and $\tau_{(B)} = |\boldsymbol{\sigma}_{\mathrm{dev}}| \overset{\mathrm{def}}{=} \sqrt{\mathrm{Tr}[\boldsymbol{\sigma}_{\mathrm{dev}}^{(\mathrm{B})} \cdot (\boldsymbol{\sigma}_{\mathrm{dev}}^{(\mathrm{B})})^{\mathrm{T}}]}$. In (6), γ_0, C and m are material parameters in addition to the elastic parameters $\mu^{(\mathrm{B})}$, $j_{\mathrm{lock}}^{(\mathrm{B})}$ and κ.

For the case of uniaxial stress state, while assuming incompressible material, we can express the deformation gradient $\boldsymbol{F}$ by the (prescribed) longitudinal stretch λ only

$$\boldsymbol{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \frac{1}{\sqrt{\lambda}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{\lambda}} \end{bmatrix} \tag{8}$$

Furthermore, we have that $\sigma_{22} = \sigma_{33} = 0$; hence from (1) we obtain (incompressibility: $\kappa \to \infty,\ J \to 1$):

$$\kappa[J-1] = \frac{\mu^{(\mathrm{A})}}{j(\boldsymbol{B}^*)} \frac{\mathcal{A}^{-1}(j(\boldsymbol{B}^*)/j_{\mathrm{lock}}^{(\mathrm{A})})}{\mathcal{A}^{-1}(1/j_{\mathrm{lock}}^{(\mathrm{A})})} \frac{1}{3} \left(\lambda^2 - \frac{1}{\lambda}\right) \tag{9}$$

which inserted into (1) gives $\sigma^{(\mathrm{A})} \stackrel{\mathrm{def}}{=} \sigma_{11}^{(\mathrm{A})}$

$$\sigma^{(\mathrm{A})}(\lambda) = \frac{\mu^{(\mathrm{A})}}{j(\lambda)} \frac{\mathcal{A}^{-1}(j(\lambda)/j_{\mathrm{lock}}^{(\mathrm{A})})}{\mathcal{A}^{-1}(1/j_{\mathrm{lock}}^{(\mathrm{A})})} \left(\lambda^2 - \frac{1}{\lambda}\right) \tag{10}$$

which is Eq. (3.23) in [5] with

$$j(\lambda) = \sqrt{\frac{1}{3}\left(\lambda^2 + \frac{2}{\lambda}\right)} \tag{11}$$

Furthermore, we obtain

$$\tau_{(B)} = \sqrt{\frac{2}{3}}|\sigma^{(\mathrm{B})}|, \qquad N^{(\mathrm{B})} = \sqrt{\frac{2}{3}}\mathrm{sgn}(\sigma^{(\mathrm{B})}) \tag{12}$$

For network B, the total stretch λ is split multiplicatively into the elastic part λ^{e} and the viscous part λ^{v} as $\lambda = \lambda^{\mathrm{e}}\lambda^{\mathrm{v}}$. We may then summarize the expression for the stress in the longitudinal direction[1] as

$$\sigma(q,\lambda) = f^{(\mathrm{A})}(\lambda) + f^{(\mathrm{B})}(\lambda^{\mathrm{e}}(q)) \tag{13}$$

where

$$\lambda^{\mathrm{e}}(q) = (\lambda^{\mathrm{v}}(q))^{-1}\lambda, \qquad \lambda^{\mathrm{v}}(q) = 1 + q \tag{14}$$

with

$$f^{(\mathrm{A})}(\lambda) \stackrel{\mathrm{def}}{=} \frac{\mu^{(\mathrm{A})}}{\mathcal{A}^{-1}\left(\frac{1}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right)} \left[\frac{\lambda^2 - \frac{1}{\lambda}}{j(\lambda)}\right] \mathcal{A}^{-1}\left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right) \tag{15}$$

and $j(\lambda)$ and $\mathcal{A}^{-1}(x)$ are defined in (11) and (2), respectively. Note that $f^{(\mathrm{A})}$ and $f^{(\mathrm{B})}$ are the same function; they only differ w.r.t the choice of elastic parameters.

