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MATHEMATICAL MODELING OF CRITICALl PHENOMENA IN SOLID SOLUTION OF SEMICONDUCTORS BASED ON A_2B_6 COMPOUNDS

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Mathematical modeling of critical phenomena in multicomponent solid solutions of semiconductors was carried out on the basis of the theory of phase transitions and the theory of catastrophes. A mathematical method is proposed for calculating the spaces of coexistence of phases in solid solutions of semiconductors of II – VI groups of the periodic system. An algorithm for calculating the zero contours of the free energy function of the system, critical spaces and spaces of phase coexistence is presented. For calculating spaces of coexistence of phases of order two in ternary solid solutions based on semiconductors of II – VI groups of the periodic system the differential topological approach was used. The calculations were carried out in the framework of the regular solution model. Interactions both of the first and the second nearest neighbor pairs of atoms and also the temperature dependence of the interaction parameter were considered additionally. Modern methods of computer simulation are used for analyzing processes of occurrence of self-organizations ordered structures. Multicomponent phase diagrams, taking into account the possibility of existence of bifurcation spaces and critical spaces and spaces of coexistence of phases of different orders were obtained. The positions of the spaces of coexistence of second-order phases for the Zn-Cd-Te system are calculated using the mathematical method proposed in this work. Multicomponent phase diagrams have been obtained, taking into account the possibility of the existence of bifurcation spaces, critical spaces and spaces of coexistence of phases of different orders, makes it possible to predict the processes of loss of stability in three-component semiconductor solutions based on compounds II - V and groups of the periodic system with different modes of their synthesis and operation.

Keywords: Computer simulation, phase diagrams, solid solutions, alloys, semiconducting II–VI materials.

Introduction

The development of modern methods of computer modeling led to the possibility of predicting the properties of multicomponent semiconductor materials. One of the promising areas is the mathematical modeling of processes leading to degradation of the properties of semiconductor compounds. Some progress has been made in this area; however, some directions in the modeling of processes in semiconductors remain poorly studied. In particular, there are practically no papers related to the modeling of spaces in which two or more phases can coexist simultaneously in solid solutions of semiconductors. This circumstance is a significant omission, since in many solid solutions, for example, obtained on the basis of A_2B_6 semiconductor compounds [1-5], metastable states associated with the formation of phases of coexistence spaces are observed. The problem of creating and investigating A_2B_6 materials, which has optimal properties for tasks of electronics, is increasingly important today. Moreover crystal properties

play the most important part for characteristic of created devices. The researches of A_2B_6 multicomponent materials received have shown that homogeneous solid solutions of semiconductors occur unstable. This leads to spinodal ordering and forming periodical structures with modulated composition. The loss of thermodynamic stability with respect to composition fluctuations, which is possible in a multicomponent solid phase, can lead to the appearance of metastable or unstable states of multicomponent solid solutions. The appearance of critical phenomena in unstable solid phases leads to the degradation of the properties of optoelectronic devices. However, the problem of predicting the possibility of appearing spaces of the coexistence of fazes in A_2B_6 solid solutions was studied not enough. In this paper, a thermodynamic model is considered in which the temperature dependences of the interaction parameter between the atoms of the first two coordination spheres are taken into account. One of the promising solid solutions based on A_2B_6 is $Zn_XCd_{1-X}Te$. On the basis of the model considered and using a differential topological approach, a spaces of coexistence of phases of order two for the Zn-Cd-Te system is obtained.

