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MODELING OF VACANCY KINETICS IN NANOSTRUCTED HEAT-RESISTANT ALLOY AT THE THERMAL FATIGUE

A.V. Galaktionova and A. K. Emaletdinov

Ufa State Aviation Technical University, K.Marks str. 12, Ufa, 450000, Russian Federation

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Abstract. The paper deals with the modeling of vacancy kinetics in nanocrystalline alloys at the thermo-mechanical loading, including cyclic tensile stress and temperature. The evolution of vacancy system determines the durability of nanostructed two-phase alloys. The vacancy kinetics is determined by the diffusion equation, considering the diffusion and thermal tensions. The excess vacancy density and the total tensions are determined. The expressions for the characteristic vacancy lifetime and the chemical potential of vacancy are obtained. The system of equations for the inhomogeneous vacancy concentration at the one-dimension task solved by numerical methods is obtained. The excess vacancy density leads to the formation of vacancy clusters.

1. INTRODUCTION

The evolution of vacancy system and the pore formation under the cyclic thermo-mechanical loading determine the durability of the nanocrystalline two-phase alloys such as superalloys, which are the composite materials consisting of the cubic γ' -phase grains with size about to 0.5 μm and connected by the thin layers of matrix γ-phase with thickness about to 0.05 μm [1-3]. The alloys are affected by a complex influence of the several operational factors: the high loads, the vibration, the uneven cyclic heating. The vacancy formation and the activation of diffusion processes occur under the influence of thermo-mechanical loads. The excess inhomogeneous non-equilibrium vacancy concentration appears during the process of loading. The tensions occurring due to the difference of thermal expansion coefficients of the phases appear under the continuous temperature change.

2. DERIVATION OF VACANCY KINETICS

The vacancy kinetics is determined by the diffusion equation with a source of vacancy occurring by the thermally activated mechanism taking into account the diffusion and thermal tensions, and the tension concentration near the inclusions [4-8]. The partial diffusion coefficients of the components are different, what leads to the occurrence of vacancy flows in the grains and in the interlayers. The vacancy flows appear under the influence of non-uniform operating tensions and temperature of the alloy. In this work, the modeling of vacancy kinetics at thermo-mechanical loading including the cyclic tensile stress, the temperature tension and the heating to the high temperature taking into account the microstructure is performed for the first time.

An infinite isotropic plate placed under the influence of constant and cyclic tensile stresses along

Corresponding author: A.V. Galaktionova, e-mail: g-arina@yandex.ru

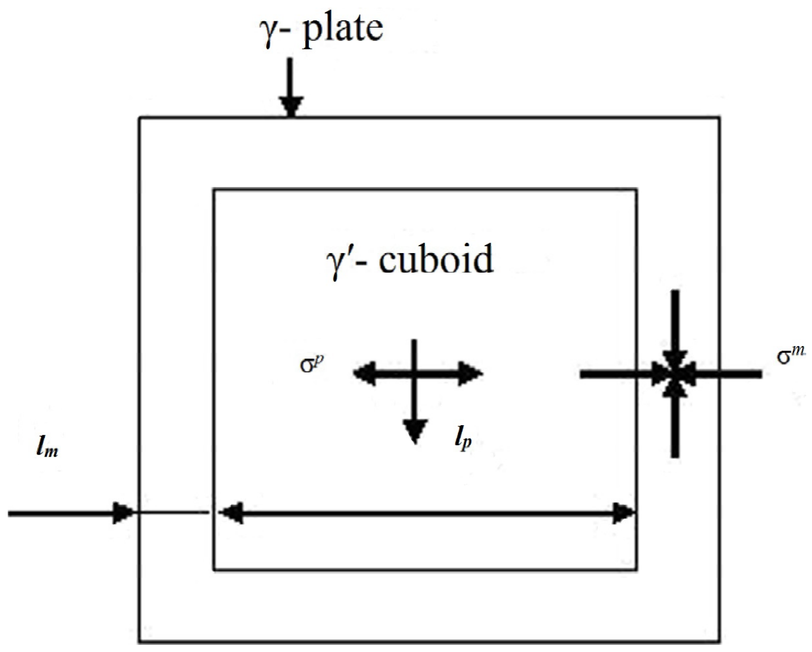

Fig. 1. The schematic microstructure of nickel superalloys.

the plate and temperature gradient across the plate is considered. It need to consider a periodic cell of γ'/γ-microstructure consisting of a γ' -cuboid surrounded by a γ-shell, which, in turn, consists of three γ-plate, three γ-blocks and small γ-cuboid to solve the problem of the phase tension determining (Fig. 1).

The interphase (coherent) tensions in the γ'/γ-microstructure of undeformed heat-resistant nickel alloys appear due to the difference between the parameters of γ- and γ'- lattices.