The evolution equation for the state variable q reads

$$\dot{q} - \lambda^{\mathrm{v}}(q)\dot{\gamma}(q)N^{(\mathrm{B})}(q) = 0, \qquad q(0) = 0 \tag{16}$$

where

$$\dot{\gamma}(q) = \gamma_0 \left[j(\lambda^{\mathrm{v}}(q)) - 1\right]^C \tau_{(B)}^m \tag{17}$$

To summarize, the material parameter set to be determined in the calibration is

$$p = \{\underbrace{\mu^{(\mathrm{A})}, j_{\mathrm{lock}}^{(\mathrm{A})}, \mu^{(\mathrm{B})}, j_{\mathrm{lock}}^{(\mathrm{B})}}_{\text{"elastic"}}, \underbrace{\gamma_0, C, m}_{\text{"viscous"}}\} \tag{18}$$

[1] We restrict to situations where the longitudinal stretch $\lambda(t)$ is prescribed.

3 Explicit expression of derivatives

3.1 Calibration - problem formulation

In [3], the model format for calibration of constitutive models under uniaxial stress state was expressed as: Find the material parameter set $p \in \mathbb{R}^m$ such that the objective function

$$\mathcal{F}(p,q) = \frac{1}{2}\sum_{i}^{N^{\text{obs}}} c_i[\sigma(p,q)(\bar{t}_i) - \sigma_i^{\text{obs}}]^2 \tag{19}$$

is minimized under the constraint that the (internal) state variable q satisfy the evolution equation

$$\dot{q} - h(p,q) = 0, \qquad q(0) = 0 \tag{20}$$

Using the format for calibration, as described in [2], the first and second derivatives of $h(p,q)$ and $\mathcal{F}(p,q)$ with respect to p and q are needed. Thus, the explicit expressions for $h'_p(p,q)$, $h'_q(p,q)$, $h''_{pp}(p,q)$, $h''_{pq}(p,q)$, $h''_{qq}(p,q)$ $\mathcal{F}'_p(p,q)$, $\mathcal{F}'_q(p,q)$, $\mathcal{F}''_{pp}(p,q)$, $\mathcal{F}''_{pq}(p,q)$ and $\mathcal{F}''_{qq}(p,q)$ will be derived below.

3.2 Derivatives of $h(p,q)$

The explicit expression for the derivatives of $h(p,q)$ are obtained after straightforward differentiation

$$h(p,q) = \lambda^{\text{v}}(q)\dot{\gamma}(p,q)N(q) \tag{21}$$

$$\begin{aligned}
\underline{h}'_p(p,q) &= \lambda^{\text{v}}(q)N(q)\underline{\dot{\gamma}}'_p(p,q) &(22)\\
h'_q(p,q) &= N(q)\dot{\gamma}(p,q) + \lambda^{\text{v}}(q)N(q)\dot{\gamma}'_q(p,q) &(23)\\
\underline{h}_{pp}(p,q) &= \lambda^{\text{v}}(q)N(q)\underline{\dot{\gamma}}''_{pp}(p,q) &(24)\\
\underline{h}''_{pq}(p,q) &= \lambda^{\text{v}}(q)N(q)\underline{\dot{\gamma}}''_{pq}(p,q) + N(q)\underline{\dot{\gamma}}'_p(p,q) &(25)\\
h''_{qq}(p,q) &= \lambda^{\text{v}}(q)N(q)\dot{\gamma}''_{qq}(p,q) + 2N(q)\dot{\gamma}'_q(p,q) &(26)
\end{aligned}$$

where it was noted that $N'_q(q) = 0$ for $q \neq 0$ and $(\lambda^{\text{v}})'_q(q) = 1$.

3.3 Derivatives of $\gamma(p,q)$

Proceeding with the explicit derivatives of $\gamma(p,q)$, we obtain

$$\dot{\gamma}(p,q) = \gamma_0\left[j(\lambda^{\text{v}}(q)) - 1\right]^C \left[\tau_{(B)}(p,q)\right]^m \tag{27}$$

$$\underline{\dot{\gamma}}'_p(p,q) = \begin{bmatrix} 0 \\ 0 \\ \gamma_0 m\left[j(\lambda^{\rm v}(q))-1\right]^C\left[\tau_{(B)}(p,q)\right]^{(m-1)}(\tau_{(B)})'_{\mu^{(\rm B)}}(p,q) \\ \gamma_0 m\left[j(\lambda^{\rm v}(q))-1\right]^C\left[\tau_{(B)}(p,q)\right]^{(m-1)}(\tau_{(B)})'_{j^{(\rm B)}_{\rm lock}}(p,q) \\ \left[j(\lambda^{\rm v}(q))-1\right]^C\left[\tau_{(B)}(p,q)\right]^m \\ \gamma_0\left[j(\lambda^{\rm v}(q))-1\right]^C\left[\tau_{(B)}(p,q)\right]^m\log(|j(\lambda^{\rm v}(q))-1|) \\ \gamma_0\left[j(\lambda^{\rm v}(q))-1\right]^C\left[\tau_{(B)}(p,q)\right]^m\log(\tau_{(B)}) \end{bmatrix} \tag{28}$$

$$\dot{\gamma}'_q(p,q) = \gamma_0 C\left[j(\lambda^{\rm v}(q))-1\right]^{C-1}\tau^m_{(B)}j'_\lambda(\lambda^{\rm v}(q)) + \gamma_0 m\left[j(\lambda^{\rm v}(q))-1\right]^C\tau^{(m-1)}_{(B)}(\tau_{(B)})'_q \tag{29}$$