Main part

Modern computer models describe the properties of semiconductor compounds based on A_2B_6 quite correctly. In [6] within the framework of the polyassociative model, a satisfactory description of the phase diagram was obtained and the thermodynamic functions of the dissociation of complexes in the Cd-Hg-Te system were found. A good agreement with the experimental data was obtained in the modeling of phase equilibrium for the Zn-Cd-Te system in [7]. Attempts are made [8, 9] to construct models for explaining intrinsic ferromagnetism in $Zn_{1-x}Cr_xTe$. The first steps have been taken to model the appearance of an additional geometric phase in semiconductor systems with a strong spin-orbit coupling [10, 11]. The static model of the formation of an exciton condensed phase with allowance of the nonequilibrium effects in a two-dimensional system is presented in [12, 13]. Modeling based on the variational approach makes it possible to study the influence of the magnetic field on the energy of the ground state of exciton-donor complexes [14]. Mixing models for studying the effective dielectric permittivity of alloys was considered in [15]. A model was proposed [16] that allows one to explain the characteristic features of the photoluminescence spectra of single quantum dots of CdMnSe/ZnSe. A model is obtained for studying the process of self-assembly of tetrahedral cells in alloys [17]. Attempts were made to construct models for explaining ferromagnetism in ZnMnO on the basis of assumptions about its intrinsic nature [18] or as a consequence of some metastable phase [19]. A model is known [20] that quantitatively describes the processes of passivity of defects in a polycrystalline CdTe:Cl. The article [21] describes a model based on a completely microscopic theory, which allows one to demonstrate the effect of high-order optical nonlinearities in the coherent control signal for ZnSe. The [22] proposed a model that allows one to explain of laser shock waves impact on a defect system in narrow-gap HgCdTe alloys. Modelling proposed in the article [23] provides calculations of internal tensions in the ZnBeSe alloys. A model has been developed [24] that makes it possible to describe the photoluminescence spectra of localized excitons of $CdS_{1-x}Se_xS$ with a hexagonal structure and alloys in which regions with a hexagonal structure and a structure with stacking faults coexist. Work continues on improving the models that explain the mechanism of the transition from 2D to 3D growth in the CdSe / ZnSe system [25]. There are contradictory models on the basis of which attempts are made to describe the growth of ZnO films on GaAs substrates by pulsed laser

deposition [26 – 30]. Model representations [31] make it possible to better understand the photoluminescence spectra of an (Cd,Mn)Te in the presence of a spin-polarized two-dimensional hole gas and can now be useful in elucidating certain properties of the magnetic phase in a quantum well.

Thermodynamic modeling of critical phenomena in solid solutions of A_2B_6 semiconductors. Simulation of the process of formation of critical spaces and spaces of coexistence of phases in multicomponent and multiphase systems may be carried out on the basis of a differential topological approach [32, 33, 37 – 42]. According to Maxwell's principle, the space of coexistence of phases arises when two (or more) global minima of potential functions of system have the same depth. The appearance of such a space corresponds to the classical phase transition of the first kind. At some points in this space, the existing phase may become unstable, creating a bifurcation subspace. Two phases in some space may be identical under certain conditions, creating a critical space of the second order. When there is three or four identical phases having critical spaces of third order or fourth respectively.

Modeling of critical phenomena for A_2B_6 we will show on an example of Zn-Cd-Te system that is of great interest as a buffer material in the formation of heterostructures strictly matched for a period of crystal lattices for infrared devices and X-ray sensors To obtain a thermodynamic model to predict of the ordering in a triple system, it is necessary to construct an expression for the free energy of the system as a potential function dependent on the system parameters. In the framework of this paper, the expression for the free energy of a $Zn_XCd_{1-X}Te$ solid solution was constructed as a function of the component concentrations and temperature of the system $F=F(X_{AB},X_{AC},T)$, where X_{AB} and X_{AC} are understood to mean the concentration of atomic pairs $Zn-Te$ and $Cd-Te$ in a quasi-binary approximation. To analyze the existence of a stable phase need conditions [32] under which the first derivative of the free energy of the system by the concentrations of the corresponding components x will be equal to zero, and the second derivative will have positive values:

$$\frac{dF}{dx}=0\,;\quad \frac{d^2F}{dx^2}>0\,. \tag{1}$$

The space of instability that is bifurcation space is calculated on the conditions of zero first and second derivatives, and the positive value of the third derivative:

$$\frac{dF}{dx}=\frac{d^2F}{dx^2}=0\,;\quad \frac{d^3F}{dx^3}>0\,. \tag{2}$$

The condition for the existence of a critical space of the second order is the correspondence with the zero values of the first, second and third derivatives simultaneously and the positive value of the fourth derivative:

$$\frac{dF}{dx}=\frac{d^2F}{dx^2}=\frac{d^3F}{dx^3}=0\,;\quad \frac{d^4F}{dx^4}>0\,. \tag{3}$$

In formulas (1–3) there are complete derivatives, which in the case of $Zn_XCd_{1-X}Te$ alloy means differentiation by X_{AB} and X_{AC}.