In works [9-11], the interphase tensions are calculated at the two-dimensional approximation (plane strain). According to the accepted assumptions, the stress condition of the periodic cell is described by two components of tension σ^m and σ^p (Fig. 1).

The formation of excess vacancies occurs by the action of thermo-mechanical loads. The kinetics of change of excess vacancy density at the first approximation is described by the equation [7]:

$$\frac{\partial c}{\partial t} + \nabla D \nabla c = \frac{c - c_0}{\tau_0}, \qquad (1)$$

where c - the excess vacancy density, c_0 - the equilibrium vacancy density, τ_0 - the average vacancy lifetime until absorption by drains (dislocations, boundaries, etc.), D - diffusion vacancy coefficient.

The characteristic vacancy lifetime until absorption by drains is estimated by the expression [7]:

$$\tau_0 = l^2 p / D, \qquad (2)$$

where l - the average distance between the drains, p - sticking coefficient of vacancy. The vacancy lifetime can vary from 10 to 10^3 seconds depending on the drain density.

The vacancies will have the chemical potential in the elastic tension σ and temperature T field in an isotropic medium, what can be represented as

$$\mu = kT \ln\left(\frac{c}{c_0}\right) - \frac{1}{3}\Omega\sigma + \frac{k_T}{cD}T, \qquad (3)$$

where Ω - vacancy power, characterizing the change of crystal volume at the vacancy formation in this crystal, k_T - thermal diffusion ratio. The first term describes the vacancy diffusion, the second and the third terms describe the vacancy drift under the influence of non-uniform tension and temperature, respectively. The equilibrium vacancy concentration is determined by the equation:

$$c_0 = \exp\left(\frac{-E + \sigma\Omega}{kT}\right), \qquad (4)$$

where E - the vacancy formation energy.

The system of equations (1)-(4) must be supplemented by boundary conditions. The concentration and diffusion tensions, the cyclic thermo-mechanical loading affect the non-equilibrium vacancy concentration. The magnitude of the concentration tensions depends on the size mismatch of atoms and the modulus of component compressibility. The diffusion tensions appear due to the unequal counter flows of the component atoms. The total tensions at the first approximation in the linear theory of elasticity will be determined by the expression [5-8]:

$$\sigma(r) = \sigma_0 + K_0\Omega c + \sigma_1 - K_0\alpha_T T(r), \qquad (5)$$

where σ_0, σ_1 - the tension values of the centrifugal forces of stretching and vibration, respectively, K_0 - the compression modulus, α_T - the coefficient of thermal expansion. The first term describes the centrifugal tensile stress, the second and the third terms describe the concentration and vibration tensions, the last term describes the thermo-elastic tensions.

The instabilities leading to the formation of vacancy clusters occur by the interaction of single excess vacancies in the tension and temperature field. The excess vacancy density c is determined by the expression:

$$\Delta c = c - c_0 = c_0 \frac{\Delta D}{D} + c_0 \exp\left(\frac{\sigma\Omega}{kT}\right). \qquad (6)$$

The solution of system of Eqs. (1)-(6) is possible only by numerical methods. Averaging over the midline of γ' -cuboid, an one-dimensional stationary task for a layered system consisting of γ' /γ-microstructure with thickness l_p/l_m, respectively, is considered to simplify the problem [5,6]. The conditions of continuity for the concentration and the vacancy flow density are given on the boundary. The qualitative profiles of non-uniform vacancy concentration