We proceed with the second derivatives, first the components of $\underline{\dot{\gamma}}''_{pp}$ (a 7×7-matrix)

$$\dot{\gamma}''_{\mu^{(\rm A)}p} = \dot{\gamma}''_{j^{(\rm A)}_{\rm lock}p} = \underline{0} \tag{30}$$

$$\dot{\gamma}''_{\mu^{(\rm B)}\mu^{(\rm B)}} = \gamma_0 m(m-1)(j(\lambda^{\rm v}(q))-1)^C\tau_B^{m-2}(\tau_B)'_{\mu^{(\rm B)}}(\tau_B)'_{\mu^{(\rm B)}} \tag{31}$$

$$\dot{\gamma}''_{\mu^{(\rm B)}j^{(\rm B)}_{\rm lock}} = \gamma_0 m(j(\lambda^{\rm v}(q))-1)^C\left[(m-1)\tau_B^{m-2}(\tau_B)'_{\mu^{(\rm B)}}(\tau_B)'_{j^{(\rm B)}_{\rm lock}} + \tau_B^{m-1}(\tau_B)''_{j^{(\rm B)}_{\rm lock}\mu^{(\rm B)}}\right] \tag{32}$$

$$\dot{\gamma}''_{\mu^{(\rm B)}\gamma_0} = \frac{\dot{\gamma}'_{\mu^{(\rm B)}}}{\gamma_0} \tag{33}$$

$$\dot{\gamma}''_{\mu^{(\rm B)}C} = \dot{\gamma}'_{\mu^{(\rm B)}}\log|j(\lambda^{\rm v}(q))-1| \tag{34}$$

$$\dot{\gamma}''_{\mu^{(\rm B)}m} = \dot{\gamma}'_{\mu^{(\rm B)}}[\log(\tau_B)+1/m] \tag{35}$$

$$\dot{\gamma}''_{j^{(\rm B)}_{\rm lock}j^{(\rm B)}_{\rm lock}} = \gamma_0 m(j(\lambda^{\rm v}(q))-1)^C\left[(m-1)\tau_B^{m-2}(\tau_B)'_{j^{(\rm B)}_{\rm lock}}(\tau_B)'_{j^{(\rm B)}_{\rm lock}} + \tau_B^{m-1}(\tau_B)''_{j^{(\rm B)}_{\rm lock}j^{(\rm B)}_{\rm lock}}\right] \tag{36}$$

$$\dot{\gamma}''_{j^{(\rm B)}_{\rm lock}\gamma_0} = \frac{\dot{\gamma}'_{j^{(\rm B)}_{\rm lock}}}{\gamma_0} \tag{37}$$

$$\dot{\gamma}''_{j^{(\rm B)}_{\rm lock}C} = \dot{\gamma}'_{j^{(\rm B)}_{\rm lock}}\log|j(\lambda^{\rm v}(q))-1| \tag{38}$$

$$\dot{\gamma}''_{j^{(\rm B)}_{\rm lock}m} = \dot{\gamma}'_{j^{(\rm B)}_{\rm lock}}[\log(\tau_B)+1/m] \tag{39}$$

$$\dot{\gamma}''_{\gamma_0\gamma_0} = 0 \tag{40}$$

$$\dot{\gamma}''_{\gamma_0 C} = \dot{\gamma}'_{\gamma_0}\log|j(\lambda^{\rm v}(q))-1| \tag{41}$$

$$\dot{\gamma}''_{\gamma_0 m} = \dot{\gamma}'_{\gamma_0}\log(\tau_B) \tag{42}$$

$$\dot{\gamma}''_{CC} = \dot{\gamma}'_C\log|j(\lambda^{\rm v}(q))-1| \tag{43}$$

$$\dot{\gamma}''_{Cm} = \dot{\gamma}'_C\log(\tau_B) \tag{44}$$

$$\dot{\gamma}''_{mm} = \dot{\gamma}'_m\log(\tau_B) \tag{45}$$

$$\tag{46}$$

where it was used in (31) that $((\tau_B)''_{\mu^{(\rm B)}\mu^{(\rm B)}} = 0)$.

