A computational crystal plasticity framework based on dislocation transport

H. Hernández[1,2], T.J. Massart[1], R.H.J. Peerlings[2], and M.G.D. Geers[2]

hhernand@ulb.ac.be, thmassar@ulb.ac.be, R.H.J.Peerlings@tue.nl, M.G.D.geers@tue.nl

(1) *Université Libre de Bruxelles.* (2) *Technische Universiteit Eindhoven.*

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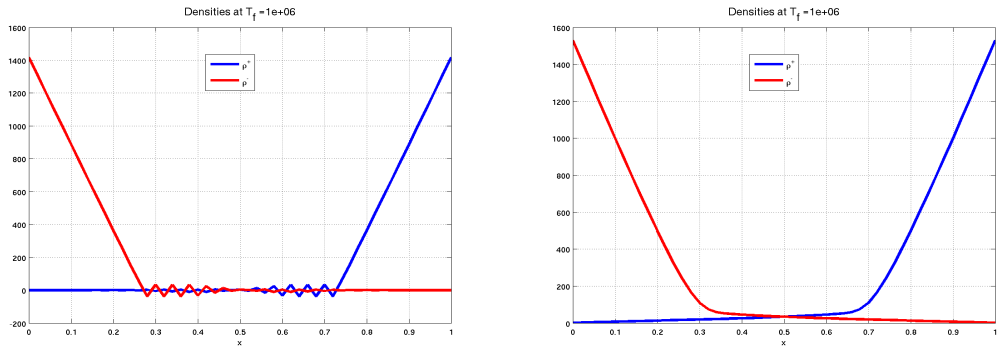
Crack initiation in crystalline materials often occurs at the boundaries between individual crystals. An important cause for this failure mechanism is that grain boundaries act as weak barriers for plastic slip. As a consequence, dislocations, which are the carriers of plastic slip, may pile-up against them, thus causing elevated local stresses. In order to properly model such stress fields, recent approaches have been developed using a higher-order crystal plasticity model which accounts for the presence and transport of dislocations in terms of dislocation densities [3, 4]. The macroscopic continuum description of the interactions of these dislocations can be expressed in terms of densities of dislocations, as illustrated in [2, 5], as a set of coupled non-linear partial partial differential equations dominated by advection. This latter feature introduces several numerical difficulties compromising the successful use of such models.

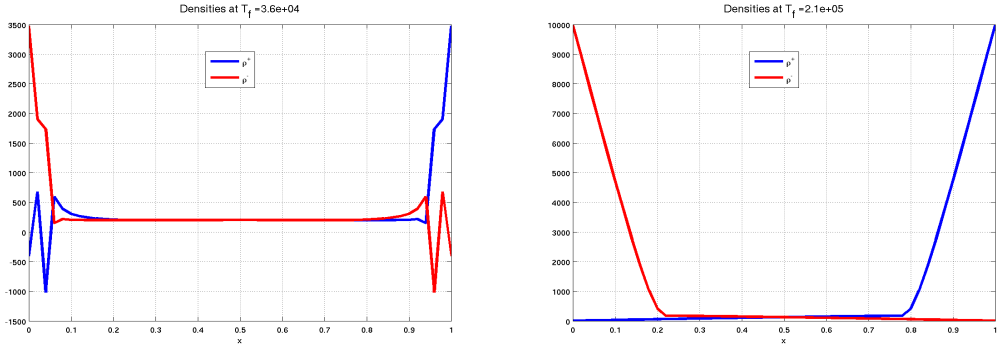
In order to overcome the difficulties associated with advection dominated problems, several stabilization techniques have been developed and are available in the literature [1, 6]. The vast majority of them developed in the context of the finite element methods have as final goal the numerical approximation of the Navier-Stokes or other sets of equations of interest for the fluid dynamics community. However, some important differences between the fluids case and the dislocation transport equations exist, such as the type of boundary conditions, the presence of the non-linearity or the nature of the coupling between the principal variables. These aspects make some of the most popular and classical stabilization techniques unsuited in the present situation if applied in a straightforward manner.

For this reason, in the first part of this project, we have developed a stabilization technique which is able to deal with the problem at hand. As a first result we show in figures 1 and 2 the distribution of densities of positive and negative dislocations for a one-dimensional benchmark problem. The two figures correspond to the case when a one-dimensional layer is subjected to shear stresses of $\sigma = 0.1\ GPa$ for Figure 1, and $\sigma = 1.0\ GPa$ for Figure 2. When increasing σ, the problem becomes more dominated by advection, causing the appearance of boundary layers which in turn harm the stability of the numerical scheme. This causes the appearance of oscillations if classical finite elements are used on a too coarse mesh, as can be observed on the left part of the figures. The right plots correspond to the case for which our stabilization technique has been applied. It can be observed that the numerical approximations



(a) Classical (b) Stabilized

Figure 1: Densities of dislocations with $\sigma = 0.1\ GPa$



(a) Classical (b) Stabilized

Figure 2: Densities of dislocations with $\sigma = 1.0\ GPa$

obtained are non-negative, smooth and free of any oscillation. The same mesh has been used in all cases. This allows envisioning the use of the developed technique for the simulation of crystalline materials with a tractable computational effort.

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