



# Gibbs–Thomson condition for the rapidly moving interface in a binary system



A. Salhoumi<sup>a,b</sup>, P.K. Galenko<sup>c,d,\*</sup>

<sup>a</sup> Université Hassan II de Casablanca, Faculté des Sciences Ben M'Sik, Laboratoire de Physique de la Matière Condensée (LPMC), BP 7955 Casablanca, Morocco

<sup>b</sup> Université Hassan II de Casablanca, Faculté des Sciences Juridiques, Economiques et Sociales Ain Sebaa, BP 2634 Casablanca, Morocco

<sup>c</sup> Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, D-07743 Jena, Germany

<sup>d</sup> Ural Federal University, Laboratory of Multi-Scale Mathematical Modeling, 620000 Ekaterinburg, Russia

## HIGHLIGHTS

- A phase-field model for fast transformations is used.
- A dynamical boundary condition for the fast interface is derived.
- Predictions of the condition are qualitatively consistent with data of atomistic simulations.

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## ABSTRACT

Using a phase-field model for fast phase transformations we derive an interface condition for the rapidly moving solid–liquid interface. The model is described by equations for the hyperbolic transport and fast interface dynamics, which are reduced to a sole equation of the phase field with the driving force given by deviations of temperature and concentration from their equilibrium values within the diffuse interface. It is shown that the obtained interface condition presents the acceleration- and velocity-dependent Gibbs–Thomson interfacial condition. This condition is identical to the advanced Born–Infeld equation for the hyperbolic motion by mean curvature with the driving force. As a limiting case, the interface condition presents “velocity-driving force” relationships found earlier as traveling wave solutions for slow and fast phase field profiles. Predictions of the analytical solutions are qualitatively compared with literature data of atomistic simulations on crystal growth kinetics.

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## 1. Introduction

The shift of the thermodynamic equilibrium at the curved interface is described by the Gibbs–Thomson condition [1,2] which presents a balance between a volumetric tendency to exchange and a surface tendency to save a shape of co-existing phases. The Gibbs–Thomson condition can be simply derived from the traditional thermodynamic analysis as well as it provides geometrical motivation for the phase field model equations [3]. Indeed, developed phase-field models and methods [4–8] are able to describe a wide spectrum of tasks arising in condensed and soft matters on the mesoscopic and diffusive length scales [9]. Being thermodynamically consistent, these methods predict known interface and bulk phase

\* Corresponding author at: Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, D-07743 Jena, Germany.  
E-mail address: [peter.galenko@uni-jena.de](mailto:peter.galenko@uni-jena.de) (P.K. Galenko).

conditions for equilibrium and near equilibrium conditions [10,11] among which the Gibbs–Thomson condition plays a central role in interpretation of governing equations for phase field modeling [12].

Traditional approaches to construct phase field models are based on the hypothesis of local equilibrium, which presents an excellent approximation for the dynamics of near equilibrium systems [4–12]. These models use parabolic types of governing differential equations and describe a rather rich variety of processes evolving close to the global thermodynamic equilibrium. For fast transformations and transitive processes, equations of a hyperbolic type have been suggested to take deviations from local equilibrium conditions into account [13–16]. In this sense, equations of a hyperbolic type were naturally derived within a spectrum of tasks arising in systems evolving far from thermodynamic equilibrium [17–21]. The validity of hyperbolic type models has been verified in molecular dynamics simulations of solute trapping effect by the rapidly moving fronts [22] and by coarse graining derivations of phase field equations [23].

The main purpose of the present paper is to formulate the condition of Gibbs–Thomson-type which follows from the hyperbolic phase field model and might be applied to the rapidly moving phase interface. As starting and concrete process we consider in this paper the rapid solidification of a metastable liquid [24] – the process which can be re-interpreted within the phase field model to other phase transformations at least in condensed media.

