SIMULATION OF PHASE TRANSPORTATIONS IN THE FIELD OF INTERNAL STRESSES

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Abstract

The main types of the internal stresses are the thermal and residual ones and fields of structural defects as well. These stresses have an essential effect on the phase transformations in materials. The kinetics of the process is described by a parabolic equation under corresponding initial and boundary conditions. The aim of this paper is simulating the phase transformations in the field of the internal stresses with logarithmic coordinate dependence. Such dependence allows the exact solution of the diffusion kinetics task to be obtained. The triple grain boundaries are considered as structural defects. They serve as stress concentrators under external loadings. This is caused by the orientation dependence of elastic and thermophysical characteristics of the contiguous grain materials. The dilatation field of considered defects depends logarithmically on the radial coordinate. The hydride phases formation within the alloys on the base of zirconium is enough to be mentioned as an illustration. This material is used for claddings of fuel elements of nuclear reactors. Analytical relations for the field of atomic hydrogen concentration near the triple grain boundaries are given. If the concentration of hydrogen atoms exceeds the solubility limit at a given temperature, hydride phases are formed in zirconium. The further growth of hydrides is limited by the diffusion supply of hydrogen atoms. The exact analytical solution task of phase transformations in the area of the triple grain boundaries is the test example for a complex field of internal stresses.

Key words: internal stresses, diffusion kinetics, phase transformations

1. INTRODUCTION

The strength of structural components in modern structures depends on the level and character of internal stresses. They occur within a material in the presence of non-uniform deformation. The main types of the internal stresses are the thermal (developed by Parkus, 1959) and residual ones and field of structural defects as well (developed by Teodosiu, 1982). The stresses change the strength properties as a result of diffusion process present. The physical mechanisms underlying changes of properties include, for example, decreasing of surface fracture energy, stress corrosion cracking and hydrogen embrittlement (on the basis of research by Varias and Massih, 2000). These mechanisms also include dif-fusion of interstitial impurities (e.g. hydrogen and oxygen) in the internal stress field. Hydrogen is dominant among these interstitial impurities. This dominance is caused by the high diffusion mobility of hydrogen atoms in a wide range of temperature. At room temperature, for example, the diffusion coefficient of hydrogen atoms is greater by several orders of magnitude than the diffusion coefficients of other substitutional and/or interstitial impurities.

Internal stresses have an essential effect on the phase transformations in materials. The kinetics of the process is described a parabolic equation under corresponding initial and boundary conditions. In general, the internal stresses fields have complex dependence on coordinates. A pleasant exclusion from a general rule is the internal stresses with loga-

rithmic coordinate dependence. Such dependence allows the exact solution of the diffusion kinetics task to be obtained. The aim of this paper is simulating the phase transformations in the field internal stresses with a logarithmic coordinate dependence. The triple grain boundaries are considered as structural defect. They serve as stress concentrators under external loadings. This is caused by the orientation dependence of elastic and thermophysical characteristics of the contiguous grain materials. The dilatation field of considered defects depends logarithmically on the radial coordinate. The hydride phases formation within the alloys on the base of zirconium is enough to be mentioned as an illustration. This material is used for claddings of fuel elements of nuclear reactors.

Internal stresses change only kinetics of a new phase growth. The impurities activity remains constant. Its changing in the stress field is not considered in this model. In general, the internal stresses fields have complex dependence on coordinates. Therefore, essential mathematical difficulties occur when solving a diffusion equation taking into account the stresses. The exact analytical solution of such problems is known only for logarithmic coordinate dependence of the internal stresses field.

2. PHYSICAL ESSENCE OF THE INTERNAL STRESSES

The internal stresses occur within a material in the presence of non-uniform deformation. Typical examples of such stresses are temperature and residual stresses as well as ones about the structural defects. Occurrence of the thermal stresses is caused by non-uniform distribution of the temperature field. In general case the temperature stresses have a rather complex dependence on coordinates. Therefore, account of their effect on the diffusion processes kinetics is of essential mathematical difficulties. However, in some cases the thermal stresses logarithmic depend on the coordinates. The thermal stresses in a hollow cylinder are the example of such dependence. It is known that interaction of an impurity atom with the thermal stresses field depends on the first invariant of the stresses tensor. For the thermal stresses in the hollow cylinder this characteristic is determined by the relation (on the basis of research by Melan & Parkus, 1953 and Timoshenko & Gudier, 1979):

$$\sigma_{ll} = \frac{2\alpha\mu(1+\nu)(T_1-T_2)}{1-\nu}\left\{\frac{1+2\ln\frac{r}{R}}{\ln\frac{R}{r_0}}+\frac{2r_0^2}{R^2-r_0^2}\right\}, (1)$$

where α is coefficient of linear expansion, μ is shear module, ν is Poisson's ratio, r_0 and R are inner and outer radius of a hollow cylinder, T_1 and T_2 are temperatures of inside and outside of a hollow cylinder correspondingly. This relation is obtained for the flat deformation conditions at the boundaries free of the stresses.