Thus, for calculating the positions of the boundaries of phase stability, it is necessary to construct an analytical expression for free energy. The application of the above mathematical

procedures will allow analytically obtain the position of the boundaries of the critical spaces of the required order. At the same time, the expressions (2) correspond to the spinodal curves indicating the thermodynamic position of a completely unstable state of the phase. To calculate the positions of the boundaries of the metastable states (binodals of decay), it is necessary to compare the expressions (1) that need to be written for each of the coexisting phases.

Thermodynamic modeling of free energy of a solid phase of $Zn-Cd-Te$ system. The free energy of the triple zinc system can be looked at as the sum of free energy contributions for pure binary solids components, i.e., zinc and cadmium systems, the free energy of the ideal mixture, without taking into account the interaction between the components and the component taking into account the deviation of the value of the free energy from the energy of the ideal solution [34, 35]:

$$F = \sum_{i=1}^{2} F_i + F^{id} + \Delta F^{ex}, \tag{4}$$

where F_i is the free energy for pure binary components with F_{Zn-Te} and F_{Cd-Te} constituents; F^{id} is the free energy of the ideal mixture without taking into account the interaction between the components; ΔF^{ex} – deviation of the value of free energy from the energy of the ideal solution. The Bethe grid, taking into account the interaction of the first and second nearest adjacent atoms, is depicted in Fig. 1. For convenience, different types of atoms, i.e. atom Te, Zn, and Cd, are indicated by the numbers 1, 2 and 3, respectively. Mark 2, 3 denotes the location of an atom of type 2 or 3.

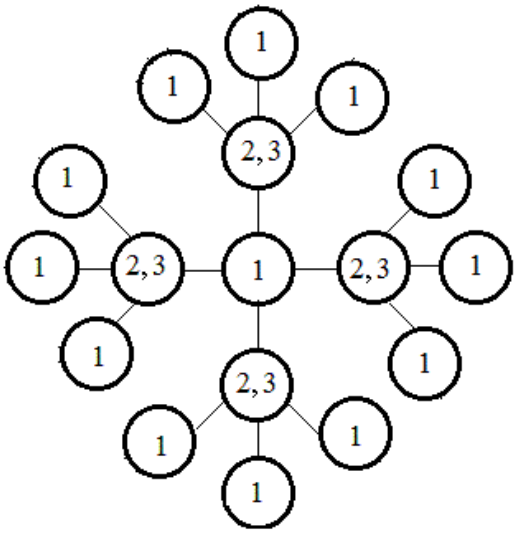

Fig. 1. Bethe grid for a triple $Zn_X Cd_{1-X} Te$ solid solution. The number 1 denotes the atom Te, 2 is the atom Zn, and 3 is the atom Cd

Then, taking into account the interactions of the atoms of the first and second coordination spheres, the components of free energy for pure binary constituents can be represented as:

$$F_{12} = \left\{ w_{12} + \frac{z_2}{z_1}(w_{11}^2 + w_{22}^1) \right\}, \tag{5}$$

$$F_{13} = \left\{ w_{13} + \frac{z_2}{z_1}(w_{11}^3 + w_{33}^1) \right\} , \quad (6)$$

where w_{12} is the binding energy between atoms Te and Zn, provided that they are the first closest neighbors. Accordingly, w_{13} denotes the binding energy between the nearest adjacent atoms of Te and Cd. The denotations w_{11}^2 and w_{11}^3 in (5) and (6) correspond to the binding energy between the second nearest neighboring atoms of Te on the condition that atom of Zn or atom of Cd is located between them respectively. Accordingly, w_{22}^1 and w_{33}^1 is the binding energies between the second nearest neighboring atoms of Zn and atoms of Cd on the condition that the Te atom is between them. Constants z_1 and z_2 in (5) and (6) are respectively the number of nearest neighboring atoms for each of the atoms (z_1=4) and second nearest neighboring atoms (z_2=12) in a zinc grid. It should be noted quite complicated problems associated with the calculation of energy connections, but in the process of obtaining derivatives, already at the stage of finding the second derivative, in connection with the linearity of expressions (5) and (6) this part of the expression (2) is completely degenerate and does not affect the verification of conditions (2) – (3).