The components of $\underline{\dot{\gamma}}''_{pq}$ are as follows

$$\dot{\gamma}''_{q\mu^{(\mathrm{A})}} = \dot{\gamma}''_{qj^{(\mathrm{A})}_{\mathrm{lock}}} = 0 \tag{47}$$

$$\begin{aligned}\dot{\gamma}''_{q\mu^{(\mathrm{B})}} &= \gamma_0 Cm[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m-1}j'_\lambda(\lambda^{\mathrm{v}}(q))(\tau_B)'_{\mu^{(\mathrm{B})}} \\ &\quad +\gamma_0 m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\left[\tau_B^{m-1}(\tau_B)''_{q\mu^{(\mathrm{B})}}+(m-1)\tau_B^{m-2}(\tau_B)'_q(\tau_B)'_{\mu^{(\mathrm{A})}}\right]\end{aligned} \tag{48}$$

$$\begin{aligned}\dot{\gamma}''_{qj^{(\mathrm{B})}_{\mathrm{lock}}} &= \gamma_0 Cm[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m-1}j'_\lambda(\lambda^{\mathrm{v}}(q))(\tau_B)'_{j^{(\mathrm{B})}_{\mathrm{lock}}} \\ &\quad +\gamma_0 m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\left[\tau_B^{m-1}(\tau_B)''_{qj^{(\mathrm{B})}_{\mathrm{lock}}}+(m-1)\tau_B^{m-2}(\tau_B)'_q(\tau_B)'_{j^{(\mathrm{B})}_{\mathrm{lock}}}\right]\end{aligned} \tag{49}$$

$$\dot{\gamma}''_{q\gamma_0} = C[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B j'_\lambda(\lambda^{\mathrm{v}}(q))+m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-1}(\tau_B)'_q \tag{50}$$

$$\begin{aligned}\dot{\gamma}''_{qC} &= \gamma_0 m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-1}\log|j(\lambda^{\mathrm{v}}(q))-1|(\tau_B)'_q \\ &\quad +\gamma_0[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B j'_\lambda(\lambda^{\mathrm{v}}(q))+\gamma_0 C(j(\lambda^{\mathrm{v}}(q))-1)^{C-1}\tau_B^{m}\log|j(\lambda^{\mathrm{v}}(q))-1|j'_\lambda(\lambda^{\mathrm{v}}(q))\end{aligned} \tag{51}$$

$$\begin{aligned}\dot{\gamma}''_{qm} &= \gamma_0 C[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m}\log(\tau_B)j'_\lambda(\lambda^{\mathrm{v}}(q))+\gamma_0[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-1}(\tau_B)'_q \\ &\quad +\gamma_0 m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-1}\log(\tau_B)(\tau_B)'_q\end{aligned} \tag{52}$$

and, finally, $\dot{\gamma}''_{qq}$ is

$$\begin{aligned}\dot{\gamma}''_{qq} &= \gamma_0 C[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m}j''_{\lambda\lambda}(\lambda^{\mathrm{v}}(q))+\gamma_0 Cm[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m-1}j'_\lambda(\lambda^{\mathrm{v}}(q))(\tau_B)'_q \\ &\quad +\gamma_0 C(C-1)[j(\lambda^{\mathrm{v}}(q))-1]^{C-2}\tau_B^{m}[j'_\lambda(\lambda^{\mathrm{v}}(q))]^2+\gamma_0 m[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-1}(\tau_B)''_{qq} \\ &\quad +\gamma_0 m(m-1)[j(\lambda^{\mathrm{v}}(q))-1]^{C}\tau_B^{m-2}[(\tau_B)'_q]^2+\gamma_0 Cm[j(\lambda^{\mathrm{v}}(q))-1]^{C-1}\tau_B^{m-1}(\tau_B)'_q j'_\lambda(\lambda^{\mathrm{v}}(q))\end{aligned} \tag{53}$$

