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Energetic approach for a sliding inclusion accounting for plastic dissipation at the interface, application to phase nucleation

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ABSTRACT

During solid-solid phase transitions, the eigenstrain introduced by the geometrical transformation in the newly formed phase is a significant issue. Indeed, it is responsible for very large elastic energy and dissipation at the continuum scale that have to be added to the total energy in order to determine if a phase transition can occur. The eigenstrain can cause sliding of the newly formed grain. In this paper, an analytical method coupled with numerical energetic optimization is derived to solve the problem of a two-dimensional circular elastic sliding inclusion accounting for plastic dissipation at the interface. Numerical calculations under plane stress assumption show that dissipation enables an effective decrease in the energy needed for the phase transformation to occur.

1. Introduction

Phase transitions are crucial for many applications. A general strategy for modeling phase transitions consists in constructing a cost function (or a global energy) by adding different energetic contributions and dissipated energies arising at different scale during phase transition. Then a minimization over possible states (i.e., a global energy balance) is considered in order to determine if phase nucleation is the most favorable option with respect to the energetic cost function as proposed for instance by Fischer and Reisner (1998).

Among the energetic contributions that should be considered, one of the most studied is the energy gain by the rearrangement of the crystal lattice (Müller et al., 2007). This contribution is associated to the free Gibbs energy variation between one phase and the other. However, the geometrical transformation from the crystalline structure of the parent phase to the crystalline structure of the product phase, amounts to impose, at the scale of continuum mechanics, an eigenstrain in the product phase. For instance within the framework of steel well known orientation models proposed by Bain and Dunkirk (1924); Nishiyama (1934); Kurdjumow and Sachs (1930) may be used to quantify this eigenstrain.

Thus, the free Gibbs energy variation between the parent phase and the product phase is not sufficient to evaluate if phase transformation may occur. Indeed, at the scale of continuum mechanics, the newly formed phase nucleates with a certain size. The geometrical transformation undergone in the inclusion is thus incompatible with the presence of the surrounding matrix, and the inclusion and the matrix will therefore experience elastic strains. Phase nucleation occurs if a lower total energy is reached. Therefore, this elastic energy tends to reduce the possibility of phase changes because the energy gained at the atomic scale by the modification of the crystal structure is compensated by the bulk energy at a larger scale. Thus, one needs to evaluate the elastic energy associated with the eigenstrain in order to correctly predict phase nucleation. For instance, within the framework of Zirconium phase transition, Hensl et al. (2015) include elastic energy in the global free Gibbs energy. Usually the well-known inclusion method proposed by Eshelby (1957) is used to evaluate the stored elastic energy due to the eigenstrain. For instance (Lambert-Perlade et al., 2004) used the Eshelby inclusion method to model self-accommodation within the framework of austenite to bainite phase transition in steel alloys. Mura et al. (1976) proposed an extension of the Eshelby inclusion method for anisotropic materials and consider applications to martensite formation. Previous works consider purely elastic materials even though non-negligible plastic strain may occur. Thus, Delannay et al. (2008) proposed to evaluate elastic-plastic accommodation by using a Finite Element model of an embedded-cell model. One can also mention a different strategy proposed by Ammar et al. (2009) based on a phase-field model of phase transition in elastic-plastic materials where the free en-

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ergy density accounts for dissipation and elastic and chemical[1] contributions.

All the previously mentioned works are based on a perfect adhesion between the inclusion and the surrounding matrix of the parent phase. However, experimental evidences of sliding inclusions have been published by Saotome and Iguchi (1987) for instance. Thus, this paper aims at developing an alternative inclusion method adapted to sliding inclusions and that takes into account plastic dissipation at the interface. The significance of sliding inclusions on the elastic energy when considering phase transitions was already investigated by Tsuchida et al. (1986) and Mura et al. (1985); Jasiuk et al. (1987) for perfectly sliding inclusions in two and three dimensions respectively. More precisely, continuity of normal traction and normal displacements at the inclusion/matrix interface is assumed as well as a condition of vanishing shear traction. Tangential displacements are discontinuous at the interface and are determined through the latter shear free condition. On this basis, it was shown that allowing for sliding reduces the energy needed for the transformation to occur. In this paper, imperfectly sliding inclusions are considered and shear stresses are not set to zero at the interface.

Imperfectly sliding inclusion problems have already been solved by Huang et al. (1993) and Ru (1998), by modeling the relative magnitude of sliding by introducing a parameter varying between zero (perfectly bounded interface) and one (perfectly sliding interface) and by Zhong and Meguid (1997) by assuming that the normal stress is proportional to the corresponding tangential displacement discontinuity which amounts to a Coulomb type friction law. Relying on the same assumption, Mogilevskaya and Crouch (2002) solved the problem of multiple circular sliding inclusions by using a Galerkin boundary integral method.

