Modeling of the mechanical behavior of interfaces by using strain gradient plasticity

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Reason is not automatic. Those who deny it cannot be conquered by it. Do not count on them. Leave them alone.

Ayn Rand

There is nothing that can be said by mathematical symbols and relations which cannot also be said by words. The converse, however, is false. Much that can be, and is, said by words cannot successfully be put into equations, because it is nonsense.

Clifford Truesdell
Preface

The research presented in this licentiate thesis was carried out at the Department of Solid Mechanics at the Royal Institute of Technology (KTH) between May 2006 and October 2009. The work have been financially supported by the Swedish Research Council (Vetenskapsrådet) which is gratefully acknowledged.

I would like to take the opportunity here to give thanks to a few people who have made it possible for me to sit here and write this. My deep gratitude goes to my two thesis advisors, Prof. Peter Gudmundson and Dr. Jonas Faleskog. Prof. Gudmundson put his trust in me and employed me to do research with him in this very exciting project. Later when Prof. Gudmundson had to quit the project Dr. Faleskog took over and have, these last two years, proved to be immensely important to me as a scientific mentor, discussion partner, motivator and colleague.

I also feel I need to thank Prof. Mårten Olsson and the late Prof. Fred Nilsson who both encouraged me to dive into the world of research after my masters degree.

I should also – to be fair – list all of my fellow PhD-students (past and present) and all the other people at the department as they have been, and are, a great driving force for me. This would be quite tedious for the reader so I will refrain from it, but there is one who deserves a special mention; Dr. Per Fredriksson. During my first year and a half at the department he was more or less constantly having to answer questions that I had, and he did it without ever getting tired and always showing great insight into some of the most complicated issues I could come up with to pester him with. The discussions we had have been invaluable to me.

This section would not be complete without mentioning my friends, both my old friends here in Sweden who have stuck with me for such a long time now, and my new friends from my travels all over the world. You are, to borrow freely from Shakespeare, like an ever-fixed mark that looks on tempests and is never shaken. You are the star to the wandering bark of my life, whose worth’s unknown although its height be taken. You have proved to be a source of inspiration, laughs, friendship and love and you have had great patience with me, such that I could not live without it now once I have known it.
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Stockholm, October 2009
List of appended papers

**Paper A:** Hardening and softening mechanisms at decreasing microstructural length scales  
Carl F. O. Dahlberg and Peter Gudmundson  
*Philosophical Magazine* 88, 2008, 3513–3525

**Paper B:** Energetic interfaces and boundary sliding in strain gradient plasticity; investigation using an adaptive implicit finite element method  
Carl F. O. Dahlberg and Jonas Faleskog  
*To be submitted for international publication*

In addition to the appended papers, the work has resulted in the following publications and presentations:

1. **Längdskaleberoende för plastisk deformation av laminat**  
Carl F. O. Dahlberg and Peter Gudmundson  
Presented at Svenska Mekanikdagar, Luleå 2007 (A,P)

2. **Hardening and softening mechanisms at decreasing microstructural length scales**  
Carl F. O. Dahlberg and Peter Gudmundson  

3. **Hardening and softening in micro and nanoplasticity**  
Carl F. O. Dahlberg and Peter Gudmundson  

4. **Effekt av interna gränsytor och plastiska töjningsgradienter vid skjuvbelastning av en flerfassolid**  
Carl F. O. Dahlberg and Jonas Faleskog  
Presented at Svenska Mekanikdagar, Södertälje 2009 (A,P)

5. **Interface and plastic strain-gradient effects on the global response of a layered solid deformed in simple shear**  
Carl F. O. Dahlberg and Jonas Faleskog  
*Proc. 7th EUROMECH Solid Mechanics Conference*, Lisbon 2009 (A,P)

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1. A = Extended abstract, P = Presentation, Pp = Proceeding paper
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Introduction

During the last half century or so the trend of making things smaller and smaller have accelerated. Nowadays words like miniaturization, micro and even nano are becoming part of the everyday stock and store vocabulary of the general public. This is of course driven by the progress the scientific and engineering communities are making in fitting more things into less space. Closest at hand as an example of this are the great leaps made by the computer and microelectronics industry. But so called micro electromechanical systems (MEMS), advances in thin film coatings and nano-engineered materials can also serve as good examples of this trend.

Together with this fairly rapid development has come the equally rapid need to understand what physically happens when things get smaller. Forces, processes, interactions and mechanisms — that usually drown in the noise of the so familiar macro world around us — might all of a sudden become important when we try to understand phenomena on a smaller and smaller scale.

