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# Relaxation of a precipitate misfit stress state by creep in the matrix

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ABSTRACT

Designed microstructures, such as the ones of high strength and creep resistant modern steels and Al-alloys, are based in many cases on the understanding of the role of precipitates. The kinetics of precipitation can be significantly influenced by the adaption of their volumetric misfit relative to the matrix where plastification and creep of the matrix are typical accommodation processes in addition to vacancy diffusion-controlled mechanisms. A solution for creep coupled with elasticity as such an accommodation mechanism is presented. The set of governing equations including the according assumptions is provided. First, an efficient numerical algorithm is presented to solve the system of two such governing differential equations. Second, necessary steps to obtain an analytical form of the rate equation of the contact pressure are outlined. This rate equation for the contact pressure can be later implemented into models for treatment of precipitation kinetics in complex systems.



## 1. Introduction

The success of advanced alloys, such as modern steels and Al-alloys, is related to designed microstructures. In many cases several kinds of precipitates influence the strength, hardness, creep resistance and other properties of high practical relevance to a remarkable extent. Consequently, understanding the evolution of precipitates can be considered as one of the most important steps in modeling of modern materials, see, e.g. the important contributions by Berveiller and coworkers for steels in Schmitt et al. (1997). In the last decade, numerous papers based on experiments and/or modeling were published addressing this topic. Many authors have contributed to bridge the gap between physical metallurgy (chemistry) and mechanics of materials, see, e.g., Glazoff et al. (2004). Here, remarkable contributions with respect to precipitates and elevated temperatures, i.e. their development and interaction with the creep behavior of the material, shall be mentioned as Morris et al. (2008), and Muñoz-Morris et al. (2009) for Fe–Al-alloys, Morra et al. (2009) for the important SAE52100 steels for bearings, Fan and Yang (2011) for two-phase titanium alloys and Basirat et al. (2012) for 9Cr–1Mo steels for power plants at temperatures higher than 500 °C and le Graverend et al. (2014) for nickel-based superalloys. Additionally, ab-initio and atomistic concepts are nowadays frequently employed. However, except for the nucleation stage, see, e.g., the corresponding treatment by Wagner et al. (Kostorz, 2001) and the recent book by Kozeschnik (2013), precipitates are known to give rise to

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an effective strengthening mechanism, once they have reached diameters of some tens or hundreds of nanometers, see, e.g. Ahmadi et al. (2014). At that scale level, the precipitates can already be regarded as continua, so the concepts of continuum thermodynamics and mechanics are applicable. Of course, the evolution of precipitates must be described in the framework of non-equilibrium thermodynamics. Ziegler's thermodynamic extremal principle, see, e.g. Ziegler (1977), Fischer et al. (2014), represents an excellent tool to formulate evolution equations, see Svoboda et al. (2004) and the numerical implementation in the MatCalc-Code (http://www.matcalc.tuwien.ac.at). It should be mentioned that Cocks and co-workers followed an equivalent approach, i.e. the minimum principle for the dissipation potential (see Fischer et al., 2014, Section 2.3 therein) for an inclusion in an elastic material, see Gill et al. (2001). The total Gibbs energy of the system, consisting of a (mostly dominant) chemical and mechanical contribution, and the total dissipation in the system are the primary functions to derive the evolution equations of the precipitates. The application of the thermodynamic extremal principle also accounts for constraints such as the mass-conservation or stoichiometric relations for the evolution of chemical composition in precipitates, see Svoboda et al. (2004) and Kozeschnik et al. (2004a,b).

