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Stress, deformation and diffusion interactions in solids – A simulation study

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ABSTRACT

Equations of diffusion treated in the frame of Manning's concept, are completed by equations for generation/annihilation of vacancies at non-ideal sources and sinks, by conservation laws, by equations for generation of an eigenstrain state and by a strain-stress analysis. The stress-deformation-diffusion interactions are demonstrated on the evolution of a diffusion couple consisting of two thin layers of different chemical composition forming a free-standing plate without external loading. The equations are solved for different material parameters represented by the values of diffusion coefficients of individual components and by the intensity of sources and sinks for vacancies. The results of simulations indicate that for low intensity of sources and sinks for vacancies a significant eigenstress state can develop and the interdiffusion process is slowed down. For high intensity of sources and sinks for vacancies a significant eigenstrain state can develop and the eigenstress state quickly relaxes. If the difference in the diffusion coefficients of individual components is high, then the intensity of sources and sinks for vacancies influences the interdiffusion process considerably. For such systems their description only by diffusion coefficients is insufficient and must be completed by a microstructure characterization.

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1. Introduction

The current work is devoted to study the interaction between diffusion and stress state, together with an according strain state. Generally, one can distinguish among three groups of works contributing to this topic.

- The first group of works accounts for the influence of the stress state by addition of stress terms to the chemical potentials of vacancies and components. The stress state can be a given load stress state and/or due to a given eigenstrain state. Most of the past, recent and actual contributions work with this concept, see an overview in Svoboda et al. (2006), Section 7 there, and Fischer and Svoboda (2014), or the book by Balluffi et al. (2005), Section 3.5.1 there. Usually, an additional chemical potential term proportional (or related) to the hydrostatic stress term σ_H is selected. As examples only some recent works and papers are mentioned, e.g. by Lindberg (2013), Yan et al. (2014), Winzer and Khader (2013) and Villani et al. (2014), applying a σ_H -term. Some authors introduce instead of σ_H the volume strain ϵ_H , as Hosseini et al. (2014), Suo and Shen (2012a, 2012b), and Allam et al. (2012). Sometimes only the dependence of the diffusion

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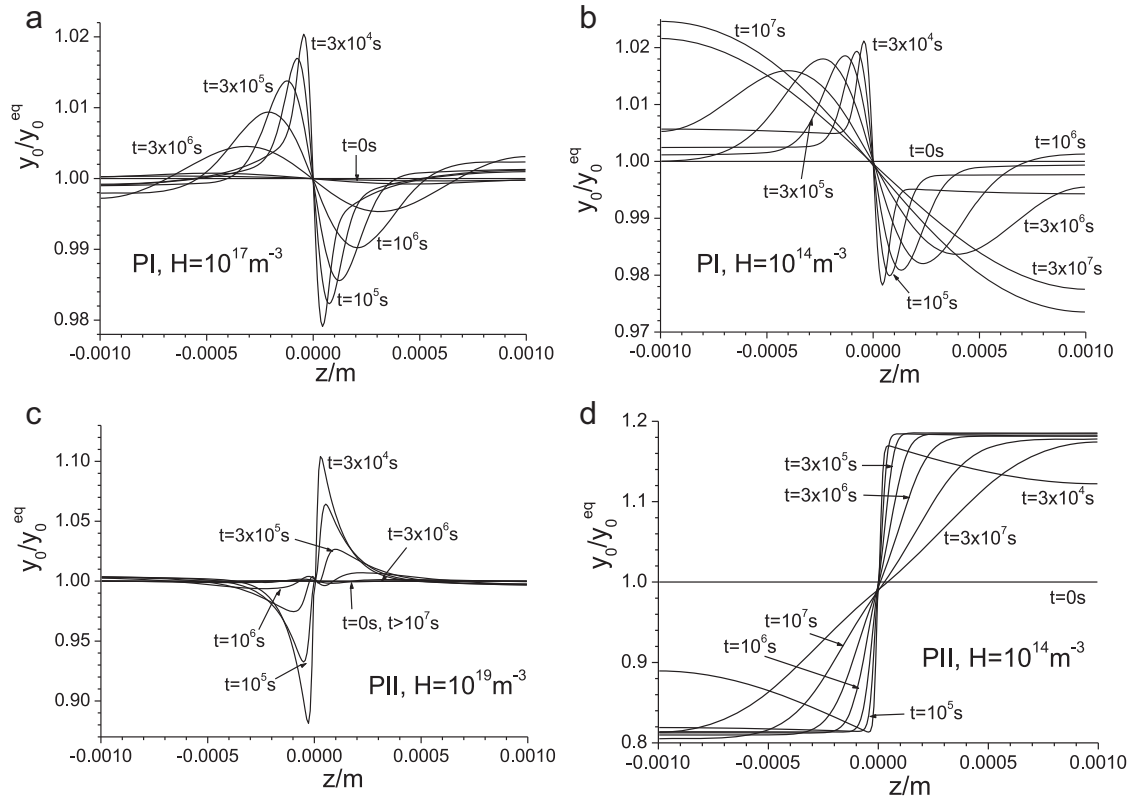