Small scale plasticity

Some of the first indications of a length scale dependence of material properties are due to Hall (1951) and Petch (1953). Their results, which have become known as the Hall–Petch relationship, showed that the yield stress ($\sigma_y$) of crystalline materials depends inversely on the grain size ($d$),

$$\sigma_y = \sigma_0 + k d^a$$  \hspace{1cm} (1)
where $\sigma_0$ is the yield stress of a coarse grained material, $k$ is a fitting parameter and the exponent $\alpha$ is usually taken as $-1/2$, at least above the nanometer size range.

More recently several experimental results have shown that not only grain size but other problem specific length scales might give rise to a strengthening effect with decreasing scale. Xiang and Vlassak (2006) have shown that the yield stress of thin films increase when the thickness is reduced. Their study also showed that when one or both sides of the film was passivated the strengthening effect was even greater. A passivated surface would introduce gradients in the plastic strain field, thus indicating that plastic strain gradients play a role in the strengthening.

The indentation depth, using a sharp indentor, have also been reported to introduce a size effect in the measures of hardness (see for instance Nix and Gao (1998)). This can be explained by the dependence of plastic strain gradients. The gradients introduce a length scale to the problem, which otherwise lacks all sense of scale since the sharp indentation problem is self similar and the results, according to conventional theories, should not change with depth. Another well known experiment that shows size dependence in the presence of plastic strain gradients is the wire torsion problem in Fleck et al. (1994).

**Strain gradient plasticity**

The above mentioned, and several other, experimental results indicate that at tiny length scales the gradient of plastic strain becomes important and should be taken into consideration. The attempts to incorporate this dependence into a continuum theory have given rise to many suggestions on how so called strain gradient plasticity (SGP) theories should be formulated. One of the early pioneers was Aifantis (1984, 1987) when trying to explain localization phenomena. Other influential work within the field can be attributed to Fleck and Hutchinson (1993, 1997, 2001), Gudmundson (2004) and Anand et al. (2005).

This thesis deals with the implementation and investigation of some of the modeling possibilities of the SGP theory of Gudmundson (2004). The theory is a higher order theory which means that the structure of the boundary value problem is changed at its core, as compared to the conventional continuum description, with additional terms appearing in the
principle of virtual work,

\[
\int_{\Omega} \left[ \sigma_{ij} \delta \varepsilon_{ij}^e + q_{ij} \delta \varepsilon_{ij}^p + m_{ijk} \delta \varepsilon_{ij,k}^p \right] \mathrm{d}V = \int_{\partial \Omega} \left[ T_i \delta u_i + M_{ij} \delta \varepsilon_{ij}^p \right] \mathrm{d}S,
\]

(2)

where the Cauchy stress \( \sigma_{ij} \), the elastic strain \( \varepsilon_{ij}^e \), the force tractions \( T_i \) and the displacements \( u_i \) are components of the conventional theory. However, an additional assumption is that the plastic strains \( \varepsilon_{ij}^p \) and the gradients of plastic strain \( \varepsilon_{ij,k}^p \) can contribute to the work performed in the body through their conjugated stress measures, the micro stress \( q_{ij} \) and the moment stress \( m_{ijk} \) respectively, which also leads to the need to balance this on the boundary by the work performed by the moment tractions \( M_{ij} \) and introduction of the plastic strains as variables.\(^2\)

The introduction of higher order terms necessitates the introduction of higher order boundary conditions, which in this case turns out to mean either prescribing the plastic strains or the moment tractions on the boundary \( \partial \Omega \). The augmented formulations can predict an increase in yield stress with decreased dimension in relation to some intrinsic material length scale(s) that appears naturally as a consequence of the formulation, as have been shown by Fredriksson and Gudmundson (2005, 2007).

The field of SGP is currently undergoing a maturing process and some proposed theories are gaining more support than others in light of their predictive powers and physical reasonableness. This in turn have lead to current research topics within SGP that are now more concerned with connecting it to experimental results and known and postulated physical processes. The prediction of a reasonable value of the Hall–Petch exponent, the application of realistic boundary conditions and internal interface modeling – all of which will be touched upon in this thesis.

**Grain boundary sliding**

The notion of *smaller is stronger* as indicated by the Hall–Petch relation and other strengthening mechanisms is generally accepted as a truth – on very good grounds. But, this trend

\(^2\)although in general not as an independent set of variables since \( u_{i,j} = \varepsilon_{ij}^e + \varepsilon_{ij}^p \)
can not go on forever, and there is a mounting number of research articles and experimental results indicating that at the most diminished length scales this trend stops or even reverses in what has been named the inverse Hall–Petch effect. The cause of the Hall–Petch effect is the increased resistance to dislocation movement by the decreased distance between barriers (grain boundaries, inclusions, phase boundaries and other internal interfaces) in the crystal lattice. At some point the free space for even a single dislocation to move in without encountering resistance tends to zero. When this happens some other deformation mechanism have to be activated and one suggestion is grain boundary sliding.