The free energy for a mixture of ideal components of a solution, that is, the second term in (4) can be found by the classical expression:

$$F^{id} = -TS^{id} ,$$

where S^{id} is the entropy of an ideal solution, in which the atoms are randomly located. The value of the configurationally entropy S^{id} can be expressed in terms of the total number of atoms in the solution N_0 and the concentration parameter x:

$$S^{id} = -R \cdot ((1-x)\ln x + x\ln x), \quad (7)$$

where R - gas constant. Taking into account the connection of the concentration parameter x with the number of pairs of atoms N_{12} and N_{13}:

$$x = N_{12} / N_0$$
$$1-x = N_{13} / N_0$$

and the number of pairs of atoms with corresponding moles of X_{12} and X_{13}:

$$N_{12} = z_1 N_0 X_{12}$$
$$N_{13} = z_1 N_0 X_{13}$$

the expression (7) can be represented as:

$$S^{id} = -z_1 R \cdot (X_{12}\ln X_{12} + X_{13}\ln X_{13}) . \quad (8)$$

The formula (8) is most convenient for differentiation.

The deviation of the value of the free energy from the energy of the ideal solution is expressed by the difference between the configuration entropy and the entropy of the ideal solution, the temperature and the mixing energy:

$$F^{ex} = -T(S - S^{id}) + \Delta E . \quad (9)$$

According to the theory of simple solutions, the mixing energy ΔE can be expressed through the interaction parameter and mole fractions of the solution components in the form:

$$\Delta E = \alpha_{12-13} \frac{X_{12} X_{13}}{X_{12} + X_{13}},$$

where α_{12-13} – interaction parameter. In the approximation $S = S^{id}$, the expression (4) taking into account (9) takes the form:

$$F = \sum_{i=1}^{2} F_i - TS^{id} + \Delta E . \quad (10)$$

Note that for the analysis of higher derivatives in terms of composition concentrations starting from the second one, in the framework of the regular approximation it suffices to consider only two last terms in (10):

$$-TS^{id} + \Delta E = z_1 TR(X_{12} \ln X_{12} + X_{13} \ln X_{13}) + \\ + \alpha_{12-13} \frac{X_{12} X_{13}}{X_{12} + X_{13}} .$$

The interaction parameter α_{12-13} within the framework of work was considered as a function of temperature T [37]:

$$\alpha_{TeZn-TeCd} = (17230 - 14{,}83\mathrm{T})\ \mathrm{J/Mole}.$$

Prediction of critical phenomena in ternary system $Zn - Cd - Te$**.** In order to analyze the probability of occurrence of critical spaces and spaces of coexistence of phases in the system $Zn - Cd - Te$, the analytical expressions of higher derivatives according to the order parameters X_{ij} for the free energy of the system were obtained and investigated. Derivatives by concentrations from the first to fourth inclusive for the free energy (4) of the solid solution $Zn_X Cd_{1-X} Te$ were calculated using the methods of matrix-vector differentiation of multidimensional systems. To obtain matrices of higher derivatives, the method of direct sums [34] was used. The algorithm for calculating the higher derivatives of free energy consisted of successive calculations of components of derivatives by corresponding concentrations, compilation of matrices from components of derivatives, calculation of their determinants and calculation of positions of zero contours. As a result of calculating the first derivative of free energy (4), components of the derivative F_i ($i = 1, 2$) of the function of two variables was obtained as two partial derivatives by X_{12} and X_{13}:

$$F_i = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix},$$

where F_1 and F_2 are partial derivatives of free energy by X_{12} and X_{13}, respectively. The obtained analytical expressions were used to calculate the components of the second derivative of the free energy of the investigated system:

$$F_i = \begin{pmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{pmatrix}, \tag{11}$$

where the element of the matrix F_{11} is the analytic expression of the partial derivative of F_1 by X_{12} concentration, F_{12} is the corresponding derivative of F_1 by X_{13} concentration, F_{21} is the derivative of F_2 by X_{12} concentrations and F_{22} is the derivative of F_2 by X_{13}. The analytical expression of the determinant of the second derivative was obtained for the components of the matrix (11) and its value was calculated according to the concentration parameter x with the given step for $x \in (0;1)$. The values found were used to obtain the null contours of the second derivative and to analyze the stable phases of the $Zn-Cd-Te$ system in accordance with (1). To obtain the highest free energy derivatives, the Maxima system's calculation tools were used [43]. The results of calculations are shown in Fig. 2.

