A Numerical Investigation for a Model of the Solid-Gas Phase in a Crystal Growth Apparatus

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Abstract. We present discretization and solver methods for a model of the solid-gas phase in a crystal growth apparatus. The model equations are coupled Eulerian and heat-transfer equations with flux boundary conditions. For a more detailed discussion we consider simpler equations and present time- and space-decomposition methods as solver methods to decouple the multi-physics processes. We present the error analysis for the discretization and solver methods. Numerical experiments are performed for the Eulerian and heat-transfer equation using decomposition methods. We present a real-life application of a crystal growth apparatus, based on underlying stationary heat conduction. Finally we discuss further error analysis and application to a more complex model of crystal growth.

AMS subject classifications: 74S10, 80A20, 47F05, 65M60, 80M25, 49M27

PACS: 02.60.Cb, 02.60.-x, 44.05.+e, 47.10.ab, 47.11.Df, 47.11.St, 47.27.te

Key words: Decomposition methods, finite-volume discretization, error analysis, heat equation, crystal growth.

1   Introduction

The modelling and numerical simulation of the solid-gas phase in complex apparatuses have become interesting tools for the improved design and optimization of numerous industrial processes such as crystal growth, for example by the physical vapour transport (PVT) method [25]. Because of the complex processes, a careful study is important for the correct design of numerical simulations [36]. The combination of discretization and solver methods is therefore an important task. We propose decomposition methods to break down complicated multi-physics into simpler physics. Time decomposition

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methods, and their extended versions with more stable behaviour, are based on operator-splitting methods [14]. With these methods a useful decoupling of the time-scales is possible and the solvers can be applied on these different time-scales. Space decomposition methods are based on Schwarz waveform relaxation methods and their accurate error estimates [10]. These methods decouple into domains with the same equation parameters. Therefore effective spatial discretization and solver methods are applicable.

The paper is organized as follows: The mathematical model is stated in Section 2, the space discretization methods are performed with finite volume discretization and are described in Section 3. The time-discretization and decomposition methods are described in Sections 4 and 5. In Section 6 we describe the numerical experiments in which we verify our decomposition methods and simulate a realistic crystal-growth apparatus. Future work and the Conclusions are presented in Section 7.

2   Mathematical model

The motivation for this study comes from the technical demand to simulate a crystal growth apparatus for single SiC crystals. The single crystals are highly valued materials for opto-electronics and electronics [34]. The silicon carbide (SiC) bulk single crystal is produced by a growth process through physical vapour transport (PVT), called the modified Lely method. The modelling of the thermal processes within the growth apparatus is done by [26] and [37]. The underlying equations of the model are as follows:

a.) In this work, we assume that the temperature evolution inside the gas region Ω_g can be approximated by considering the gas to be pure argon. The reduced heat equation is

$$\rho_g \partial_t U_g - \nabla \cdot (\kappa_g \nabla T) = 0, \tag{2.1}$$
$$U_g = z_{Ar} R_{Ar} T, \tag{2.2}$$

where T is the temperature, t is the time, and U_g is the internal energy of the argon gas. The density of the argon gas is ρ_g, κ_g denotes the thermal conductivity, z_{Ar} is the configuration number, and R_{Ar} is the gas constant for argon.

b.) The temperature evolution inside the region of solid materials Ω_s, for example inside the silicon carbide crystal, the silicon carbide powder, the graphite, and the graphite insulation, is described by the heat equation

$$\rho_s \partial_t U_s - \nabla \cdot (\kappa_s \nabla T) = f, \tag{2.3}$$
$$U_s = \int_0^T c_s(S) \, dS, \tag{2.4}$$

where ρ_s is the density of the solid material, U_s is the internal energy, κ_s is the thermal conductivity, and c_s is the specific heat. Here, f represents the heat source in the material Ω_s.