The approach developed in this paper differs from previous solutions to the extent that there is no assumption on shear traction at the interface and no a priori relationship between tangential displacement discontinuity and normal traction. The problem of an inclusion subject to a known eigenstrain and prescribed sliding is solved with continuity of normal and shear traction and continuity of normal displacement at the interface. The whole solution depends on the prescribed slip and energetic arguments are eventually used in order to determine the actual slip that the system will reach.

These energetic arguments come from experimental observations performed by Saotome and Iguchi (1987) that enable to interpret sliding as localized plasticity at the interface. Therefore, dissipated energy should be taken into account. This is not allowed by the previously mentioned papers, where sliding is determined by an arbitrary proportionality relation between normal traction and tangential displacement discontinuity or by setting shear traction to zero. The energetic approach, that ultimately enables to determine sliding, classically consists in minimizing a global energy that takes into account bulk energy and plastic dissipation. Within the framework introduced for instance by Fedelich and Ehrlacher (1997) and Mielke (2003), dissipation can be seen as a cost (or a distance) that the system has to pay (or to cross) to get a new state, therefore the state variables are those that optimize the bulk energy accounting for the cost to reach this new state. It should be noted that plasticity is considered only at the interface (shear band) and not in the inclusion or matrix bodies.

In the present work, these ideas are applied to the two-dimensional problem of a circular inclusion subject to a given eigenstrain and surrounded by an infinite matrix. An approximate solution to the problem of an inclusion subject to a given eigenstrain and an arbitrary sliding prescribed at the interface is first derived in the context of complex analysis and the works of Muskhelishvili (1953). A numerical minimization of the sum of elastic and dissipated energies at the interface (given as a function of the prescribed sliding) is then performed, in order to determine the actual sliding that the system will reach when loaded by the eigenstrain. A yield strength for the boundary is introduced in order to compute the dissipated energy. This variational method ensures that the von Mises yield criterion is met for sliding to occur. The numerical results thus obtained are then compared with results from a finite element method calculation performed on Abaqus in the case of free slip. Note that the general case of a finite yield strength would require the introduction of interface elements with a plastic behavior between the inclusion and its surroundings, which does not appear to be implemented in Abaqus to the best of the authors' knowledge. One contribution of this work is thus the ability of the method to deal with a perfectly plastic interface. Finally, the behavior of the solution proposed with finite yield strength is investigated. The convergence of the results with the truncation of the expansions is also investigated, and a Gibbs phenomenon is naturally observed when the tangential component becomes discontinuous.

The approximate solution developed here is eventually used to estimate the mechanical energy that has to be provided by the surroundings to the system for a single circular region of space to undergo a phase transition with a given eigenstrain. The plastic dissipation at the interface is shown to be non neglectable with respect to the elastic energy stored during the process. The total energy, that is the sum of the elastic energy and the plastic dissipation, is thus interpreted as the energy that is needed for this phase transition to occur locally.

2. Semi-analytical solution to the problem of a circular sliding inclusion with non-zero tangential component of the interfacial tractions

The semi-analytical solution to the problem of a sliding circular inclusion subject to a given uniform eigenstrain expressed in its principal directions is derived in this section. Let the Ox and Oy axes of the Cartesian coordinate system be the principal directions of the eigenstrain $\boldsymbol{\varepsilon}^*$, so that the matrix associated with $\boldsymbol{\varepsilon}^*$ in this coordinate system is:

$$\boldsymbol{\varepsilon}^* = \begin{pmatrix} \varepsilon^*_{xx} & 0 \\ 0 & \varepsilon^*_{yy} \end{pmatrix} \tag{1}$$

Both the inclusion and the matrix are linear elastic and plane theory of elasticity is considered. The Lamé coefficients of the inclusion and the matrix are denoted by (λ_I, μ_I) and (λ_M, μ_M), where I and M stand for *inclusion* and *matrix* respectively. The following derivation uses complex potentials and expansions into power series, Laurent series and Fourier series. The solution that is derived here can be broken down into three parts. First, the solution to the problem of a disk with prescribed surface tractions at the boundary, and the solution to the problem of a matrix with a circular hole with prescribed surface tractions along the hole and no displacement at infinity are addressed in Sections 2.2 and 2.3 respectively. These solutions are obtained by expanding the prescribed surface tractions into a Fourier series and is quite analogous to the solutions given by Muskhelishvili (1953). Then, using these two preliminary solutions, the problem of a circular inclusion subject to a given uniform eigenstrain and a prescribed trial sliding along the interface is derived in Section 2.4. The trial sliding is denoted by $g(\theta)$ where r, θ are polar coordinates. Eventually the actual sliding that the system will reach is denoted by $g^S(\theta)$ where S stands for *solution*. To solve this sliding inclusion problem, the prescribed surface tractions are eliminated using continuity conditions on the displacement (accounting for the trial sliding $g(\theta)$)

[1] which represents the difference of structural state between phases.