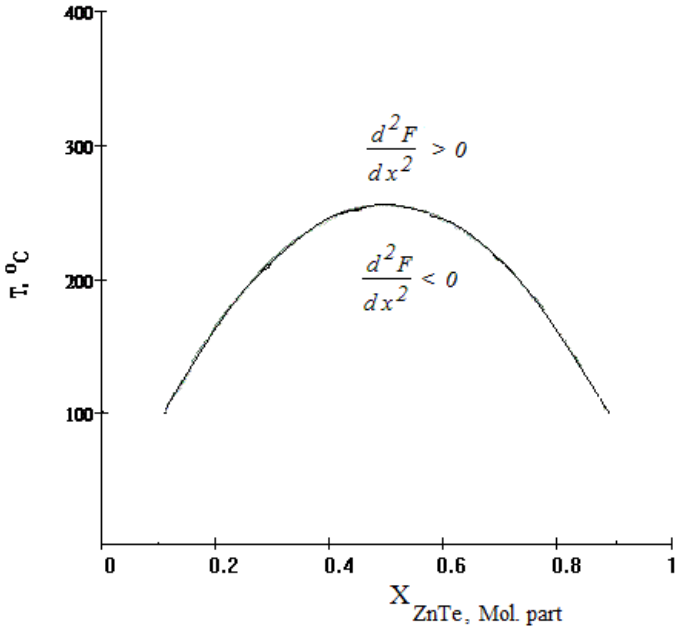

Fig. 2. The cross section of the existence of solid solutions phase diagram of $Zn-Cd-Te$ system. The results of numerical calculations of the zero contour of the second derivative of the free energy of the system are shown

The points satisfying the condition $\det F_i = 0$ were reflected on the cross section for the existence of solid solutions of the state diagram of the $Zn-Cd-Te$ system. After that, areas were determined in which the values of the respective determinants were positive or negative. In

the next step, each of the elements F_{ij} of the matrix (1.3.2) differentiated by concentrations X_{ij}. As a result of the differentiation, two matrices of partial derivatives were obtained. The first of them consisted of the components of the F_{ij} obtained by differentiation by X_{12}, the second one from the components obtained by differentiation in X_{13}:

$$F_{ij1} = \begin{pmatrix} F_{111} & F_{121} \\ F_{211} & F_{221} \end{pmatrix}, \quad F_{ij2} = \begin{pmatrix} F_{112} & F_{122} \\ F_{212} & F_{222} \end{pmatrix}. \tag{12}$$

The expression for the determinant of the third derivative was obtained on the basis of the direct sum method as the sum of the determinants of the matrices (12):

$$DetF_{ijk} = DetF_{ij1} + DetF_{ij2}. \tag{13}$$

The calculations of the values of the determinants (13) were used to calculate the instability spaces, that is, the bifurcation spaces under the conditions (2). The results of calculations of zero contour are shown in Fig. 3.

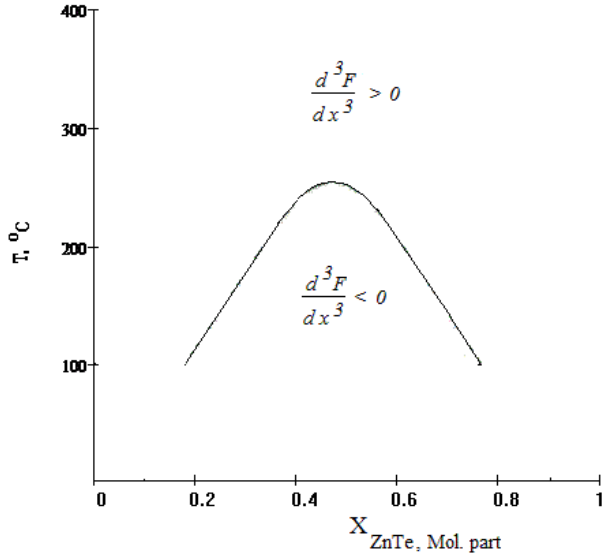

Fig. 3. The cross section of the existence of solid solutions phase diagram of $Zn-Cd-Te$ system. The results of numerical calculations of the zero contour of the third derivative of the free energy of the system are shown

To obtain the analytical expression of the determinant of the fourth derivative of free energy, the matrices of the partial derivatives of the components (12) were calculated:

$$F_{ij11} = \begin{pmatrix} F_{1111} & F_{1211} \\ F_{2111} & F_{2211} \end{pmatrix}, \quad F_{ij12} = \begin{pmatrix} F_{1112} & F_{1212} \\ F_{2112} & F_{2212} \end{pmatrix} \quad F_{ij21} = \begin{pmatrix} F_{1121} & F_{1221} \\ F_{2121} & F_{2221} \end{pmatrix},$$
$$F_{ij22} = \begin{pmatrix} F_{1122} & F_{1222} \\ F_{2122} & F_{2222} \end{pmatrix}. \tag{14}$$