Such coordinate dependence is peculiar to the residual stresses in the hollow cylinder. The latter occur in the material when carrying out various technological operations. Let us consider the following version of the residual stresses formation. The cutting edges of the cylinder are moved apart by angle ω, and the missing material is placed there. During this operation the area about outer cylinder surface is under as-pressed condition, and about the inner cylinder surface – as-tensed condition. The first invariant of the residual stresses tensor for the flat deformation conditions also has the logarithmic coordinate dependence:

$$\sigma_{ll} = \frac{\omega\mu(1+\nu)}{2\pi(1-\nu)}\left\{1+2\ell n\frac{r}{R}+\frac{2\left(\frac{r_0}{R}\right)^2}{1-\left(\frac{r_0}{R}\right)^2}\ell n\frac{r_0}{R}\right\} (2)$$

where ω is angle of the cutting edges opening of the hollow cylinder. The rest notations correspond to the ones adopted before. The dilatation field in the area of the triple grain boundaries is simulated by the wedge disclination. The first invariant of the internal stresses tensor also has the logarithmic coordinate dependence similar to the formula (2), where ω is modulus of disclination rotation vector, r_0 and R are inner and external radiuses of the wedge disclination.

3. SEGREGATION OF IMPURITIES IN THE STRESSES FIELD

The typical size of the substitutional impurity is usually more (less) than the corresponding size of a basic material atom. The sizes of interstice (octa- and tetrahedral), as a rule, are less than the substitutional impurities size. Such inconsistency of the typical sizes leads to elastic interaction of the impurity atoms with the internal stresses. The interaction

potential is defined by the known relation (Vlasov et al. (2001) researched the interaction potential V):

$$V = -\frac{\sigma_{ll}}{3}\delta\upsilon \qquad (3)$$

where σ_{ll} is first invariant of tensor stresses, $\delta\upsilon$ is change of metal volume at an impurity atom placement. For $\sigma_{ll} > 0$ (tension stresses) and $\delta\upsilon > 0$ (an impurity atom increases a crystal lattice parameter) potential V takes a negative value. It corresponds to attraction of an impurity atom to the tension stresses area and its displacement from the compression stresses area. Relation (3) takes into account only dimensional effect in the energy of the impurity atom connection with the internal stresses field. In other words, inconsistency between the impurity atom sizes and the volume for its placement is accompanied by the elastic interaction of the impurity atom with the stresses fields. The other types of interactions (module, electrostatic, chemical ones) can be easily estimated by renormalization of the constants in relation (3).

The impurity concentration field is determined from the solution of the equation of a parabolic type under the corresponding initial and boundary conditions (on the basis of research by Vlasov & Fedik, 2002; Vlasov & Fedik, 2006):

$$\frac{1}{D}\frac{\partial C}{\partial t} = \Delta C + \frac{\nabla(C\nabla V)}{kT}, \ r_0 < r < R,$$

$$C(r,0) = C_0, C(r_0,t) = C_p^1, C(R,t) = C_p^2 \qquad (4)$$

where D is coefficient of atoms diffusion, k is Boltzmann constant, T is absolute temperature, C_0 is average concentration of impurity atoms, r_0 and R are inner and outer radiuses of the internal stresses action, C_p^1 and C_p^2 are equilibrium concentrations of the impurity atoms on the boundaries of the discussed field. Equation (4) connects physics and mechanics when simulating material damages in the internal stresses field. The complicated coordinate dependence of potential V does not allow us to obtain an analytical solution of task (4) in the class of the known functions and their combinations. This difficulty can be overcome successfully for the logarithmic coordinate dependence of potential V. It is caused by the fact that in this case potential V is a harmonic function, and its gradient is inversely proportional to a radius in the polar coordinate system. Physical meaning of the initial and boundary conditions of task (4) is quite evident. At start time the impurity atoms concentration is equal to an average value. Equilibrium impurities concentration is quickly set on the area boundary and then kept in accordance with potential V on the outer cavity too. From equation (4) one can see that segregation of the impurity atoms is proportional to the gradient of potential V. Therefore, the constants in the relations for σ_{ll} disappear when differentiating. It simplifies the solution of diffusion kinetics task. Keeping commonality, let us consider the internal stresses in the triple grain boundaries. The first invariant of the stresses tensor is determined by relation (2). Taking into account (2) and (3) after simple mathematical conversions we will obtain:

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1+\beta}{r}\frac{\partial C}{\partial r}, \ r_0 < r < R,$$

$$C(r,0) = C_0, C(r_0,t) = C_p^1, C(R,t) = C_p^2, \qquad (5)$$

$$\beta = \frac{\mu\omega(1+v)\delta\upsilon}{3\pi(1-v)kT}.$$

The dimensionless parameter of task β defines the relation between the binding energy of impurity atoms with the field of the internal stresses and heat motion. In the case $\beta \ll 1$, the internal stresses field is slight disturbance of a diffusion flux as a result of the concentration gradient. For $\beta \gg 1$ the internal stresses field gives the main contribution into the process kinetics. At $\beta \cong 1$ diffusion fluxes of the impurity atoms are commensurable at the expense of the concentration gradients and interaction potential. The estimations show that for some systems (for example, Zr-H) value $|\beta| \cong 1$. Taking $\beta = -1$ ($\omega < 0$ for accepted scheme of the internal stresses), we obtain a rather simple variant of task (5):

$$\frac{1}{D}\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2}, \quad r_0 < r < R,$$

$$C(r,0) = C_0, C(r_0,t) = C_p^1, C(R,t) = C_p^2. \qquad (6)$$

An interesting feature of the obtained equation should be noted. It is seen the internal stresses change symmetry of the diffusion equation. Kinetics of the impurity segregations in the hollow cylinder runs according to the law of flat symmetry. The solution of task (6) gives distribution of the impurity atoms concentration taking into account the internal stresses field

$$C - C_0 = \frac{R\left(C_p^1 - C_0\right) - r_0\left(C_p^2 - C_0\right) + r\left(C_p^2 - C_p^1\right)}{R - r_0} +$$

$$+ \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[(-1)^n \left(C_p^2 - C_0\right) - \left(C_p' - C_0\right) \right] \times \qquad (7)$$

$$\times \sin \frac{\pi n (r - r_0)}{R - r_0} \exp\left(-\frac{\pi^2 n^2 D t}{(R - r_0)^2} \right).$$

As times goes by, the concentration field of the impurity atoms takes a stationary character in accordance with the interaction potential. In this case redistribution of the impurity atoms takes place when keeping their integral concentration. The strength characteristics of the material are changed and it has a disposition to damages. The limiting link of this process is diffusion of the alloying elements of the alloy in the internal stresses field. If in a local volume of the material the concentration of the impurity atoms exceeds the solubility limit at given temperature, a new phase separations are formed. So for example, in Zr-H system hydrides are formed.

4. NEW PHASES FORMATION IN THE STRESSES FIELD

The new phases are characterized by considerable volume changes in relation to the basic material. The stresses occur on the interphase boundaries, and microcracks are formed. The example of such damage is metal embrittlement when forming hydride phases (Wäppling et al (1997) researched the hydride-induced embrittlement in zirconium - based alloys). The internal stresses also have an effect on kinetics of a new phase growth. Let us consider the internal stresses in the triple grain boundaries. Maximal concentration of the impurity atoms occurs on the area boundary, where the new phase formation takes place. Its further growth is realized at the expense of impurity atoms diffusion. The task of defining kinetics of the new phase growth in the triple grain boundaries is mathematically formulated as follows

$$\frac{1}{D} \frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial r^2} + \frac{1 + \beta}{r} \frac{\partial C}{\partial r},$$

$$C(R_1,t) = C_2, \ C(r,0) = C_0 \ (r \geq R_0), \ C(\infty, t) = C_0, \qquad (8)$$

$$\left(C_1 - C_2\right) \frac{dR_1}{dt} = D \left\{ \left| \frac{dC}{dr} \right| + \left| \frac{C\beta}{r} \right| \right\}_{r=R_1},$$

where R_0 is radius of the a phase centre, R_1 is current radius of a new phase. The rest notations are correspond to the ones accepted before. On the moving

interphase boundary the concentration of the impurity atoms is changed in leaps and bounds: $C = C_1$ for the new phase and $C = C_2$ in the surrounding matrix ($C_1 > C_2$, $C_2 < C_0$, where C_0 is average concentration of the impurity atoms). It is supposed that a typical size of the new phase centre is considerably less than the wedge disclination radius. Such supposition allows us to consider the new phase growth in an unlimited matrix and obtain the analytical solution of task (8). Change of the new phase radius obeys the law $R_1(t) = \delta \sqrt{Dt}$, where δ - dimensionless parameter of the task. Its value is determined from the mass balance equation on the interphase boundary. For $\beta = -1$ approximately to "stationary interphase boundary" we will obtain a quadratic equation for determining parameter δ

$$\delta^2 - \frac{2\delta}{\sqrt{\pi}} \left| \frac{C_2 - C_0}{C_1 - C_2} \right| - \left| \frac{2C_2}{C_1 - C_2} \right| = 0. \qquad (9)$$