The calculation of the mechanical contribution to the Gibbs energy due to formation of the precipitates and their according elastic misfit-strains relative to the surrounding matrix has already been covered, see, e.g., the overview by Fratzl et al. (1999), essentially going back to the pioneering work of Eshelby (1957). However, the mechanical dissipation due to relaxation of the stress field around the precipitate is still an open issue and needs some further research. For an elastic–plastic matrix surrounding a spherical precipitate solutions are already available, see, e.g., the contributions by Fischer and Oberaigner (2001) or the recent paper by Song et al. (2014) for precipitates. In this context, also the solutions for voids, see Fischer and Antretter (2009) and Levitas and Altukhova (2011), and for bubbles or melted zones are mentioned, see, e.g., Levitas and Altukhova (2012a) and Levitas (2012b). Since the dominant size of precipitates is in the range of some hundred nanometers and even smaller, pure slip of only very few dislocations can be activated, see, e.g. the pioneering paper by Ohashi (2004); dislocation plasticity plays only a reduced role. The formation of precipitates mostly takes place at elevated temperatures, e.g. >600 °C in steels. Thus, relaxation by dislocation creep in the matrix is much more relevant than its plastic behavior exclusively by dislocation slip. Dislocation creep is represented by the time and temperature-dependent plastic deformation significantly below the yield stress due to combination of dislocation slip and climb. Dislocation creep can be described phenomenologically by constitutive equations based on models published in a series of seminal contributions by Weertman, see e.g. Weertman (1955), relating the creep rate and applied stress by a power law with the exponent $n \in \langle 3, 5 \rangle$.

Solutions for the accommodation of a precipitate by a creeping matrix are rather scarce and mostly valid only for incompressible materials, which is certainly not the case for precipitates embedded in the matrix with often significantly different elastic properties. As an example for a numerical solution concept, we refer to the paper by Gilormini and Germain (1987) and references therein. Of course, one may pertinently argue that this problem can easily be solved by structural mechanics codes such as ABAQUS (http://www.simulia.com). However, models for complex systems require formulating the evolution equations for the stress state in precipitates in a closed analytical form taking advantage of standard system and material parameters and their rates. For this purpose, simply applicable analytical expressions are lacking to date.

Therefore, the goal of this paper is to develop an expression for the rate $\dot{p}$ of the pressure $p$ acting on the surface of an elastic precipitate embedded in an elastic and creeping matrix. Here, it should be mentioned that also a pure vacancy mechanism, such as vacancy annihilation or generation at the interface between the precipitate and the matrix coupled with diffusion of vacancies in the matrix, is capable of relaxing the pressure, see the studies by Svoboda et al. (2005, 2006) and two further papers, Svoboda and Fischer (2011) and Levitas and Attariani (2012c), dealing with voids (hollows as "quasi-soft" precipitates) in nanospherical particles. However, here we understand creep in the matrix as a combination of dislocation slipping and climbing, which can be considered as classical power-law creep. For specific situations, the rate $\dot{p}$ is calculated based on the derived analytical expressions and calibrated with numerical calculations considered as "exact" reference solutions. The energetic consequences of creep in the matrix surrounding the precipitate are also demonstrated.

## 2. Problem formulation and definitions

All relations concerning the mechanics of the problem can be found in several textbooks, e.g., Malvern (1969), App. II.4 therein.

The investigated configuration is given as follows

(I) The precipitate is assumed as a spherical inclusion (subscript I) with the radius $R$ in an infinite matrix (subscript M). The elastic properties of the inclusion are $E_{\rm I}$, $\nu_{\rm I}$ and those of the matrix $E_{\rm M}$, $\nu_{\rm M}$. The quantity $E$ refers to Young's modulus, $\nu$ to Poisson's ratio. The subscripts will henceforth only be provided where necessary. They will be omitted in equations common for both the inclusion and the matrix.

(II) A spherically symmetric system is assumed, where the deformation is determined only by the radial displacement $u = u(r)$, $r$ being the radial coordinate with the origin in the center of the precipitate. The strain tensor $\boldsymbol{\varepsilon}$ has a radial component $\varepsilon_{\rm r} = \partial u/\partial r = u'$ and the two tangential components $\varepsilon_{\varphi} = \varepsilon_{\vartheta} = u/r$; other components are zero. The differential quotient $\partial g/\partial r$ is abbreviated as $g'$ for an arbitrary function $g(r, t)$.