3.4 Derivatives of $\tau_B(p,q)$

Recalling (12)

$$\tau_{(B)} = \sqrt{\frac{2}{3}}|\sigma^{(\mathrm{B})}| = \sqrt{\frac{2}{3}}|f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q))| \tag{54}$$

we obtain

$$(\underline{\tau}_{(B)})'_p(p,q) = \sqrt{\frac{2}{3}}\mathrm{sgn}(f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q)))(\underline{f}^{(\mathrm{B})})'_p(p,\lambda^{\mathrm{e}}(q)) \tag{55}$$

$$(\tau_{(B)})'_q(p,q) = -\sqrt{\frac{2}{3}}\mathrm{sgn}(f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q)))(f^{(\mathrm{B})})'_{\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q))(1+q)^{-2}\lambda \tag{56}$$

where it was used that $(\lambda^{\mathrm{e}})'_q(q) = -(1+q)^{-2}\lambda$. The second derivatives are

$$(\underline{\tau}_{(B)})''_{pp}(p,q) = \sqrt{\frac{2}{3}}\mathrm{sgn}(f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q)))(\underline{f}^{(\mathrm{B})})''_{pp}(p,\lambda^{\mathrm{e}}(q)) \tag{57}$$

$$(\underline{\tau}_{(B)})''_{pq}(p,q) = -\sqrt{\frac{2}{3}}\mathrm{sgn}(f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q)))(\underline{f}^{(\mathrm{B})})''_{p\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q))(1+q)^{-2}\lambda \tag{58}$$

$$(\tau_{(B)})''_{qq}(p,q) = \sqrt{\frac{2}{3}}\text{sgn}(f^{(\text{B})}(p,\lambda^{\text{e}}(q)))(f^{(\text{B})})'_{\lambda^{\text{e}}}(p,\lambda^{\text{e}}(q))2(1+q)^{-3}\lambda - \sqrt{\frac{2}{3}}\text{sgn}(f^{(\text{B})}(p,\lambda^{\text{e}}(q)))(f^{(\text{B})})''_{\lambda^{\text{e}}\lambda^{\text{e}}}(p,\lambda^{\text{e}}(q))[(1+q)^{-2}\lambda]^2 \quad (59)$$

where it was used that $(\lambda^{\text{e}})''_{qq}(q) = 2(1+q)^{-3}\lambda$.

3.5 Derivatives of $f^{(\text{A})}(p,\lambda)$

Recall the expression for $f^{(\text{A})}$ from (15):

$$\underline{f}^{(\text{A})}(p,\lambda) = \frac{\mu^{(\text{A})}}{\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)}\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right]\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right) \quad (60)$$

$$(f^{(\text{A})})'_{\mu^{(\text{A})}}(p,\lambda) = \frac{1}{\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)}\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right]\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right) \quad (61)$$

$$(f^{(\text{A})})'_{j^{(\text{A})}_{\text{lock}}}(p,\lambda) = \frac{\mu^{(\text{A})}}{(j^{(\text{A})}_{\text{lock}})^2}\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right] \cdot \left[\frac{(\mathcal{A}^{-1})'\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right) - j(\lambda)\,(\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)}{\left[\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)\right]^2}\right] \quad (62)$$

and remaining p-derivatives vanish.

Furthermore for λ, we have

$$(f^{(\text{A})})'_{\lambda}(p,\lambda) = \frac{\mu^{(\text{A})}}{\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)}\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right](\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right)\frac{j'_{\lambda}(\lambda)}{j^{(\text{A})}_{\text{lock}}} + \frac{\mu^{(\text{A})}}{\mathcal{A}^{-1}\left(\frac{1}{j^{(\text{A})}_{\text{lock}}}\right)}\left[\frac{\left(2\lambda+\frac{1}{\lambda^2}\right)j(\lambda) - j'_{\lambda}(\lambda)\left(\lambda^2-\frac{1}{\lambda}\right)}{(j(\lambda))^2}\right]\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(\text{A})}_{\text{lock}}}\right) \quad (63)$$

Proceeding with the second derivatives of $f^{(\text{A})}$.

$$(f^{(\text{A})})''_{\mu^{(\text{A})}\mu^{(\text{A})}}(p,\lambda) = 0 \quad (64)$$

$$(f^{(A)})''_{\mu^{(A)} j^{(A)}_{\text{lock}}}(p,\lambda) = \frac{(f^{(A)})'_{j^{(A)}_{\text{lock}}}(p,\lambda)}{\mu^{(A)}} \tag{65}$$

$$\begin{aligned}(f^{(A)})''_{j^{(A)}_{\text{lock}} j^{(A)}_{\text{lock}}}(p,\lambda) &= -\frac{2(\underline{f}^{(A)})'_{j^{(A)}_{\text{lock}}}(p,\lambda)}{j^{(A)}_{\text{lock}}} \\ &+ G\left[\frac{j(\lambda)^2\,(\mathcal{A}^{-1})''\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right) - (\mathcal{A}^{-1})''\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)}{\left[\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\right]^2}\right] \\ &+ 2G\,(\mathcal{A}^{-1})'\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\left[\frac{(\mathcal{A}^{-1})'\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right) - j(\lambda)\,(\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)}{\left[\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\right]^3}\right]\end{aligned} \tag{66}$$

