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Diffusion under a Stress in Interstitial Alloys and Simulation of Atom Redistribution Near the Crack Tip.

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1. Introduction

Elastic fields, generating by defects of the structure, influence the diffusion processes. In addition, as a result, it leads to the alteration of the phase transformation kinetic, segregation formation and changes of the system properties. However, understanding the effects of pressure and strain on diffusion in solids is now limited. 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. Equation (1) is similar to one, describing the electric field influence on the diffusion flux. At the same time, this expression does not take into account the principal difference between the effect of electrical field, which directly affects a jumping atom and the elastic field, the influence of which is realized through the neighbors, surrounding this atom. It is clear, that for the second case the effect must depend on the geometry of the arrangement of neighbor atoms and, consequently, on crystallographic structure. One of the chief aims of our approach [2,3] is to obtain the general equations for the diffusion fluxes under strain that give the possibility for using these equations at low temperatures, as in this case, the strain influence on the diffusion fluxes is manifested in maximal degree. In presented paper, we have done the next step in the development of approach: general equations for the fluxes in interstitial alloys and new equations for the strain influence on diffusion (SID) coefficients are obtained. For an illustration of our approach possibilities we examine an interstitial atom segregation formation near the crack tip.

2. Theory of diffusion under stress and simulation of segregation formation

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 flow. In this case, the flux depends on matrix of diffusion coefficients. Each of these coefficients depends on strain tensor components in the 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. If we substitute the obtained expressions for fluxes in the equation of continuity, then we get the diffusion equation, in which the influence of elastic stress on flows is taken into account. In particular, this equation gives the possibility to describe interstitial redistribution under stress near defects.

The second part is modeling of interstitial segregation based on a nonlinear diffusion equation taking strain fields generated by the defect into account. Calculations were made for C and H in α-Fe and in FCC Ni. The distribution of H atoms near the crack tip in α-Fe is presented on Fig.1. The results of this simulation show that the distribution of the interstitials near the crack tip has a quite complicated character. A corresponding function $c(x,y)$ in the normal plane to the crack has some ridges and valleys between them. This distribution cardinally differ from the one obtained on the basis equation (1).

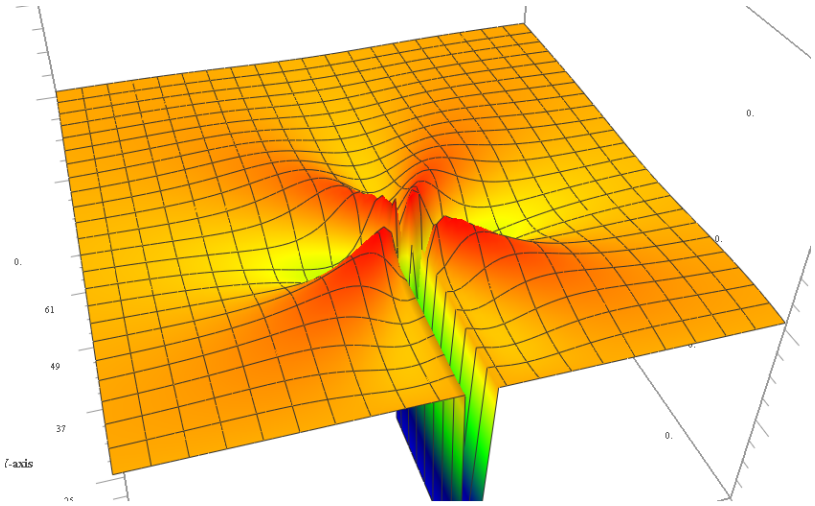

Fig. 1. Distribution of the H atoms near the crack tip in iron.

3. Conclusion

Based on the theoretical approach, developed earlier, the nonlinear equation for interstitial diffusion in bcc and fcc structures has been derived. A new model of diffusion, allowing taking into account influence of stress on redistribution of interstitial atoms near the crack tip is developed.

References

[1] P.G. Shewmon, Diffusion in Solids, McGraw-Hill Company, 1963.
[2] A.V. Nazarov, A.A .Mikheev, Def. and Dif. Forum, **143-147** (1997) 177-185.
[3] A.V. Nazarov and A.A. Mikheev, Physica Scripta, **T108**, (2004) 90-95.