HERMITE finite elements in numerics of second gradient elasticity

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Abstract

In order to account for the so-called size effect in micro-/nanomaterials, second gradient continuum theories are promising and used in elasticity to a great extent. Additional material length scale parameters are introduced and the problems of static beam and plate bending are analyzed. Moreover, it is attempted to look at the EINSTEIN–DE-HAAS–effect from that end. To be more specific, body-couples are applied to a solid and connected to second gradients of displacements. Balance equations of a generalized continuum theory are presented and higher-order stress-strain relations are derived. In order to account for second gradients of displacements, which manifest themselves in the higher-order strain energy density, a global C^1–continuous displacement field is desirable as a solution. The so-called HERMITE finite element formulation allows for merging gradients between the elements and therefore is a good candidate in order to achieve at least node-wise C^1–continuity. Element stiffness matrices as well as global stiffness matrices are developed for some specific elastic problems. Convergence, C^1–continuity, and the size effect are demonstrated in each numerical simulation. The resultant material behavior is compared to experiments for the bending stiffness of differently sized micro-beams made of the polymer SU-8.

Keywords: continuum mechanics, computational mechanics, second gradient elasticity, size-effect, Hermite finite elements

1. Introduction

Materials with intrinsic micro or nano-structure may show size-dependent material behavior, which is reflected, *e.g.*, in a stiffer elastic response to external forces, when the size of the material body is reduced. A quantitative understanding of a size effect is of great importance when modeling Micro- and Nano-Electro-Mechanical Systems (MEMS/NEMS). Driven by the miniaturization as an improvement of the performance of MEMS, the requirement of reliability in simulation techniques increases. Experimental validation therefore is given in, *e.g.*, [1, 2, 3, 4]. Second Gradient (SG) continuum theories can be used, if the elastic deformation behavior of the material body depends on the thickness, while in the absence of strain gradients (*e.g.*, in uniaxial tensile tests [2]) it is not used. Those materials are referred to as "non-simple materials of the gradient type" and are in reality, for example, polymers at a small scale. Since conventional continuum theories based on the CAUCHY continuum are not able to predict size effects, the present work deals with the *Modified Strain Gradient theory* (MSG) developed in, *e.g.*, [5, 6]. The application of conventional Finite Element (FE) strategies may lead to inaccurate results if finite element formulations are used, which only fulfill global C^0–continuity. The scope of this work is, to develop FE formulations based on HERMITE polynomials in order to fulfill node-wise C^1–continuity of the solution.

2. A second gradient theory of elasticity

2.1. Strain energy formulation

The EINSTEIN summation convention is used on repeated indices and spatial partial derivatives in the Cartesian coordinate system are denoted by comma-separated indices. The present work is based on one of the three reduced forms of the strain energy densities for small deformations, u^{SG}, as postulated by MINDLIN (1962) [5]. A modified strain gradient energy density (acc. to [7, 8, 9]) is derived from MINDLIN's second form of a linear isotropic strain energy density:

$$\begin{aligned} u^{\mathrm{MSG}} &= 2G\varepsilon_{ij}\,\varepsilon_{ij} + \lambda\varepsilon_{kk}\,\varepsilon_{ii} + 2G\ell_0^2\varepsilon_{mm,i}\,\varepsilon_{kk,i} + \\ &\quad + 2G\ell_1^2\eta^{(1)}_{ijk}\,\eta^{(1)}_{ijk} + 2G\ell_2^2\chi^{\mathrm{S}}_{ij}\,\chi^{\mathrm{S}}_{ij}\ , \end{aligned} \tag{1}$$

where λ and G are LAMÉ's constants, whereas ℓ_0, ℓ_1 and ℓ_2 denote additional material length scale parameters. These parameters are of the dimension of squared length in order to guarantee a positive definite problem in the energy minimization. The normalization of the higher-order terms by G is arbitrary. With respect to a formulation of the problem in terms of displacements u_i, the strain and higher-order strain tensors are:

$$\begin{aligned} &\varepsilon_{ij} = \tfrac{1}{2}\left(u_{i,j} + u_{j,i}\right)\ , \quad \chi^{\mathrm{S}}_{ij} = \tfrac{1}{4}\left(\epsilon_{ilk}\,u_{k,lj} + \epsilon_{jlk}\,u_{k,li}\right)\ , \\ &\eta^{(1)}_{ijk} = \tfrac{1}{3}(u_{k,ij} + u_{i,jk} + u_{j,ki}) - \tfrac{1}{15}\big(\delta_{ij}\left(u_{k,mm} + u_{m,mk} + u_{m,km}\right) \\ &\quad + \delta_{jk}\left(u_{i,mm} + u_{m,mi} + u_{m,im}\right) + \delta_{ki}\left(u_{j,mm} + u_{m,mj} + u_{m,jm}\right)\big). \end{aligned} \tag{2}$$

2.2. Deformation assumptions

The present work deals with the following restrictions to the displacement field in order to derive partial differential equations (PDE) and their weak forms by the help of variational calculus.