The paper is organized as follows. Main equations of the phase field model are summarized in Section 2. A method to treat phase field equations based on the averaging procedure is given in Section 3. A central result of the work obtained as acceleration- and velocity-dependent Gibbs–Thomson condition is derived in Section 4. We discuss the obtained condition in comparison with previously derived equations in Section 5. Specifically, a quantitative comparison of linear and nonlinear equations for interface motion which are following from the obtained interface condition is given in this discussing section. Finally, Section 6 presents a summary of our conclusions.

## 2. The model

Consider a binary dilute system consisting of A atoms (solvent) together with a tiny amount of B atoms (solute) with the concentration  $C$  under constant temperature  $T$  and constant pressure. Then the evolution of the system to equilibrium is described by the following equations of hyperbolic type [21,24]

$$\tau_D \frac{\partial^2 C}{\partial t^2} + \frac{\partial C}{\partial t} = \nabla \cdot \left[ M_C \left( \frac{\partial^2 f}{\partial C^2} \nabla C + \frac{\partial^2 f}{\partial C \partial \phi} \nabla \phi \right) \right], \quad (1)$$

$$\tau_\phi \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial \phi}{\partial t} = M_\phi \left( \varepsilon_\phi^2 \nabla^2 \phi - \frac{\partial f}{\partial \phi} \right), \quad (2)$$

where  $f$  is the free energy density,  $C$  is the solute concentration (of B-atoms),  $\tau_D$  is the relaxation time for the diffusion flux,  $M_C$  is the mobility of B-atoms,  $\tau_\phi$  is the time scale for the relaxation of the rate of change of the phase field  $\partial\phi/\partial t$ , and  $M_\phi$  is the mobility of the phase field.

Note that, in comparison with the parabolic type of phase field model equations [10–12], hyperbolic equations (1)–(2) refine the time scale  $\tau$  due to second derivative of  $C$  and  $\phi$  with respect to  $t$ . If the time scale of parabolic equations is limited by the thickness  $\delta$  of the diffuse interface:  $\tau < \delta^2/(M_\phi \varepsilon_\phi^2)$ , the system of hyperbolic equations (1)–(2) should take into account time scales  $\tau_D$  and  $\tau_\phi$  for relaxation of the fast variables the values of which depend on concrete system. For example, these relaxation times can be estimated in ranges of  $10^{-11}$  (s)  $< \tau_D < 10^{-10}$  (s) and  $10^{-13}$  (s)  $< \tau_\phi < 10^{-11}$  (s) as for a Ni–Cu concentrated alloy or for the Si–As semiconductor system solidification [24].

Following model [25], the local equilibrium free energy density  $f$  is chosen as the ideal solution of a dilute binary system

$$f(C, \phi) = f^A(T_A) - (T - T_A)s(\phi) + \varepsilon(\phi)C + \frac{RT}{v_m} (C \ln C - C) + Wg(\phi), \quad (3)$$

where  $f^A(T)$  is the free energy density of a pure system consisting of a solvent (pure A-atoms),  $T_A$  is the solidification temperature of the solvent,  $R$  is the gas constant,  $v_m$  is the molar volume (assumed equal for A- and B-atoms), and  $W$  is the height of the energetic barrier which is modeled by the double-well function

$$g(\phi) = \phi^2 (1 - \phi)^2. \quad (4)$$

The entropy density  $s(\phi)$  and the internal energy density  $\varepsilon(\phi)$  are derived using the dilute alloy approximation

$$s(\phi) = \frac{s_s + s_l}{2} - p_s(\phi) \frac{L}{2T_A}, \quad p_s(\phi) = 1 - 2p(\phi), \quad (5)$$

$$\varepsilon(\phi) = \frac{\varepsilon_s + \varepsilon_l}{2} - p_\varepsilon(\phi) \frac{RT}{2v_m} \ln k_e, \quad (6)$$

$$p_\varepsilon(\phi) = \frac{2}{\ln k_e} \ln [k_e + p(\phi)(1 - k_e)] - 1,$$

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