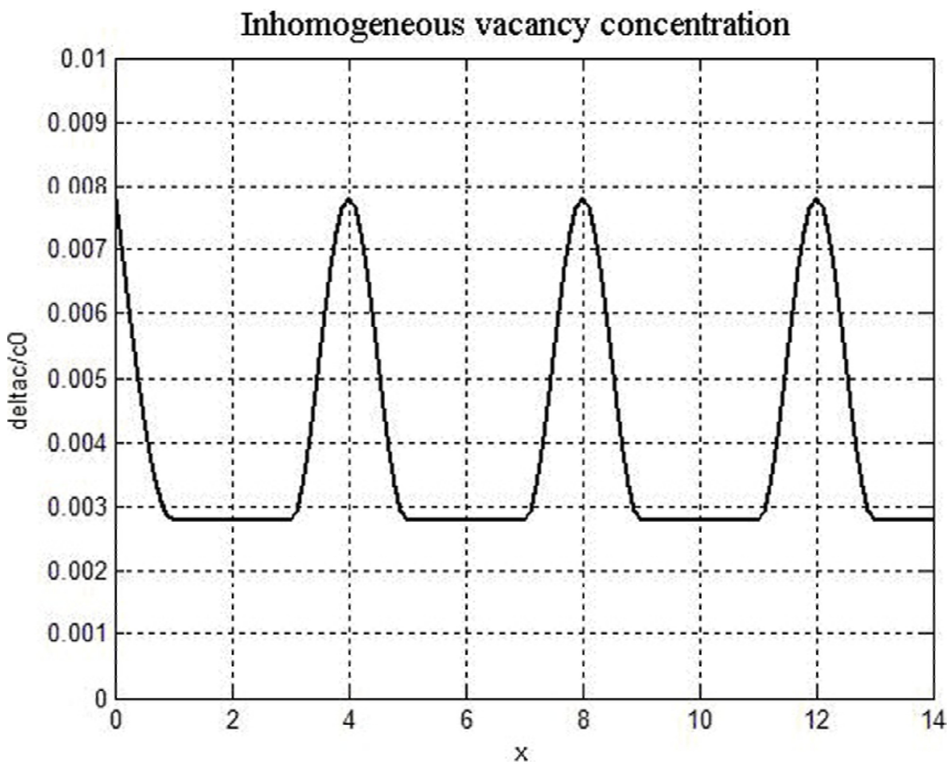

Fig. 2. The profile of non-uniform stationary vacancy concentration in the grains of γ' -phase 1 and γ-interlayer 2 under the thermo-mechanical loading.

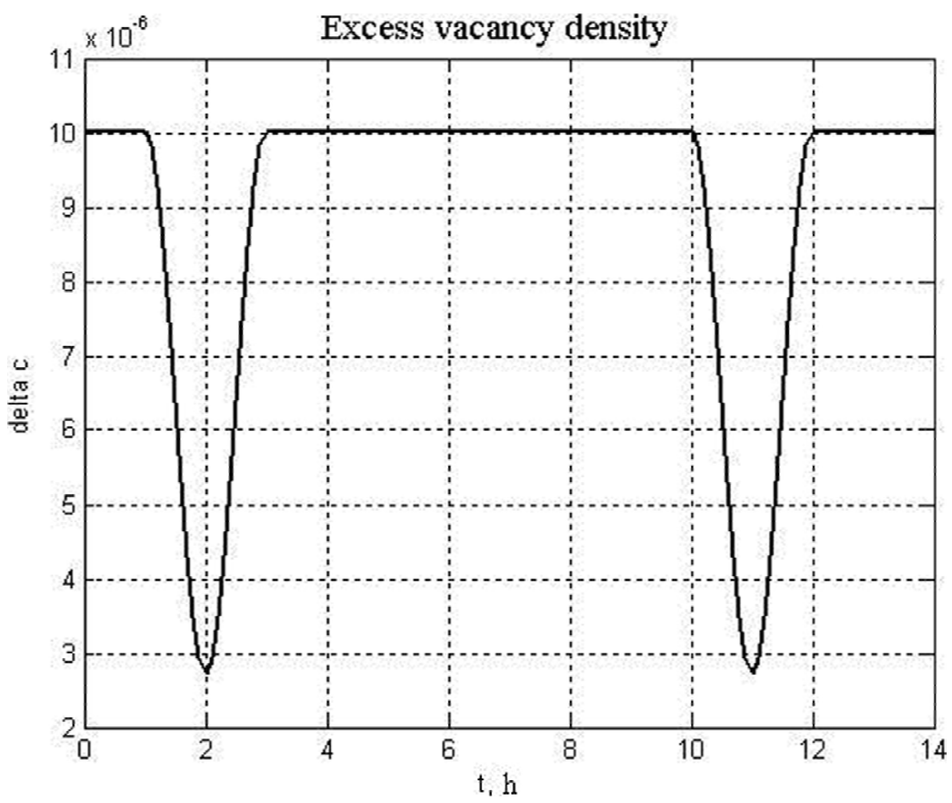

Fig. 3. The changing of the excess vacancy density under the thermo-mechanical loading.

in the γ'/γ-microstructure obtained by numerical calculations of the stationary one-dimensional problem are shown on Fig. 2.

Solving the above equations, we obtain the dependence of the pore growth rate and the pore size changes (Figs. 2-5).

3. CONCLUSIONS

The experimental data show the values of stationary distributions of fluctuations with a period which equal to 2.5*x*, whereas the theoretical calculations give the value which equal to 1.5*x*. The changing of excess vacancy density occurs at the stationary conditions in the form of the distribution of fluctuations caused by cyclic tension and temperature. The non-uniform vacancy concentration also has the form of periodic distributions. Thus, the excess vacancy density leads to the formation of vacancy clusters.

