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Modeling single crystals: time integration, tangent operators, sensitivity analysis and shape optimization

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Abstract

In this paper, a comprehensive overview of the numerical analysis of single crystalline materials at high temperatures is presented, including implicit higher order time integration, consistent linearization and respective sensitivity analysis. Both a phenomenological and a crystallographic model are employed to simulate the mechanical isothermal behavior of the nickel-based superalloy CMSX-4 at 950°C in a finite element environment. A shape optimization methodology for testing specimen design based on extensive finite element computations is presented. The sensitivity analysis according to the chosen time integration scheme is performed leading to an algorithm for simultaneous analysis and design (SAND). Examples for the shape optimization of a cruciform specimen for biaxial tensile experiments at high temperatures are given and discussed in detail.

Keywords: B. Single crystals; B. Elastic–viscoplastic materials; C. Finite elements; C. Optimization; Sensitivity analysis

1. Introduction

Single crystalline materials are typically used for high temperature applications, where polycrystalline alloys fail due to the weakening effects of grain boundaries acting as dislocation sources in highly loaded states. These so-called *superalloys* exhibit a pronounced anisotropic elastic *and* viscoplastic behavior under mechanical

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loading. Special material models of unified type are utilized for the description of such phenomena. The development of these alloys is mainly motivated from applications in gas turbines and aircraft engines. The energetic ratio of efficiency of these constructions is principally dependent on the maximum process temperature where consideration of the Carnot process allows for a simple estimate of a theoretical maximum efficiency. The higher the temperature in the first row of vanes is, the greater the theoretical maximum efficiency is.

Material models for such alloys are intensively discussed in current research. The following list of publications is by far not complete, it is rather a brief sketch of selected research topics associated with single crystalline materials. The short time viscoplastic behavior of such alloys is for example investigated by Choi and Krempl (1989), Sutcu and Krempl (1990), Dane and Stouffer (1988) or Jordan and Walker (1992). All models are based on some kind of Hill-type plasticity and referred to as *first generation models*. Méric et al. (1991), Nouailhas and Culié (1991) and Nouailhas and Cailletaud (1995) proposed anisotropic models at small strains of the *second generation* with Chaboche-type hardening variables motivated from micromechanical observations on slip system levels on an atomistic length scale λ^* (cf. Fig. 1). Forest et al. (1997) formulated an extension to large deformations in a Cosserat framework. However, Shu (1998) considers size effects in single crystalline structures. Creep deformations on a large time scale are modeled, for instance, by Brehm and Glatzel (1998) and Qi and Bertram (1997). Balke and Estrin (1994) concentrate on the development of shear bands leading to a macroscopic failure of the assembly. An approach towards an efficient numerical assessment of these models in a finite element context was given by Cuitiño and Ortiz (1992). A methodology for the determination of suitable sets of material parameters for these complex material models was proposed by Kunkel and Kollmann (1996), who concentrated on the Choi and Krempl (1989) model with not less than 30 free parameters.

This short overview on research activities concerns mainly the mechanical modeling. Numerical approaches specially for single crystals are not yet that elaborated. Kirchner and Simeon (1999) present an implicit higher order time integration scheme and apply it successfully to a first generation model. Recently, Kirchner (1999) gave a generalization of this approach allowing for straightforward application to (almost) any kind of small strain plasticity models, provided an additively decomposable strain measure is used. Herein, the most important points of the argumentation will be reviewed to demonstrate the necessities to fulfil in order to apply this quite simple but nevertheless efficient method in plasticity.

One problem for single crystalline materials at high temperature is the experimental testing and respective identification of the model parameters. Circular cross sections perpendicular to the specimen axis do not necessarily remain circular shaped under uniaxial tensile loading which is obviously in contradiction to the classical assumption usually met for isotropic materials (see, for instance, Anand and Kothari, 1997) that the uniaxial deformation in the measuring length of the specimen is homogeneous. It is therefore necessary to account for the resulting inhomogeneity in a sophisticated identification procedure. More elaborated two- and three-dimensional tests and respective identification procedures are thus needed. The