Journal of the Mechanics and Physics of Solids 60 (2012) 1243–1256

Contents lists available at SciVerse ScienceDirect

Journal of the Mechanics and Physics of Solids

journal homepage: www.elsevier.com/locate/jmps

# A phase field model incorporating strain gradient viscoplasticity: Application to rafting in Ni-base superalloys

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A R T I C L E I N F O

*Article history:*
Received 8 November 2011
Received in revised form
6 April 2012
Accepted 10 April 2012
Available online 16 April 2012

*Keywords:*
Phase transformation
Size effect
Phase field modeling
Strain gradient plasticity
Superalloys

A B S T R A C T

The first formulation of a phase field model accounting for size-dependent viscoplasticity is developed to study materials in which microstructure evolution and viscoplastic behavior are strongly coupled. Plasticity is introduced using a continuum strain gradient formalism which captures the size effect of the viscoplastic behavior. First, the influence of this size effect on the mechanical behavior of the material is discussed in static microstructures. Then, the dynamic coupling between microstructure evolution and viscoplastic activity is addressed and illustrated by the rafting of the microstructure observed in Ni-base superalloys under creep conditions. It is found that the plastic size effect has only a moderate impact on the shape of the rafts but is crucial to reproduce the macroscopic mechanical behavior of that particular material.



## 1. Introduction

Phase transformations play a major role for designing new materials with new properties, for improving the performance of existing materials, or defining new processes. It is indeed possible to combine the properties of different coexisting phases in an optimal way thanks to particular morphologies, which introduce internal scales besides the scale of interfaces. The phase distribution and morphology may be quite complex because they often result from complex evolutions controlled by the interaction between different phenomena: e.g. chemical diffusion, interfacial energies, mechanics (elasticity, plasticity, etc.) or electromagnetism. In the solid state, the mechanical behavior of the phases, from elasticity to elasto-viscoplasticity, has a major influence on the microstructure evolution. Indeed, phase transformations most often generate internal stresses coming from eigenstrains associated with changes in crystalline structure and in chemical composition. In the case of coherent precipitation (in the absence of plasticity) these stresses induce very anisotropic long-range interactions between precipitates at the origin of complex patterns (Khachaturyan, 1983). However, in many industrial materials, plasticity is likely to partially relax stresses when those reach the yield stress. This indeed may happen in three cases: (i) First, internal stresses can reach significant magnitudes as in bainites or martensites in steels where plasticity is responsible for the change in their morphologies (Li et al., 1998). (ii) Second, yield stresses are generally small at high temperature where diffusive phase transformations generally proceed. Hence, even rather small eigenstresses may be relaxed as during the late stage of $\gamma'$ precipitation in superalloys (Yang et al., 2007). (iii) Finally, in service, materials are often submitted to external loadings and temperature changes. In that case, the microstructure evolution and the plastic activity are also obviously coupled.

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0022-5096/$ - see front matter 
http://dx.doi.org/10.1016/j.jmps.2012.04.003

Despite some early attempts (Ganghoffer et al., 1994; Wen et al., 1996; Ganghoffer et al., 1997; Su et al., 2006) the coupling of plastic relaxation with phase transformations has not been extensively investigated so far from a modeling point of view, because this requires efficient methods to handle microstructure evolution.

These last two decades, the phase field method (PFM) has emerged as the most powerful method for such a task, especially when stresses are involved in solids. Indeed, this method has been able (i) to explain the formation of complex microstructures, such as cuboidal microstructures in Ni-base superalloys (Wang et al., 1998; Boisse et al., 2007; Boussinot et al., 2009), twin structures in martensites (Wang et al., 2004; Finel et al., 2010), chessboard structures (Le Bouar et al., 1998) or hydrides precipitation in zirconium (Thuinet and Legris, 2010) and (ii) to capture subtle kinetic processes such as the slow down of coarsening in the presence of high elastic inhomogeneity (Onuki and Nishimori, 1991) or transitions between growth modes in ternary alloys involving slow and fast diffusing species (Viardin, 2010). So, it appears natural to include plasticity into a PFM to investigate its role in phase transformations.