The determinant of the complete fourth derivative of free energy was obtained as the sum of the determinants of the matrices (14):

$$DetF_{ijkl} = DetF_{ij11} + DetF_{ij12} + DetF_{ij11} + DetF_{ij22}$$

The results of the calculation of the zero contours of the complete fourth derivative of the free energy of the system are shown in Fig. 4.

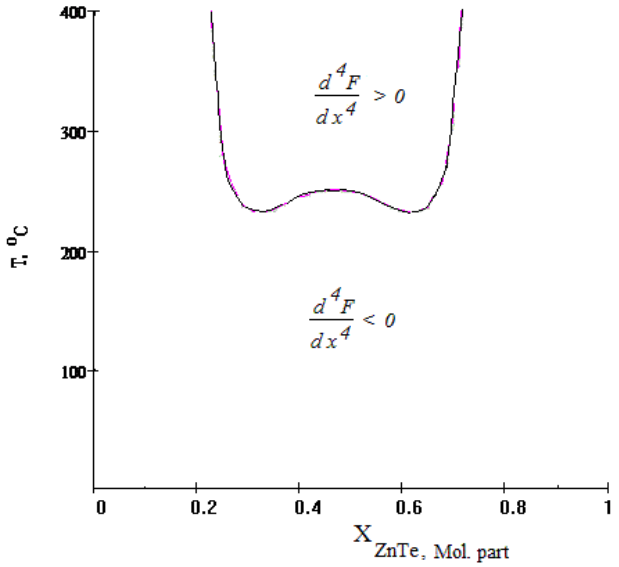

Fig. 4. The cross section of the existence of solid solutions phase diagram of $Zn-Cd-Te$ system. The results of numerical calculations of the zero contour of the fourth derivative of the free energy of the system are shown

In order to verify the condition (3) and calculate the domains of the second-order critical space were used the results of calculating the values of the determinants of the matrices (11), (12) and (14), as well as the positions of the zero contours depicted on Fig.2. - 4. The region in which the most probable occurrence of critical spaces of the second order is shown in Fig. 5:

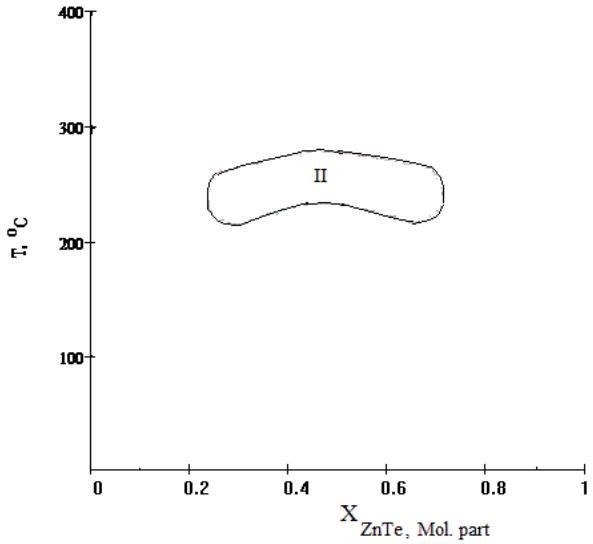

Fig. 5. The cross section of the existence of solid solutions phase diagram of $Zn-Cd-Te$ system. The results of numerical calculations of the region of the conditions for forming the spaces of coexistence of phases of order two are shown (the region found is indicated by the mark II)

Conclusion

Within the framework of thermodynamic modelling, the zero contours of the free energy derivatives from the first to the fourth inclusive was calculated and plotted for the $Zn_XCd_{1-X}Te$ solid solution on the diagrams of the state of the $Zn-Cd-Te$ system. The space in which the simultaneous occurrence of two kinds of solid phases is most probable was found for the $Zn-Cd-Te$ system. The results are obtained for temperatures in the range from 100 to 400 degrees Celsius. From the results of the calculations, it follows that the most probable region of the concentration space in which space of coexistence of phases of the order of two can form corresponds to concentrations in the range of 0.25 – 0.75 at temperatures of the 210-290 degrees Celsius. The data obtained during the simulation are important from a practical point of view, since they are related to the difficulties in the synthesis of $Zn_XCd_{1-X}Te$ layers and allow the development of recommendations for the process of their growing under different conditions. The study of the obtained positions of the zero contours of higher derivatives of free energy in the framework of the considered model opens the possibility of estimating the occurrence of periodic oscillations of the composition. The proposed model allows us to analyze the processes of formation of concentration domains in the volume of material while providing the necessary conditions for the synthesis of $Zn_XCd_{1-X}Te$ solid solutions.

