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Modeling the thermoelastic–viscoplastic response of polycrystals using a continuum representation over the orientation space

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Abstract

Conventional methodologies towards polycrystal plasticity use an aggregate of single crystals and this choice of the aggregate affects the response of the polycrystal. In order to address this issue, a continuum approach is presented for the representation of polycrystals through an orientation distribution function over the orientation space. Additionally, a constitutive framework for thermoelastic–viscoplastic response of metals based on polycrystal plasticity is presented along with a coupled macro–micro, fully implicit Lagrangian finite element algorithm. Numerical examples that highlight the accuracy, performance and benefits of the proposed approach are presented.

Keywords: Crystal plasticity; Orientation distribution function; Lagrangian analysis; Finite elements; Thermo-mechanical processes

1. Introduction

Material properties and processing techniques are severely affected by the underlying microstructural features in the material. These microstructural features

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include texture, grain sizes and shapes, grain boundary motion and secondary phase particles, etc., and their adequate representation is necessary for an accurate prediction of material response. Polycrystal models have primarily characterized the polycrystal through a discrete aggregate of crystals, as in Bronkhorst et al. (1992), Kalidindi et al. (1992), Maniatty et al. (1992), Beaudoin et al. (1993), Maniatty and Yu (1996), Kothari and Anand (1998), Marin and Dawson (1998) and Balasubramanian and Anand (2002). This approach works on the idea of combining discrete, preselected, single crystal responses with a suitable macro–micro linking hypothesis. Such discrete aggregate models, though simple, do not characterize texture effectively. There also exists no means by which one can compare and quantify differences between textures associated with distinct discrete aggregates. An alternate approach is a continuum representation of crystals based on quantifying texture through an ODF (orientation distribution function) which expresses the distribution of crystal orientations over the orientation space (Clément, 1982). In these methods, the evolution of a polycrystal generally demands the numerical solution of an ODF conservation equation. Some of the implementation techniques are based on the series representation of the ODF through schemes like spherical harmonics, infinite polynomial series or tensorial Fourier series. These schemes are not only complex but also lack the capability to adequately represent sharp textures. In order to overcome the above-mentioned difficulties, the approach developed in Kumar and Dawson (1996, 1997, 2000), Acharjee and Zabaras (2003) and Ganapathysubramanian and Zabaras (2004) is used, where the ODF was defined through finite element piecewise polynomial functions over an explicit discretization of the orientation space. The advantages of such an approach are substantial and are discussed in Kumar and Dawson (1997) and Ganapathysubramanian and Zabaras (2004).

Over the last four decades, researchers have been interested to study the plastic anisotropy developed during deformation and to formulate models that predict the experimentally observed behavior, see for example Hutchinson (1969), Kocks et al. (1975, 1976), Lubarda and Lee (1981), Frost and Ashby (1982), Pierce et al. (1983), Asaro and Needleman (1985), Boyce et al. (1989), Rashid and Nemat-Nasser (1990), Aravas and Aifantis (1991), Cuitiño (1992), Prantil et al. (1993), Beaudoin et al. (1994) and Steinmann and Stein (1996). Most models for crystalline materials are restrictive in the sense of a limited operating region of processing conditions. However, almost all modern applications of interest lie in a very broad operating regime – from quasi-static strain rate applications to ballistic applications (Hoge and Mukherjee, 1977; Beaudoin et al., 1993), and from cold rolling of plates to hot forging of engine components. Elastic effects have also been neglected in many studies at large plastic strains, for example in Beaudoin et al. (1993, 1994) and Marin and Dawson (1998), even though it has been shown by Maniatty and Yu (1996) that these elastic effects do play a significant role.

Critical investigations to develop accurate descriptions of material behavior (incorporating thermal response) include Kocks et al. (1975) and Frost and Ashby (1982). In order to model thermal effects, it is necessary to understand the thermal activation of dislocations. The activation rate of dislocation events depends on the