If $\beta = 0$, the internal stresses field is not taken into account. For determining parameter δ_1 of relations $R_1(t) = \delta_1 \sqrt{Dt}$ we will obtain a transcendental equation

$$\delta_1 = \frac{2}{\sqrt{\pi}} \left| \frac{C_2 - C_0}{C_1 - C_2} \right| \frac{K_1\left(\delta_1 \frac{\sqrt{\pi}}{2} \right)}{K_0\left(\delta_1 \frac{\sqrt{\pi}}{2} \right)}, \qquad (10)$$

where $K_0(x)$ and $K_1(x)$ are modified cylindrical functions. Keeping commonality, we take $C_0 = 2\times10^{-4}$ (at), $C_2 = 10^{-4}$ (at) and $C_1 = 3\times10^{-4}$ (at). From the solution of equations (9) and (10) we obtain $\delta = 1.3$ and $\delta_1 = 0.8$. The internal stresses field accelerates the diffusion process of the new phase growth. The other values of the boundary conditions change a numerical value of parameters δ and δ_1. The volume changes of the new phase cause the stresses on the interphase boundary. If the stresses level exceeds a critical value, the microcracks formation takes place (developed by Smith, 1997). The material damage is observed in a macroscopic scale. Simulation of this process also includes kinetics of the new phase growth.

Appearance of hydride phases in the shape of long cylindrical inclusions (needles) with the following growth of hydride plates in the radial direction has been observed experimentally. It is rather possible that hydride needles are formed just near the line

of the triple grain boundaries. Then the process covers abutting grain boundaries, i.e. the hydride plates occur in the radial direction.

5. CONCLUSIONS

The internal stresses have an essential effect on kinetics of diffusion processes in metals and alloys. When changing the concentration of the alloying elements, reducing the strength material characteristics takes place, and probability of damaging under the external load increases. Kinetics of the impurity atoms segregation obeys the equation of a parabolic type under corresponding initial and boundary conditions. The complicated coordinate dependence of the internal stresses field makes difficulties in obtaining the analytical solution of the diffusion equation in the stresses field. A good exclusion from the general rule is the internal stresses with a logarithmic coordinate dependence. Such dependence allows the analytical solution of the diffusion kinetics task to be obtained. It is caused by the fact that potential V is a harmonic function, and its gradient ∇V is inversely proportional to the radius in the polar coordinate system. The analytical dependences for the impurity atoms concentration taking into account the internal stresses in the triple grain boundaries have been obtained. Under the definite conditions some changes in the diffusion equation symmetry have been revealed. Kinetics of the impurity atoms segregation for cylindrical geometry runs according to the flat symmetry law. It increases a rate of the impurity segregation.

Analytical relations for the field of atomic hydrogen concentration near the triple grain boundaries are given. If the concentration of hydrogen atoms exceeds the solubility limit at a given temperature, hydride phases are formed in zirconium. The further growth of hydrides is limited by the diffusion supply of hydrogen atoms. The influence of a stress field is that, in addition to the concentration gradient, the hydrogen atoms migrate due to the stress field gradient of the triple grain boundaries. Because of this, the velocity of the hydride phase boundary increases.

Numeral simulation of the material phase transformations process taking into account the internal stresses field includes a definite sequence of the mathematical operations. These operations define the algorithm of the material phase transformations calculation: definition of the first invariant of the internal stresses tensor, mathematical formulation of the task of impurity atoms diffusion followed by the new phase formation. The exact analytical solution task of phase transformations in the area of the triple grain boundaries is the test example for a complex field of internal stresses.

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MODELOWANIE PRZEMIAN FAZOWYCH W POLU NAPRĘŻEŃ WEWNĘTRZNYCH

Streszczenie

Głównymi typami naprężeń wewnętrznych są naprężenia termiczne i rezydualne, a także obszary defektów materiałowych. Naprężenia te posiadają znaczący wpływ na przemiany fazowe w materiale. Kinetyka takich zjawisk opisana jest poprzez równanie paraboliczne z odpowiednimi warunkami początkowymi i brzegowymi. Celem niniejszego artykułu jest symulacja przemian fazowych w obszarze naprężeń wewnętrznych z logarytmiczną zależnością współrzędnych. Zależność taka umożliwia otrzymanie dokładnego rozwiązania zagadnienia kinetyki dyfuzji. Natomiast potrójna granica pomiędzy ziarnami brana jest pod uwagę jako defekt materiału i jest miejscem koncentracji naprężeń. Jako przykład pokazano strukturę stopów na bazie cyrkonu charakteryzującą się formowaniem faz hybrydowych. Dokładne rozwiązanie analityczne zagadnienia transformacji fazowych w obszarze potrójnych granic ziaren stanowi przykład testowy dla analizy kompleksowego pola naprężeń wewnętrznych.

COMPUTER METHODS IN MATERIALS SCIENCE