The results obtained in this paper open up the possibility of studying the possibility of the emergence in a solid solution of spaces of coexistence of phases of higher orders [40, 41], when three or more simultaneously coexisting spaces may arise in the solid phase.

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ КРИТИЧЕСКИХ ЯВЛЕНИЙ В ТВЕРДЫХ ПОЛУПРОВОДНИКОВЫХ РАСТВОРАХ СОЕДИНЕНИЙ A_2B_6

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Математическое моделирование критических явлений в многокомпонентных твердых растворах полупроводников было проведено на основе теории фазовых переходов и теории катастроф. В работе разработан метод математического моделирования для вычисления пространств сосуществования фаз второго порядка в тройных твердых растворах на основе соединений II - V групп периодической системы. Представлен алгоритм расчета нулевых контуров функции свободной энергии системы, критических пространств и пространств сосуществования фаз. Нулевые контуры функции свободной энергии системы находились с использованием дифференциально-топологического подхода. Вычисления положений пространств сосуществования фаз проводились в рамках приближения регулярного раствора с помощью свободного пакета компьютерной

алгебры Maxima. Математическое моделирование пространств сосуществования фаз были выполнены в приближениях взаимодействия как первой, так и второй ближайших соседних пар атомов, а также температурной зависимости параметра взаимодействия. Для анализа процессов возникновения самоорганизованно упорядоченных структур используются современные методы компьютерного моделирования. Рассчитаны положения пространств сосуществования фаз второго порядка для системы полупроводников с использованием предложеного в работе математического метода. Получено многокомпонентные фазовые диаграммы с учетом возможности существования бифуркационных пространств, критических пространств и пространств сосуществования фаз различных порядков, дает возможность прогнозировать процессы потерю стабильности в трехкомпонентных полупроводниковых растворах на основе соединений II - V и групп периодической системы с различными режимами их синтеза и эксплуатации.

Ключевые слова: математическое моделирование, фазовые диаграммы, твердые растворы полупроводников II – VI групп.

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ КРИТИЧНИХ ЯВИЩ У ТВЕРДОМУ РОЗЧИНІ НАПІВПРОВІДНИКІВ СПОЛУК A_2B_6

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Математичне моделювання критичних явищ у багатокомпонентних твердих розчинах напівпровідників було проведено на основі теорії фазових переходів і теорії катастроф. В роботі розроблено метод математичного моделювання для обчислення просторів співіснування фаз другого порядку у потрійних твердих розчинах на основі сполук II – VI груп періодичної системи. Надано алгоритм обчислення нульових контурів функції вільної енергії системи, критичних просторів і просторів співіснування фаз. Нульові контури функції вільної енергії системи знаходились за використанням диференціально-топологічного підходу. Обчислення положень просторів співіснування фаз проводились у рамках наближення регулярного розчину за допомогою вільного пакету комп'ютерної алгебри Maxima. Математичне моделювання просторів співіснування фаз було виконано у наближеннях взаємодії як першої, так і другої найближчих сусідніх пар атомів, а також температурної залежність параметра взаємодії. Для аналізу процесів виникнення самоорганізовано впорядкованих структур використовуються сучасні методи комп'ютерного моделювання. Обчислено положення просторів співіснування фаз другого порядку для системи напівпровідників з використанням запропонованого в роботі математичного методу. Отримано багатокомпонентні фазові діаграми з урахуванням можливості існування біфуркаційних просторів, критичних просторів та просторів співіснування фаз різних порядків, що надає змогу прогнозувати процеси втрату стабільності у трьохкомпонентних напівпровідникових розчинах на основі сполук II – VI груп періодичної системи за різними режимами їх синтезу та експлуатації.

Ключові слова: математичне моделювання, фазові діаграми, тверді розчини напівпровідників II – VI груп.