- EULER-BERNOULLI beams

$$u_1 = -x_3\frac{\mathrm{d}w}{\mathrm{d}x_1}\ ,\ u_2 = 0\ ,\ u_3 = w(x_1) \tag{3}$$

- TIMOSHENKO beams

$$u_1 = -x_3\phi(x_1)\ ,\ u_2 = 0\ ,\ u_3 = w(x_1) \tag{4}$$

- KIRCHHOFF-LOVE plates

$$u_1 = -x_3\frac{\partial w}{\partial x_1}\ ,\ u_2 = -x_3\frac{\partial w}{\partial x_2}\ ,\ u_3 = w(x_1, x_2) \tag{5}$$

- and plane strain assumptions

$$u_3 = 0\ ,\ \frac{\partial u_i}{\partial x_3} = 0\ . \tag{6}$$

3. C^1–continuous finite element approach

3.1. *Governing differential equations*

The reduced generalized balance equations of (linear) momentum and spin [10],

$$\sigma_{ij,i} = 0\,, \qquad \mu_{ij,i} = -\rho l_j\,, \tag{7}$$

where μ_{ij} is the couple stress tensor and l_j the body-moments, are used to derive the following PDEs: The weak form for EULER-BERNOULLI beams is

$$Sw''v'' + Kw'''v''' = 0\,, \tag{8}$$

where S and K are constants that include geometry and material coefficients, and $v(x_1)$ denotes the test-function (variation of w). The system of PDEs for TIMOSHENKO beams read

$$\begin{aligned} \left[T(\phi - w') - K\phi'' - Nw'' + S\phi^{\mathrm{IV}}\right] &= -m(x_1)\,,\\ \left[T(w'' - \phi') + Pw^{\mathrm{IV}} + N\phi'''\right] &= q(x_1)\,, \end{aligned} \tag{9}$$

where T, N and P are constants of the system, and m and q denote force and moment distributions, respectively. The PDE for KIRCHHOFF-LOVE plates becomes

$$R\Delta\Delta\Delta w(x_1,x_2) + H\Delta\Delta w(x_1,x_2) = p(x_1,x_2)\,, \tag{10}$$

where Δ is the Laplacian, R and H are system constants and p is the load distribution prependicular to the plate.

3.2. *HERMITE finite elements*

HERMITE finite elements consist of the HERMITE polynomials

$$\begin{aligned} H_1 &= 2\zeta^3 - 3\zeta^2 + 1\,, \qquad & H_2 &= \zeta^3 - 2\zeta^2 + \zeta\,,\\ H_3 &= -2\zeta^3 + 3\zeta^2\,, \qquad & H_4 &= \zeta^3 - \zeta^2, \end{aligned} \tag{11}$$

which are linearly superposed and multiplicatively connected to form either 1D or 2D trail- and test-functions w^{e} and v^{e} per element, e,

$$v^{\mathrm{e}}(\zeta,\xi) = \sum_{\alpha=1}^{4}\sum_{\beta=1}^{4} H_\alpha H_\beta\,, \quad w^{\mathrm{e}}(\zeta,\xi) = \sum_{\delta=1}^{4}\sum_{\gamma=1}^{4} c^{\mathrm{e}}_{\delta\gamma} H_\delta H_\gamma\,. \tag{12}$$

By inserting them into one of the respective weak form, we worked out the element's stiffness matrix for equidistantly distributed elements.

3.3. *Results*

t	W	L	E	$\ell_0 = \ell_1 = \ell_2$	F
100 µm	$2t$	$20t$	1.44 GPa	17.6 µm	1 µN

Table 1: Thickness t, width W, length L, elastic modulus E, material length scale parameters ℓ and the force F used for the beam simulations.

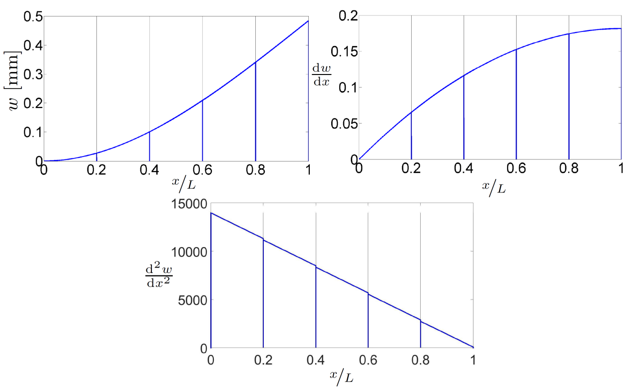

Figure 1: Plot of the C^1–continuous bending line w of an EULER-BERNOULLI beam, solved with five elements and its first and second derivative.

The curves in Fig. 1 represent the exact HERMITE base polynomials, without any interpolation. Convergence and size effect behavior can be shown to be fulfilled.

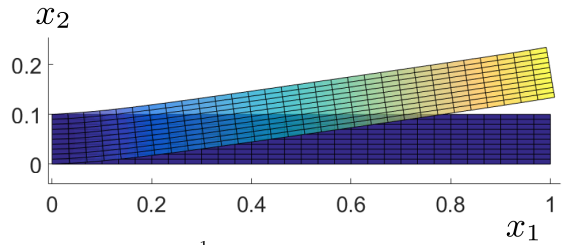

Figure 2: Plot of the C^1–continuous displacements for the plane strain assumptions, loaded only by the body-couples l_3.

The EINSTEIN–DE-HAAS effect exposes a relationship between magnetism, angular momentum, and the spin of elementary particles, driven by an external magnetic field. This effect gives rise to a simulation how body-couples (or -moments) will act on a beam, *cf.*. Fig. 2. There, a field of specific static moments penetrates the beam, which is fixed at one end and free at the other. As a result, the beam bends.

4. Conclusions

A modified second gradient continuum theory of elasticity was elaborated. Different restrictions on the displacement field were carried out in order to derive the corresponding partial differential equations and weak forms, respectively. In order to keep the first derivative of the solution continuous we discretized the problem using HERMITE finite elements. It follows that the resulting FE approximations show a size effect, as expected from the higher-order theory, as well as convergence in terms of increasing degrees of freedoms in the FE algorithm. This will allow us simulating elastostatic problems of arbitrary geometries for micromechanical applications, when considering a higher-order material behavior. So far this approach is restricted to equidistantly constructed meshes, and it is accompanied by a larger number of element coefficients than in conventional FEM.

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