with

$$G = \frac{\mu^{(A)}}{(j^{(A)}_{\text{lock}})^4}\frac{\lambda^2 - \frac{1}{\lambda}}{j(\lambda)} \tag{67}$$

$$\begin{aligned}(f^{(A)})''_{\lambda j^{(A)}_{\text{lock}}}(p,\lambda) &= \frac{\mu^{(A)}}{(j^{(A)}_{\text{lock}})^2}\left[\frac{\left(2\lambda + \frac{1}{\lambda^2}\right) j(\lambda) - j'_\lambda(\lambda)\left(\lambda^2 - \frac{1}{\lambda}\right)}{(j(\lambda))^2}\right] \\ &\cdot \left[\frac{(\mathcal{A}^{-1})'\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right) - j(\lambda)\,(\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)}{\left[\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\right]^2}\right] \\ &+ \frac{j'(\lambda)\mu^{(A)}}{(j^{(A)}_{\text{lock}})^3}\frac{\lambda^2 - \frac{1}{\lambda}}{j(\lambda)} \\ &\cdot \left[\frac{(\mathcal{A}^{-1})'\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)(\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right) - j^{(A)}_{\text{lock}}\,(\mathcal{A}^{-1})'\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right) - j(\lambda)\,(\mathcal{A}^{-1})''\left(\frac{j(\lambda)}{j^{(A)}_{\text{lock}}}\right)\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)}{\left[\mathcal{A}^{-1}\left(\frac{1}{j^{(A)}_{\text{lock}}}\right)\right]^2}\right]\end{aligned} \tag{68}$$

$$
\begin{aligned}
(f^{(\mathrm{A})})''_{\lambda\lambda}(p,\lambda) = D &\left[\frac{\left(2\lambda+\frac{1}{\lambda^2}\right) j(\lambda) - j'_\lambda(\lambda)\left(\lambda^2-\frac{1}{\lambda}\right)}{(j(\lambda))^2}\right] \left(\mathcal{A}^{-1}\right)' \left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right) \frac{j'_\lambda(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}} \\
&+ D\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right] \left(\mathcal{A}^{-1}\right)'' \left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right) \left(\frac{j'_\lambda(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right)^2 \\
&+ D\left[\frac{\lambda^2-\frac{1}{\lambda}}{j(\lambda)}\right] \left(\mathcal{A}^{-1}\right)' \left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right) \frac{j''_{\lambda\lambda}(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}} \\
&+ D\left[\frac{\left(2\lambda+\frac{1}{\lambda^2}\right) j(\lambda) - j'_\lambda(\lambda)\left(\lambda^2-\frac{1}{\lambda}\right)}{(j(\lambda))^2}\right] \left(\mathcal{A}^{-1}\right)' \left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right) \frac{j'_\lambda(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}} \\
+D &\left[\frac{\left(2-\frac{2}{\lambda^3}\right) j(\lambda) - 2j'_\lambda(\lambda)\left(2\lambda+\frac{1}{\lambda^2}\right) - j''_{\lambda\lambda}(\lambda)\left(\lambda^2-\frac{1}{\lambda}\right) + \frac{2}{j(\lambda)}[j'_\lambda(\lambda)]^2\left(\lambda^2-\frac{1}{\lambda}\right)}{(j(\lambda))^2}\right] \mathcal{A}^{-1}\left(\frac{j(\lambda)}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right)
\end{aligned} \tag{69}
$$

with

$$
D = \frac{\mu^{(\mathrm{A})}}{\mathcal{A}^{-1}\left(\frac{1}{j_{\mathrm{lock}}^{(\mathrm{A})}}\right)} \tag{70}
$$

It is noted that the first and fourth terms in (69) are identical.

The expressions for $f^{(\mathrm{B})}$ and corresponding derivatives are similar to that of $f^{(\mathrm{A})}$; however with parameters $\mu^{(\mathrm{B})}$, $j_{\mathrm{lock}}^{(\mathrm{B})}$ instead of $\mu^{(\mathrm{A})}$, $j_{\mathrm{lock}}^{(\mathrm{A})}$, respectively.

