Modelling of plastic deformation of metal crystals by using the energy criterion of path stability

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In solving rate-independent plasticity problems at finite deformation, there is a difficulty related to non-uniqueness of incremental solutions. In the crystal plasticity problems, the non-uniqueness appears already at a material point level when the set of active slip-systems is to be determined for an indefinite slip-system interaction matrix. By employing the concept of path stability, the solution of physical meaning can be selected using the computational approach based on the incremental energy minimization. However, this requires the incremental update problem to be converted first to a potential problem, which has been achieved in [1] by including the proposed selective symmetrization of the slip-system interaction matrix. Here, the incremental problem of crystal plasticity is of non-potential type on account of the preserved non-symmetry of the interaction matrix.

A new computational algorithm for calculations of the time-independent response of metal crystals is presented, based on the recently proposed quasi-extremal energy principle (QEP) [2]. The criterion of path stability embedded in the QEP provides the method of selection of the solution among multiple alternatives. The major difference with respect to [1] is that the present approach does not require any symmetrization. Nevertheless, it has been shown that only minor modifications of the previous computational algorithm are needed to extend it to the non-potential problem of crystal plasticity handled by the QEP. The augmented Lagrangian method has been applied to solve the minimization subproblem of QEP and implemented within the Wolfram *Mathematica* environment.

Effectiveness of the algorithm is demonstrated by the examples of large deformation of a (fcc) metal crystal. The approach enables step-by-step simulation of the material response along with crystallographic lattice rotations and related multiple automatic changes of active slip-systems. Along the stable solution paths, the number of simultaneously active slip systems never exceeded five. In uniaxial tension in a high-symmetry orientation, as opposed to rate-dependent models, only single or double slip activity is predicted due to the instability of a fully symmetrical deformation path.

References

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