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A study of a fully implicit integration algorithm for a rate-independent single crystal plasticity with dislocation density

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ABSTRACT

A fully implicit stress integration algorithm for a rate-independent single crystal plasticity with dislocation density is presented and its computational efficiencies are investigated within the numerical simulations of single crystal and polycrystalline aggregate.

The non-classical single crystal plasticity models based on the dislocation mechanism have been developed for the characterization of the single crystal material behavior consistent with the experimental and theoretical knowledge. Also both macro- and microscopic material behavior can numerically be reproduced, applying such constitutive model to two-scale finite element analysis. In the two-scale analysis, the intra- and intergrainular deformations play an important role in associating the heterogeneous stress and strain fields inside grain with dislocation mechanism. In the nature of the modeling methodology, the numerical analysis demands high resolution, i.e. fine discretization at each grain for the accurate evaluation. And then it becomes not only high nonlinear and heterogeneous but also computationally expensive. Therefore it is essential to improve the computational performance in the calculation of the constitutive model. Terada and Watanabe[1] applied the implicit computational methodology with the return-mapping algorithm and the exponential discretization of deformation gradient to a classical rate-independent single crystal elastoplasticity at finite strain and examined the computational performance. With their approach, the discretization error can be almost completely removed. The algorithm is expected to be effective in a newly-proposed single crystal plasticity. And so we derive an implicit algorithm for a rate-independent single crystal plasticity which contains the dislocation density as an internal variable with the computational framework proposed by Terada and Watanabe[1] in this study.

In the rate-independent single crystal plasticity, the yield criterion of each slip system is described as a difference between the resolved shear stress $\tau^{(\alpha)}$ and the critical resolved shear stress $q^{(\alpha)}$. Following the Bailey-Hirsch model extended to single crystal plasticity[2], the critical resolved shear stress for the α-th slip system is defined as

$$q^{(\alpha)} := \tau_0 + a\mu b\sqrt{\sum_{\beta=1}^{n_{\mathrm{slip}}} \Omega^{(\alpha\beta)}\rho^{(\beta)}} = \tau_0 + a\mu b\frac{c}{\bar{x}^{(\alpha)}} \qquad \forall\, \alpha \in \{1, 2, \cdots, n_{\mathrm{slip}}\} \tag{1}$$

where τ_0 is the resistance irrespective of the dislocation mechanics (or the initial yield stress), $a,\ c$ are material constants, μ is elastic shear constant, b is a magnitude of Burgers vector, $\Omega^{(\alpha\beta)}$ is an interaction matrix for dislocation density of each slip system, $\rho^{(\alpha)}$ and $\bar{x}^{(\alpha)}$ are the dislocation density and the mean free path of dislocation of α-th slip system respectively, and n_{slip} is the number of slip systems. In addition to equation (1), we employ the relationship between the dislocation density $\rho^{(\alpha)}$ and the accumulated plastic slip $\xi^{(\alpha)}$ on α-th slip plain[3].

$$\xi^{(\alpha)} = \rho^{(\alpha)} b \bar{x}^{(\alpha)} \qquad \forall\ \alpha \in \{1, 2, \cdots, n_{\mathrm{slip}}\} \tag{2}$$

We here formulate the computational algorithm of these constitutive equations with the principle of maximum dissipation and the associated flow rule, based on the framework of multi-surface plasticity. The employment of equation (2) is regarded as attaching the compatibility equations for dislocation density, corresponding to yield criterions in the rate-independent crystal plasticity. As shown in equation (1), the mean free path of dislocation of α-th slip system $\bar{x}^{(\alpha)}$ involves the dislocation densities of every slip systems, expressed in nonlinear form. The nonlinear simultaneous equation related with the dislocation densities and the accumulated plastic slips must numerically be solved again.

For the verification and demonstration of proposal algorithm, firstly the basic features of the constitutive model and the computational performance of the proposed computational algorithm are examined in the numerical analyses of single crystal. Afterward the constitutive model of single crystal is applied to two-scale finite element analysis method[4] for the simultaneous evaluation of macro- and microscopic material behavior. Finally we carry out numerical experiment of polycrystalline metals and discuss the computational performance in the two-scale analysis.

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