3.6 Derivatives of $j(\lambda)$

We recall (11) above as

$$
j(\lambda) = \sqrt{\frac{1}{3}\left(\lambda^2+\frac{2}{\lambda}\right)} \tag{71}
$$

with derivatives

$$
j'_\lambda(\lambda) = \frac{1}{\sqrt{3}}\left[\lambda^2+\frac{2}{\lambda}\right]^{-\frac{1}{2}}\left[\lambda-\frac{1}{\lambda^2}\right] \tag{72}
$$

$$
j''_{\lambda\lambda}(\lambda) = \frac{1}{\sqrt{3}}\left[\lambda^2+\frac{2}{\lambda}\right]^{-\frac{1}{2}}\left[1+\frac{2}{\lambda^3}\right] - \frac{1}{\sqrt{3}}\left[\lambda^2+\frac{2}{\lambda}\right]^{-\frac{3}{2}}\left[\lambda-\frac{1}{\lambda^2}\right]^2 \tag{73}
$$

3.7 The inverse Langevin function

We recall the inverse Langevin function from (2)

$$
\mathcal{A}(x) = \coth(x) - \frac{1}{x} \tag{74}
$$

and we note that there is no explicit expression for $y = \mathcal{A}^{-1}(x)$. One possibility is to utilize the rule for derivatives of inverse functions (obtained by differentiating the identity $\mathcal{A}(\mathcal{A}^{-1}(x)) = x$)

$$(\mathcal{A}^{-1})'(x) = \frac{1}{\mathcal{A}'(\mathcal{A}^{-1}(x))} \tag{75}$$

Instead of numerically computing $y = \mathcal{A}^{-1}(x)$ for given x by solving for y from $A(y) = x$, an approximation formula is used in practice. A Taylor series is not an option since it gives poor approximation close to the singular point $x \pm 1$. Padé approximations have been proposed, however [5] suggests the simple formula

$$\mathcal{A}^{-1}(x) = \begin{cases} 1.31446\tan(1.58986x) + 0.91209x & |x| < 0.84136 \\ \frac{1}{\mathrm{sgn}(x)-x} & 0.84136 \le |x| < 1 \end{cases} \tag{76}$$

From this, the derivatives are

$$(\mathcal{A}^{-1})'(x) = \begin{cases} \frac{1.31446\times 1.58986}{\cos^2(1.58986x)} + 0.91209 & |x| < 0.84136 \\ \frac{1}{(\mathrm{sgn}(x)-x)^2} & 0.84136 \le |x| < 1 \end{cases} \tag{77}$$

$$(\mathcal{A}^{-1})''(x) = \begin{cases} \frac{2\times 1.31446\times 1.58986^2 \sin(1.58986x)}{\cos^3(1.58986x)} & |x| < 0.84136 \\ \frac{2}{(\mathrm{sgn}(x)-x)^3} & 0.84136 \le |x| < 1 \end{cases} \tag{78}$$

4 The objective function

In (19), the objective function was defined. Upon differentiating, we obtain

$$\mathcal{F}(p,q) = \frac{1}{2}\sum_i^{N^{\mathrm{obs}}} c_i[\sigma(p,q)(\bar{t}_i) - \sigma_i^{\mathrm{obs}}]^2 \overset{\mathrm{def}}{=} \frac{1}{2}\sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]^2\Big|_{\bar{t}_i} \tag{79}$$

$$\mathcal{F}'_p(p,q) = \sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]\underline{\sigma}'_p(p,q)\Big|_{\bar{t}_i} \tag{80}$$

$$\mathcal{F}'_q(p,q) = \sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]\sigma'_q(p,q)\Big|_{\bar{t}_i} \tag{81}$$

$$\mathcal{F}''_{pp}(p,q) = \sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]\underline{\sigma}''_{pp}(p,q) + c[\underline{\sigma}'_p(p,q)][\underline{\sigma}'_p(p,q)]^{\mathrm{T}}\Big|_{\bar{t}_i} \tag{82}$$

$$\mathcal{F}''_{pq}(p,q) = \sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]\underline{\sigma}''_{pq}(p,q) + c[\underline{\sigma}'_p(p,q)]\sigma'_q(p,q)\Big|_{\bar{t}_i} \tag{83}$$

$$\mathcal{F}''_{qq}(p,q) = \sum_i^{N^{\mathrm{obs}}} c[\sigma(p,q) - \sigma^{\mathrm{obs}}]\sigma''_{qq}(p,q) + c[\sigma'_q(p,q)]^2\Big|_{\bar{t}_i} \tag{84}$$