Because plasticity in crystals is mainly due to the movement of dislocations, several works have explicitly introduced mobile dislocations in a PFM (Rodney, 2001; Wang et al., 2001; Koslowski et al., 2002) using an analogy between a dislocation loop and a thin precipitate. Dislocations are described with continuous fields for each slip system. The main advantage of this framework is that the elastic interactions between dislocations and/or precipitates are automatically accounted for. But it has two major flaws (i) first, the dislocations cores spread over several grid spacings: consequently realistic short-range interactions between dislocations require either subnanometer grid spacings, or a discrete description as in Rodney et al. (2003). (ii) Second, mechanisms other than dislocations glides (e.g. climb and cross slips at high temperatures, or twining in materials with law stacking faults energy) are not accounted for currently.

To circumvent these drawbacks, plasticity can be introduced into PFMs through plastic strain field defined at mesoscale, supplied by internal variables such as hardening variables. As usual in continuum mechanics, evolution equations in the form of ordinary differential equations are postulated to describe plastic flow and hardening with parameters identified from experimental data. This approach has the advantage to phenomenologically include all the physical processes at the origin of plasticity. Works along this route have been only very recently proposed by several groups using mesoscale plasticity models differing by their descriptions of hardening, viscosity and plastic anisotropy.

The first attempts to couple a diffuse interface model with an isotropic plasticity model have been proposed in 2005. In Guo and Shi (2005), a PFM has been coupled to an isotropic plasticity model to study stress fields around defects such as holes and cracks. In Ubachs et al. (2005), a general formalism incorporating phase field and isotropic viscoplasticity with non-linear hardening has been proposed to investigate tin–lead solder joints undergoing thermal cycling. Since these pioneering works, similar approaches including isotropic plasticity models have been developed to study crystal growth (Uehara et al., 2007), martensites (Yamanaka et al., 2008), superalloys (Gaubert et al., 2008) and kinetics issues in diffusion controlled growth (Ammar et al., 2009, 2011). Finally, in the context of rafting in Ni-base superalloys, a few works have extended PFM with *anisotropic* plasticity model, either in a perfectly plastic model (Zhou et al., 2010), or in a crystal plasticity framework including both hardening and viscosity (Gaubert et al., 2010). It is worth mentioning that in Zhou et al. (2010), the yield stress as well as any hardening effects are not included.

Despite significant successes achieved by these models, they miss an important feature of the plastic behavior: the so-called *size effect*, also known as the Hall–Petch effect in polycrystals (Hall, 1951): the smaller the domains involved by plasticity, the harder the material. This size effect becomes significant when sizes involved are below a few microns, which is typically the case in an evolving microstructure.

The aim of the present work is precisely to demonstrate how a phase field method can be coupled to a mesoscale viscoplastic model accounting for the size effect of the plastic behavior within a framework similar to the one previously proposed by Gaubert et al. (2010). This size effect can only emerge from a viscoplastic model in which an intrinsic length is included and therefore, the viscoplastic model has to be chosen within the framework of the mechanics of generalized continua (Anand et al., 2010; Forest and Sievert, 2003).

The paper is divided as follows: In a first part, the phase field method and the viscoplastic model are presented, as well as their coupling within a coherent thermodynamic framework. In a second part, the predictions of the coupled model are analyzed. We first analyze static microstructures and we explain how the size effect modifies plastic activity and the resulting macroscopic mechanical behavior. Finally, the dynamic coupling between microstructure evolution and viscoplastic activity is addressed and illustrated by the rafting of the microstructure observed in Ni-base superalloys under creep conditions.

## 2. Model description

### 2.1. Phase field model

The coupling between phase field method and mesoscale viscoplastic model is presented in the context of the microstructural evolution in Ni-base superalloys. In these alloys, the disordered $\gamma$ phase and the ordered $\gamma'$ phase coexist at equilibrium. Following Boussinot et al. (2010), the superalloy is modeled as an effective binary alloy. In that case, in addition to the local concentration field $c(\underline{\boldsymbol{r}},t)$, three non-conservative structural fields $\eta_{i=1,3}(\underline{\boldsymbol{r}},t)$ are introduced to account for the degeneracy of the low temperature $\gamma'$ phase. The four translational variants of $\gamma'$ are described by the following long-range order parameters: $\{\eta_1,\eta_2,\eta_3\}=\eta_0\{1,1,1\}$, $\eta_0\{\overline{1},\overline{1},1\}$, $\eta_0\{\overline{1},1,\overline{1}\}$, $\eta_0\{1,\overline{1},\overline{1}\}$.