Early experimental evidence of a reversed Hall–Petch effect from indentation of nanocrystalline copper and palladium (Chokshi et al. (1989)) suggested grain boundary activity as the reason behind the reversal in strength. This have been at least partially backed now with the advent of molecular dynamics simulations and results showing that ultra fine grained polycrystals deform mainly at the grain boundaries, as shown in Figure 1. In Figure 2 a schematic of how the deformation mechanisms changes with length scale is presented.

![Figure 1: A change in deformation mode from dislocation mediated deformation (yellow) to grain boundary activity (red) is indicated when the grain size is reduced, from Schiotz and Jacobsen (2003).](image)

It is here natural to postulate that there are (at least) two competing deformation mechanisms for plasticity in metallic materials. One is the fairly well understood dislocation mediated plasticity which will give an increase in yield stress with decreasing length scale.
Figure 2: A deformation-mechanism map where it is shown how the dominating deformation mechanism changes, expressed in units of stress ($\sigma$) and inverse grain size ($d$). The parameters $\sigma_{\text{inf}}$ and $r_0$ are functions of the stacking fault energy and the elastic properties. Taken from Yamakov et al. (2004).

This behavior can be captured with SGP. The other is the less well known grain boundary mediated deformation, here assumed to be a irreversible slip displacement. To model this behavior, a constitutive descriptions for interface slip have to be added, so that the two phenomena may compete and predict a maximum in yield stress at some intermediate length scale.

**Numerical treatment of higher order theories**

The numerical implementation of SGP have proved to be problematic. The structure of the boundary value problem is such that it is not very straight forward to implement it into existing commercial finite element codes. Simplifying assumptions may be employed to very idealized test problems such that they admit analytical solutions, but this approach is severely restricting. To solve more general problems with SGP an explicit (Euler forward type) finite element algorithm is usually employed.
The explicit approach has several drawbacks, one being the large number of load steps needed to find a sufficiently accurate solution. The forward integration also requires finding the rates of increments of the degrees of freedom, instead of solving for the increments of the degrees of freedom directly in each load step. The problem will usually need to be artificially decoupled to find the rates of the increments and this introduces yet another approximation, leading to the need of even more load steps. Finally the explicit methods will need to be seeded with some initial solution so that the forward tangents can be established to start with, and this might have an effect on the final solution if not done with care.

In this thesis an implicit method (Euler backward type) is presented as an alternative. Together with a choice of rate dependent constitutive relations that give an initial stiffness that is finite and adaptive step size control this method proves to be very stable. The number of load steps needed to reach a solution is controlled mainly by the need to resolve the load history response and is orders of magnitude lower than the number of steps needed to solve equivalent problems with an explicit method. The inherent numerical stability of an implicit algorithm have made it possible to approach the rate independent limit with rate sensitivity exponents that again are orders of magnitude closer to rate independence than in the explicit case. The fully coupled problem is solved directly for the increments of the degrees of freedom, further reducing the numerical errors.
Summary of appended papers

**Paper A:** *Hardening and softening mechanisms at decreasing microstructural length scales.*

In this paper a laminate structure with varying lamina thickness is used as a simple model of grain size. The SGP of Gudmundson (2004) is used to predict an increased yield stress and an interface slip mechanism is introduced to model competing softening. The SGP formulation is simplified by assuming that the bulk behaves energetically in the higher order moment stress and that only the micro stress contribute to the dissipation. A rate independent deformation type theory under the assumption of monotonically increasing load leads to analytical solutions. The introduction of a interface energy does however necessitate a numerical evaluation of the solution since solving for the boundary and interface conditions requires solution of a non-linear system of equations. The introduction of the interface slip mechanism then leads to a qualitative representation of a peak in the yield stress at some intermediate lamina thickness and then a reversal of the strengthening trend.

**Paper B:** *Energetic interfaces and boundary sliding in strain gradient plasticity; investigation using an adaptive implicit finite element method.*

This paper presents an implicit finite element procedure in 1D, but it can easily be generalized to higher dimensions. The paper investigates the effects of interfaces on the macroscopic response of a layered solid deformed in simple shear. The bulk is modeled as isotropic elastic-viscoplastic, with both plastic strains and plastic strain gradients contributing to the dissipation. The interface is modeled by introduction of a free surface energy that depends on the plastic strain state at the interface, and slip is incorporated in the model in a physically more sound way than in Dahlberg and Gudmundson (2008). It is shown how the interface energy can be used to model intermediate types of boundary conditions in addition to giving rise to an energetic contribution to the hardening in the post yield behavior. Owing to the more consistent formulations of the dissipative bulk strengthening, and the competing interface slip softening, a clear maximum in macroscopic yield stress can be predicted.
Bibliography