where

$$\sigma(p,q) = f^{(\mathrm{A})}(p,\lambda) + f^{(\mathrm{B})}(p,\lambda^{\mathrm{e}}(q)) \tag{85}$$

$$\underline{\sigma}'_p(p,q) = (\underline{f}^{(\mathrm{A})})'_p(p,\lambda) + (\underline{f}^{(\mathrm{B})})'_p(p,\lambda^{\mathrm{e}}(q)) \tag{86}$$

$$\sigma'_q(p,q) = (\lambda^{\mathrm{e}})'_q(q)(f^{(\mathrm{B})})'_{\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q)) \tag{87}$$

$$\underline{\sigma}''_{pp}(p,q) = (\underline{f}^{(\mathrm{A})})''_{pp}(p,\lambda) + (\underline{f}^{(\mathrm{B})})''_{pp}(p,\lambda^{\mathrm{e}}(q)) \tag{88}$$

$$\underline{\sigma}''_{pq}(p,q) = (\lambda^{\mathrm{e}})'_q(q)(\underline{f}^{(\mathrm{B})})''_{p\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q)) \tag{89}$$

$$\sigma''_{qq}(p,q) = (\lambda^{\mathrm{e}})''_{qq}(q)(f^{(\mathrm{B})})'_{\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q)) + [(\lambda^{\mathrm{e}})'_q(q)]^2(f^{(\mathrm{B})})''_{\lambda^{\mathrm{e}}\lambda^{\mathrm{e}}}(p,\lambda^{\mathrm{e}}(q)) \tag{90}$$

recall that $(\lambda^{\mathrm{e}})(q) = (1+q)^{-1}\lambda \rightsquigarrow (\lambda^{\mathrm{e}})'_q(q) = -(1+q)^{-2}\lambda$ and $(\lambda^{\mathrm{e}})''_{qq}(q) = 2(1+q)^{-3}\lambda$.

For the dual computation of sensitivities, we need

$$\mathcal{F}''_{p\sigma^{\mathrm{obs}}}(p,q) = -\sum_{i}^{N^{\mathrm{obs}}} c\underline{\sigma}'_p(p,q)\Big|_{\bar{t}_i} \tag{91}$$

$$\mathcal{F}''_{q\sigma^{\mathrm{obs}}}(p,q) = -\sum_{i}^{N^{\mathrm{obs}}} c\sigma'_q(p,q)\Big|_{\bar{t}_i} \tag{92}$$

5 Verification

The expressions given in this report have been verified by comparing analytical results with results from numerical differentiation using the following finite difference schemes

$$\frac{\partial g(x,y)}{\partial x} \approx \frac{g(x+d_x,y) - g(x-d_x,y)}{2d_x} \tag{93}$$

$$\frac{\partial^2 g(x,y)}{\partial x^2} \approx \frac{g(x+d_x,y) - g(x,y) + g(x-d_x,y)}{d_x^2} \tag{94}$$

$$\frac{\partial^2 g(x,y)}{\partial x \partial y} \approx \frac{g(x+d_x,y+d_y) - g(x+d_x,y-d_y) + g(x-d_x,y+d_y) - g(x-d_x,y-d_y)}{4d_xd_y} \tag{95}$$

REFERENCES

[1] B. Vexler. *Adaptive Finite Element Methods for Parameter Identification Problems.* PhD thesis, University of Heidelberg, 2004.

[2] H. Johansson and K. Runesson. Parameter identification in constitutive models via optimization with a posteriori error control. *International Journal for Numerical Methods in Engineering*, 62(10):1315–1340, 2005.

[3] H. Johansson and K. Runesson. Calibration of a class of nonlinear viscoleasticity models with sensitivity assessment based on duality. *In preparation for submission to International Journal for Numerical Methods in Engineering*, 2005.

[4] J.S. Bergström and M.C. Boyce. Constitutive modeling of the large strain time-dependent behavior of elastomers. *Journal of the Mechanics and Physics of Solids*, 46:931–954, 1998.

[5] J.S. Bergström. *Large Strain Time-Dependent Behavior of Elastomeric Materials.* PhD thesis, Massachusetts institute of technology, 1999.

[6] J.S. Bergström and M.C. Boyce. Large strain time-dependent behavior of filled elastomers. *Mechanics of Materials*, 32:627–644, 2000.

[7] E.M. Arruda and M.C. Boyce. A three-dimensional constitutive model for the large stretch behaviour of rubber elastic materials. *Journal of the Mechanics and Physics of Solids*, 41(2):389–412, 1993.