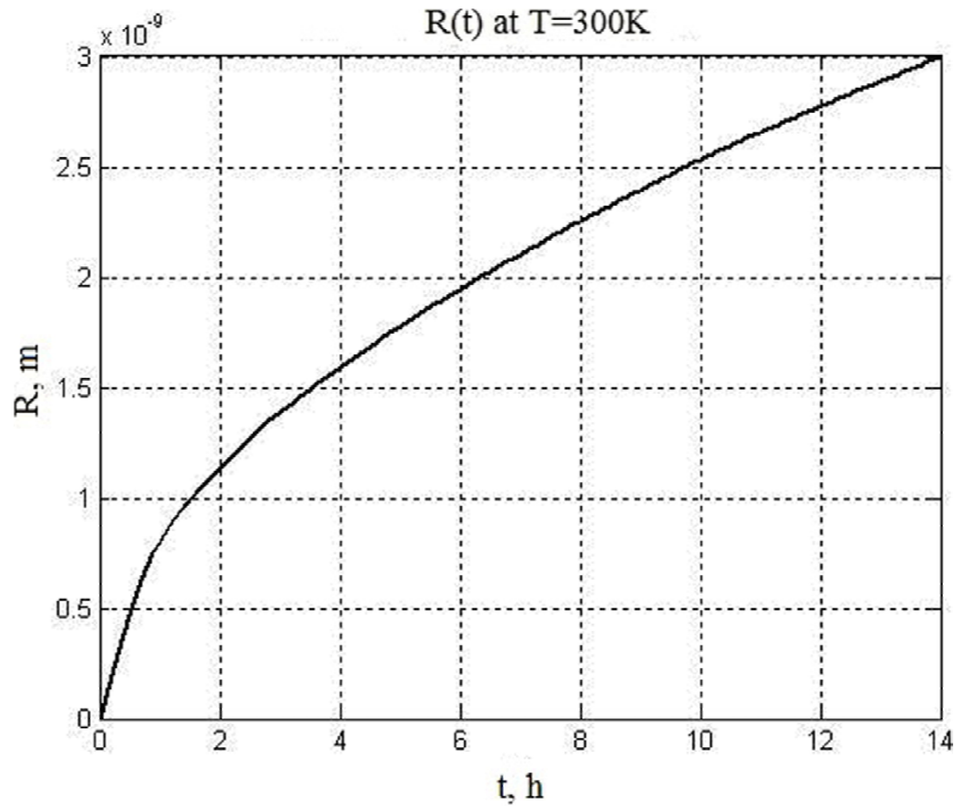

Fig. 4. The changing of pore size depending on time at 300K.

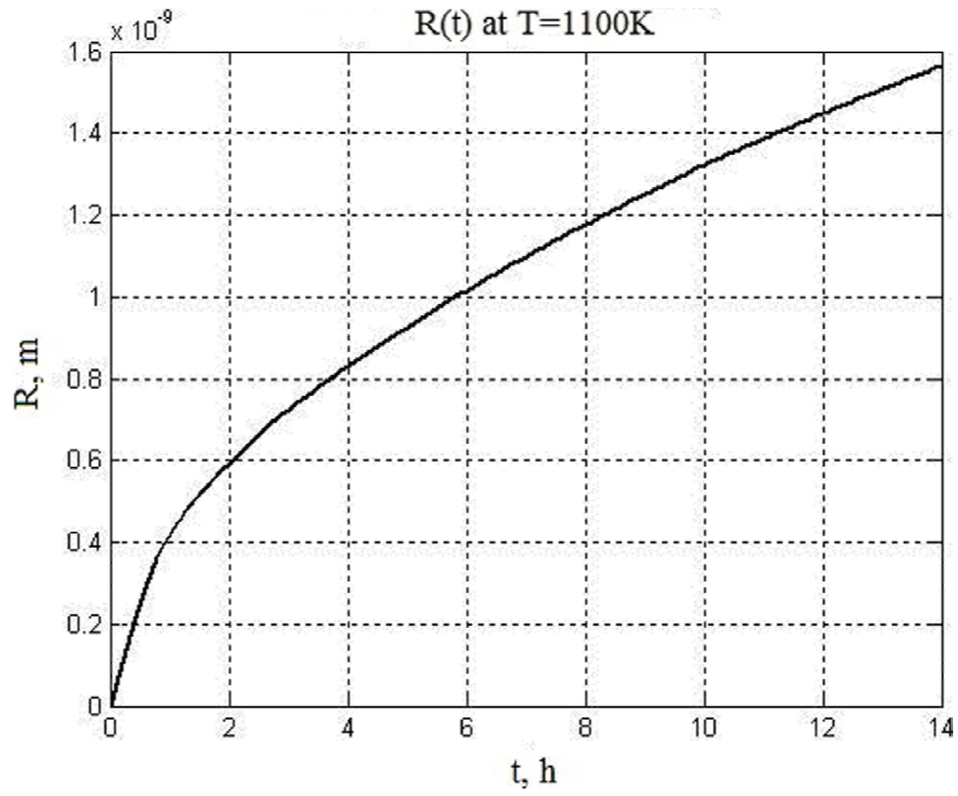

Fig. 5. The changing of pore size depending on time at 1100K.

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