



Thermomigration (thermodiffusion) and convection in molten semiconductor–metal layers

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ABSTRACT

Thermomigration or thermomigration phenomenon and the presence of convection are investigated in a binary molten semiconductor–metal layer heated from top or bottom. These phenomena may be locally present in the zone melting temperature gradient (ZMTG) method used for the fabrication of semiconductor devices and solar cells. Thermomigration is studied using the linear nonequilibrium thermodynamics, whereas convection is studied by solving the transport equations numerically in a stationary molten cell. An expression is obtained to estimate thermomigration factor in stationary binary semiconductor–metal mixtures. The presence of convection in various cases is studied as well. In the absence of any experimental data on stationary semiconductor–metal mixtures, the prediction power of the developed expression is tested against the experimental data of the moving melting zone in the ZMTG process on mixtures comprised of silicon as a semiconductor and aluminum, gallium, and gold as metal dopants. The expression can only qualitatively predict the migration velocity of the melting zone, perhaps due to the inadequacy of the nonequilibrium thermodynamics to model this process, and the uncertainties in the experimental data due to the presence of both thermomigration and the gravity-induced convection in the molten zone.

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1. Introduction

Mass diffusion due to a temperature gradient in a gas, liquid or solid mixture is called thermomigration, also Ludwig–Soret or Soret effect. In a non-isothermal mixture, thermomigration coexists with a temperature-induced diffusion, which is in fact the ordinary or mutual diffusion. Thermomigration in semiconductor and metal mixtures and in the crystal growth literature is often called thermomigration or thermotransport. Owing to the increasing applications of thermomigration through using the temperature gradient zone melting method (TGZM) in the fabrication of semiconductor devices, micro-electro-mechanical systems (MEMS), and thin films [1–11], and its theoretical and fundamental importance as a hydrodynamic problem, the goal of the present paper is to investigate the thermomigration process and convection in a stationary molten semiconductor–metal layer, which also resembles the migration of the molten zone in the TGZM method. The difference between the ideal case of a stationary molten layer and the moving zone in the TGZM is discussed later.

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Some of the crystal growth techniques are as follows: melt growth (e.g., horizontal and vertical boat growth, pulling and floating zone methods), solution growth (e.g., simple solution growth, temperature gradient zone melting (TGZM) or traveling solvent, traveling heater, solute solution diffusion, solvent evaporation and hydrothermal synthesis methods), and vapor phase growth (e.g., direct synthesis, physical and chemical vapor transport and solid phase reaction methods) [12]. The TGZM method was initially introduced as a crystal growth method by Pfann, e.g., [13]; this method has been used to grow several semiconductors, such as GaP and ZnTe [12]; however, it is more considered as a route to modify semiconductors by doping in microelectronics and MEMS applications.

Thermomigration in a stationary layer is easy to understand. A temperature gradient applied to a mixture, which is initially homogenous, activates the species. Owing to the displacement of the species a concentration gradient is induced also, which causes ordinary diffusion in the mixture. In steady state, i.e. when the mass fluxes vanish, it is observed that the temperature gradient has caused relative separation of the two components such that one of the components is segregated more on the cold side and the other component has segregated on the hot side. In the TGZM method, a liquid zone (usually a molten substance, single or multicomponent), which is initially formed on a solid surface or a thin film,