Fig. 1. Time evolution of the y_0/y_0^{eq} profiles for parameter sets (a) PI and $H = 10^{17} \text{ m}^{-3}$, (b) PI and $H = 10^{14} \text{ m}^{-3}$, (c) PII and $H = 10^{19} \text{ m}^{-3}$ and (d) PII and $H = 10^{14} \text{ m}^{-3}$.

coefficients on σ_H , see, e.g., [Bailakanavar et al. \(2014\)](#), the consideration of the elastic strain energy, as in the phase field method, see, e.g., [Kamachali et al. \(2013\)](#), and taking into account the (elastically) deformed lattice, see [Di Leo et al. \(2014\)](#) and [Miehe et al. \(2014\)](#) are assumed as sufficient. A more general formulation of the chemical potential was recently published by [Levitas and Attariani \(2014\)](#) taking into account not only the σ_H -term but also the stress deviator, described in a large strain setting.

- The second group of works deals with the diffusion of vacancies and its relation to the material velocity. Here we refer to the paper by [Andersson and Ågren, 1992](#), who introduced for their treatment several “frames of reference” in a three-dimensional space. A later comprehensive presentation of this topics in the one-dimensional space can be found in [Balluffi et al. \(2005\)](#), Section 3.1 there. However, as outlined by the authors ([Svoboda et al., 2006](#)), Section 2.3, a direct relation between the flux of vacancies and the material velocity is only possible, if ideal sources and sinks for vacancies are assumed and the actual velocity field includes a divergence-free term, which is necessary to meet the boundary condition. This term cannot be ignored as it is commonly done. Furthermore, if one assumes that the partial molar volumes of vacancies and of substitutional atoms are the same, then diffusion itself represented by exchanges of vacancies with atoms cannot lead to any deformation of the system. The assumption of such a direct relation between the flux of vacancies and the material velocity, without the mentioned divergence-free term, motivated [Berdichevsky et al. \(1997\)](#) to analyze diffusional creep and to formulate a creep strain rate $\dot{\epsilon}_{gc}$ as eigenstrain rate and as possible reason of an eigenstress state. This concept has been used later by several authors, see, e.g., by [Grychanyuk et al. \(2004\)](#) and [Tsukrov et al. \(2008\)](#), but has not been critically evaluated up to now with respect to its immanent prepositions.
- The third group of works deals with generation of an eigenstrain ϵ_{gc} , represented by the rate $\dot{\epsilon}_{gc}$,
 - due to the formation, i.e. generation or annihilation, of vacancies, and
 - due to the diffusion of elements with different partial molar volumes Ω_k , with k representing the respective component, see below.

The consistent theory for diffusion and eigenstrain rate $\dot{\epsilon}_{gc}$ has been presented in the works by the authors, see, e.g., [Svoboda et al. \(2006\)](#) and [Fischer and Svoboda \(2014\)](#). It must be emphasized that both processes, diffusion and formation of vacancies, are physically independent ones; however, they can occur simultaneously and can be coupled. The diffusion of substitutional elements is conditioned by only one type of defects, namely the vacancies. The formation of vacancies is, however, conditioned by existence of further types of defects like jogs at dislocation lines, grain boundaries, free surfaces and incoherent interfaces. Also irradiation can produce vacancies and vacancy complexes. In case of no formation of

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