Abstract Diffusion in multi-component alloys can be characterized (a) by the vacancy mechanism for substitutional components, (b) by the existence of sources and sinks for vacancies, and (c) by the motion of atoms of interstitial components. The description of diffusive and massive phase transformation of a multi-component system is based on the principle of maximum dissipation rate by Onsager; the finite thickness of the interface between both phases can be respected. A new computational model (its one-dimensional, in general non-stationary version is presented here) covers both (a) and (c) and is open to involve (b) in a natural way. The mathematical analysis results in an initial-value problem for a system of partial differential equations of evolution with certain non-local integral term; the unknowns are the mole fractions of particular components (and some additional variables in case (b)). The numerical construction of approximate solutions comes from the method of lines and from the finite difference and other numerical techniques, namely the numerical integration formulae and the spectral analysis of linear operators. The original software code is supported by MATLAB and partially by MAPLE.

5.1 Introduction

The basic principles of diffusion controlled phase transformation have been known for a long time. In general the diffusion in a multi-component system can be characterized by the well-known relation from [11], rewritten in some (more or less general) form in most later monographs or papers, as [2, 5] or [3]. The diffusive flux for every component can be evaluated as a product of the matrix of kinetic coefficients and the gradient of chemical potentials of particular components, understood as
functions of concentrations (or some equivalent characteristics, as mole fractions). In the more general context the diffusive flux may be substituted by some “extensive quantity” and the chemical potential by some “intensive variable”, for illustration of the terminology cf. [14], p. 5, and [16], p. 1370. Onsager showed that such linear phenomenological equation (originally for a heat production in an anisotropic system) can be derived from the requirement of maximum of a functional, having a close relation to the total entropy production of the system, and formulated the “thermodynamic extremal principle” (TEP). Making simplifying assumptions, in case of binary systems it was possible to derive analytic or semi-analytic solutions, useful in the field of material development. However, under more general assumptions or in systems including more than two components this approach turned out to be insufficient.

The thermodynamics of multi-component systems has its own scientific history, covering the evolution of the concept of deriving the thermodynamic functions of a system from all available experimental data, the reliable setting of kinetic parameters, etc.; much more information and references to results from the last four decades can be found in [14], p. 3. Both theoretical and experimental works yield that the diffusion in multi-component alloys can be characterized by three attributes:

(a) The vacancy mechanism for “slowly” diffusing substitutional components
(b) The existence of certain sources or sinks of vacancies
(c) The “quick” motion of atoms of interstitial components

In the following formal mathematical description of a system only the attributes (a) and (c) will be incorporated properly; the attribute (b) will be left to the concluding remarks. We also limit the discussion to isothermal and isobaric conditions. Let us notice that most papers, as [14], p. 6, or [16], p. 1373, need simplifying assumptions on the equilibrium of vacancies; only [17], p. 3046, attempt to handle the quite general case with non-ideal sources and sinks and vacancies.

Another serious problem is connected with the description of the (usually very thin) interface, separating two phases during the phase transformation. Under the assumption of the sharp interface (whose thickness is assumed to be negligible) it is not easy to formulate realistic interface conditions (as boundary conditions for particular phases) [14], p. 9, introduce three types of such conditions: the so-called local equilibrium conditions with partitioning, the local equilibrium conditions with negligible partitioning and the para-equilibrium conditions. Nevertheless, it is possible to avoid all such (rather tricky) conditions, respecting the finite thickness $h$ of the interface, as explained in [20], p. 3954, where the material behaviour in the centre of the interface corresponds to the ideal liquid phase; consequently the results for the sharp interface can be derived from those for the thick interface, using the limit passage $h \rightarrow 0$.

Several further simplifications in our considerations could be removed, but has been accepted here to generate a relatively simple mathematical formulation. Following [14], p. 6, we shall assume that the insertion of an interstitial component does not change the lattice geometry. We shall write all relations for a hypothetical one-dimensional problem, thus the interface motion in other directions will be