Phase diagram calculation of $A^{III}B^{V}$ binary solutions of the eutectic type in the generalized lattice model

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Abstract. The present work is devoted to the phase diagrams calculation of $A^{III}B^{V}$ systems within the framework of the generalized lattice model taking account of volume effects. The theoretically calculated phase diagram is compared with the corresponding experimental diagrams.

1. Introduction
Calculation of phase diagrams is one of the most interesting problem of physics of multicomponent systems. In particular, investigation of the thermodynamic properties and phase equilibria in $A^{III}B^{V}$ binary systems is of great importance for micro- and nanoelectronics. The aim of this work is a theoretical calculation of the phase diagram of $A^{III}B^{V}$ binary systems (In–Sb, In–As, Al–P, Al–Sb) within the generalized lattice model [1].

2. Model
It is well known, that the phase diagrams of the In–Sb, In–As, Al–P, Al–Sb systems are eutectic type phase diagrams with one intermediate phase of constant composition. The phase diagram of the eutectic type with intermediate phase of constant composition is schematically presented in Figure 1.

It is easy to see that the left and right parts of the initial phase diagram are similar to a conventional phase diagram of the eutectic type. The fundamental difference between both parts of the phase diagram in Figure 1 and the phase diagram of the eutectic type is that the mole fractions $x$ of the $B$ component vary in the range $0 \leq x \leq n/(m+n)$ for the left subsystem $A_mB_n$ and in the range $n/(m+n) \leq x \leq 1$ for the right subsystem $A_mB_n-B$. As a consequence, the lengths of the segments that correspond in the concentration axis to the left and right parts of the diagram are not equal to unity, whereas the length of the concentration axis in any phase diagram should be equal to unity. These differences do not permit one to directly use the well-developed methods for calculating phase diagrams in the case of simulation of the components of phase diagrams for systems with intermediate phases. The method of calculation of phase diagrams of such type has been proposed in paper [2]. The method is based on the nonlinear transformations of the concentration axes and makes it possible to correctly reduce the calculation of the phase diagrams with several intermediate phases to a sequence of phase diagrams of individual subsystems. These cases were studied in detail in papers [2,3]. For
Figure 1. Phase diagram of the eutectic type with intermediate phase of constant composition in the absence of the mutual solubility of the components in the solid state.

According to the basic principles of the generalized lattice model, the chemical potentials of a homogeneous binary solution (per mole of a material) can be represented in the following form

\[
\mu_1 = \mu_{10} + RT \ln x + W \frac{1-x}{x + \lambda(1-x)}^2, \\
\mu_2 = \mu_{20} + RT \ln(1-x) + W \frac{x}{x + \lambda(1-x)}^2,
\]

where \(\mu_{10}\) is the standard chemical potential of the \(i\)th component, \(R\) is the universal gas constant, \(T\) is the temperature of the system, \(x\) is the mole fraction of the first component, \(W\) is an analog of the energy of mixing in the generalized lattice model, \(\lambda = \omega_2/\omega_1\), and \(\omega_i\) is the characteristic atomic volume of the \(i\)th component.

Further let us consider the subsystem of an \(A_{m}B_{n}\)–\(B\) binary solution of eutectic type (see Figure 1). We can obtain all parameters of general lattice model for binary solutions of the eutectic type taking into account the chemical equilibrium in the three-phase system, i.e., equating the chemical potentials of the components in the solid and liquid phases.

Equations of the chemical equilibrium in the three-phase system form a closed system, whose solution allows us to find the concentration dependences of the liquidus branches and, hence, to construct the phase diagrams of binary system \(A-A_{m}B_{n}\) in the framework of the generalized lattice model.

It should be noted that the chemical equilibrium in the subsystem of an \(A_{m}B_{n}-B\) binary solution is considered in a similar way.
3. Phase diagram calculation
Using the technique developed in [2] calculation phase equilibria in the In–Sb, In–As, Al–P, Al–Sb systems was carried out (see, Figures 2,3). The parameters of the model are correspond to theoretical calculations of the phase diagrams was obtained (see, Table 1). It should be noted here we use the notation introduced work [2].

![Figure 2](image1)
![Figure 3](image2)

**Figure 2.** Phase diagrams of the the In–Sb, In–As systems. Dashed lines are the experimental data taken from [5]. Solid lines indicate the results obtained from theoretical calculations.

**Figure 3.** Phase diagrams of the the Al–Sb, Al–P systems. Dashed lines are the experimental data taken from [5]. Solid lines indicate the results obtained from theoretical calculations.

In addition it should be noted that explicit account of “volume” effects was carried by introducing ”specific” the atomic volumes of components within the generalized lattice model.

It can been seen from Figures 2, 3 that the phase diagrams are consistent with the experimental data available in the literature [5].

Thus, comparison with experimental data shows that the theoretical approach can be used to adequately description and prediction of the phase equilibria in the A\text{III}B\text{V} binary solutions.
Table 1. Parameters of the generalized lattice model.

| $A-B$    | $x_0$  | $T_0, ^\circ C$ | $q_{AB}$ | $\lambda$ | $W/R, K$ |
|----------|--------|-----------------|----------|-----------|----------|
| In–InSb  | 0.007  | 155.0           | 15.37    | 0.473     | -1722    |
| InSb–Sb  | 0.663  | 494.0           | 15.37    | 1.272     | 496      |
| In–InAs  | 0.003  | 155.2           | 13.99    | 0.045     | -439     |
| InAs–As  | 0.875  | 731.0           | 13.99    | 1.516     | -1569    |
| Al–AlSb  | 0.004  | 657.0           | 23.53    | 0.178     | -799     |
| AlSb–Sb  | 0.992  | 627.0           | 23.53    | 2.256     | -6016    |
| Al–AlP   | 0.001  | 659.7           | 18.00    | 0.162     | -4459    |
| AlP–P    | 0.999  | 44.0            | 18.00    | 25.001    | -4281    |

Acknowledgments. This study was supported by the Ministry of Education and Science of the Russian Federation (project 1755).

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