diffusion-fundamentals
The Open-Access Journal for the Basic Principles of Diffusion Theory, Experiment and Application

Kinetic of Void Growth in fcc and bcc Metals.

Andrei V. Nazarov[1,2], *A.A.Mikheev*[3], *I.V.Valikova*[1], *Aung Moe*[1], *A.G.Zaluzhnyi*[1,2]

[1]Moscow Engineering Physics Institute (State University), Kashirskoe shosse, 32, 115409, Moscow, RUSSIA, [1]avn46@mail.ru

[2]Institute of Theoretical and Experimental Physics, Moscow, RUSSIA

[3]Moscow State University of Design and Technology, RUSSIA

1. Introduction

We examine how elastic stress, arising from voids, influences the diffusion vacancy fluxes and growth of voids in cubic metals. Usually, the equation of diffusion in the presence of stress field has the following form [1]:

$$\vec{\boldsymbol{J}} = -\boldsymbol{D}\left(\nabla \boldsymbol{c} + \boldsymbol{c}\frac{\nabla \boldsymbol{U}}{\boldsymbol{kT}}\right) \quad , \tag{1}$$

where $\boldsymbol{U}$ is an interaction potential of the diffusing atoms with the defects generating stress fields. Some authors consider point defects as the centers of dilatation [2]. In this approximation**:**

$$\boldsymbol{U} = \beta \frac{4}{3}\pi r_0^3 \boldsymbol{Sp}\,\sigma \tag{2}$$

where r_0 is the radius of the matrix atom, $r_0(1 + \beta)$ is the effective radius for impurity atom or a defect and $\boldsymbol{Sp}\sigma$ is the trace of stress tensor. Note that in a case of elastic stress, arising from void, $\boldsymbol{Sp}\sigma = \boldsymbol{Const}$**,** and a second term in Eq.(1) equals zero [2]. Consequently, the elastic stress, arising from voids, does not influence the diffusion vacancy fluxes and growth of voids. This queer result is a sequent of the Eq.(1). In particular therefore some authors considered a possibility of generalization of this equation [3-5].

The aim of our work is to examine the elastic stress influence on diffusion flux of vacancies using the approach, developed by us earlier [4] and to obtain a kinetic equation for the growth rate of voids in cubic metals

2. Main moments of theory of diffusion under stress and simulation of void growth

This approach takes into consideration, that the strains can alter the surrounding atom configuration near the jumping one and consequently the local magnitude of the activation barrier. Knowing this change, we can calculate the atomic jump rate and obtain an equation for the vacancy flow [4]. In this case, the vacancy flux depends on the matrix of the diffusion coefficients. Each of these coefficients depends on the strain tensor components in a nonlinear way. In corresponding nonlinear equations, the functional dependence on strain is determined by coefficients, which are the main characteristics of the strain influence on diffusion (SID coefficients). These coefficients are very sensitive to atomic structure in the nearest vicinity of defect and still more to atomic structure of the saddle-point configuration. We have built an advanced model to evaluate them. SID coefficient simulation is the first step of this work.

Then we used the results of theory of elasticity concerned with the displacement field around a sphere and obtained the equation for vacancy flux, where the influence of elastic stress near the void on this flux was taken into account.

Next step is the calculation of the dependence of the diffusion coefficient on the coordinates near the different size voids. To analyze these complicated dependences we used visualization.

The diffusion equation for vacancies in which the influence of elastic stress near the void on flux was taken into account is linearized and resolved. The obtained kinetic equation for the growth rate of voids contains the additional terms conditioned by strains, arising from voids. These terms change the kinetics of void growth (See Fig.1). Using this kinetic equation, we simulate void growth in fcc and bcc metals for different temperatures and vacancy supersaturation.

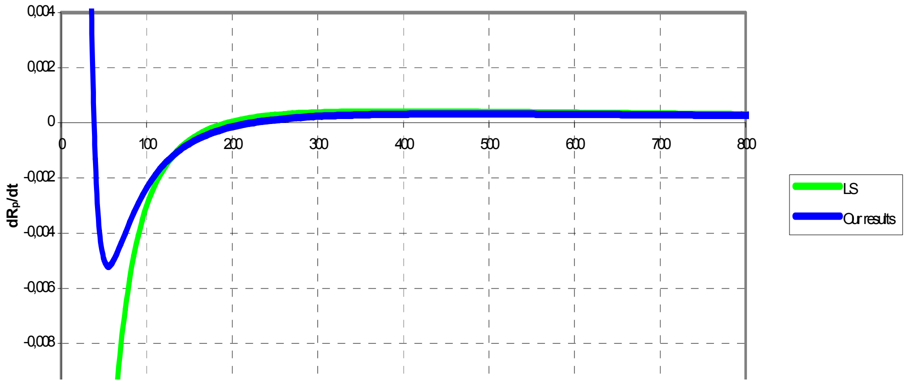

Fig. 1. Growth rate of voids versus their radius (A) in Cu. (T=250 C).

3. Conclusion

We have developed the model of growth rate of voids taking into consideration the elastic stress, arising from voids. It is shown that this elastic stress can fundamentally alter the kinetics of void growth in fcc and bcc metals

References

[1] P.G. Shewmon, Diffusion in Solids, McGraw-Hill Company, 1963.
[2] B.Ya. Lybov, Kinetic Theory of Phase Transformations, Metallurgiya, Moscow, 1969.
[3] J. Philibert, Metal Phys. and Adv. Technologies, .**21**, (1999) N1, 3-9.
[4] A.V. Nazarov, A.A .Mikheev, Def. and Dif. Forum, **143-147** (1997) 177-185.
[5] A.V. Nazarov and A.A. Mikheev, Physica Scripta, **T108**, (2004) 90-95.