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Theory of Diffusion under Stress

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1. Introduction

The elastic fields, generated by precipitates, cracks, dislocations and other defects of the structure, influence the diffusion processes. As a result, it leads to an alteration of the phase transformation kinetics, segregation formation and changes of the system properties. However, the understanding of the effects of pressure and strain on diffusion in solids is still limited. Usually, the equation of diffusion in the presence of a stress field has the following form [1]:

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

where c is the concentration of impurity atoms or defects, D is the diffusion coefficient under zero strain, 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]. The equation (1) is similar to one, describing the influence of the electric field on the diffusion flux. At the same time, this expression does not take into account the principal difference between the effect of the 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 in the second case the effect must depend on the geometry of the arrangement of the neighboring atoms and, consequently, on the crystallographic structure. Eq.(1) is too crude for objects of atomic size. This one and some other approximations [3] do not take into account the atomic structure in the neighborhood of the defect and the stresses, which essentially influence the energy of a jumping atom. Morever, only a very few papers have considered that shear stress can modify the atomic jump frequency [3].

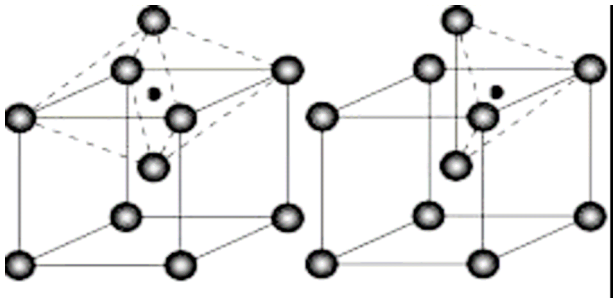

Fig. 1. Positions of an interstitial atom in the bcc structure.

Consider for example an interstitial atom in a bcc lattice (Fig. 1). The interstitial atom energy depends on the distance between the atom s and its neighbouring atoms: $E_s = E(\mathbf{r}_k - \mathbf{r}_s)$, $k \in (1,...,n)$, where n is the number of atoms in the system.
The displacement field changes the distances between atoms and, consequently, the interstitial atom energy.
$E_s = E(\mathbf{r}_k + \mathbf{u}_k - \mathbf{r}_s - \mathbf{u}_s)$. Here $\mathbf{u}_k \equiv \mathbf{u}(\mathbf{r}_k)$ is the displacement of atom k, which is a function of its location $\mathbf{r}_k$. This is true both for the equilibrium configuration and for the saddle-point configuration, and it is the starting point of our approach[4-6].

2. Main aspects of the theory of diffusion under stress and its applications

Some time ago, we suggested a new approach to resolve the problem of the influence of the elastic stresses on the vacancy jump rate for atomic diffusion in crystals [4]. It is based on the assumption that, as the stress fields can alter the atomic configuration of the defect environments, the height of the activation barrier for a defect transition is altered in accordance with the configuration change. Thus, it was obtained, that the change of the activation barrier depends on the displacement field, the symmetry of the crystal, the atomic structure near the point defects and the interatomic interaction. Knowing this change we can calculate the atomic jump rate and obtain an expression for the vacancy flow [4]. In these nonlinear equations, the influence of a deformation tensor component on the diffusion flux is determined by coefficients, which depend on the atomic interaction. One of the aims of the present work is to generalize our approach taking into account N-body interatomic interaction and to calculate the mentioned coefficients which represents the main characteristics of the strain influence on diffusion.

Recently we applied a similar approach to study the stress influence on diffusion fluxes in interstitial alloys with fcc and bcc structures [5]. The equation type depends on the crystallographic structure and the structure of the saddle-point configuration. Now we analyzed the role of the structure in diffusion under stress. The simulation results of the interstitial redistribution near defects, such as a crack tip, are presented.

In our work [6] using the suggested approach we analyzed diffusion under pressure in some cases and obtained an equation for the migration volume. The generalization of this approach is presented in a second poster.

3. Conclusion

In our presentation we are going to discuss the main moments of theory of diffusion under stress, the directions of its development and its applications.

References

[1] P.G.Shewmon, Diffusion in Solids, McGraw-Hill Book Company, Inc., 1963.
[2] B. Ya.Lybov, Kinetic Theory of Phase Transformations, Metallurgiya, Moscow, 1969.
[3] J.Philibert , Metal Physics and Advanced Tecnologies, .**21**, (1999) N1, 3-7.
[4] A.V.Nazarov, A.A. Miheev, Defect and Diffusion Forum, **143-147**, (1997) 177-184.
[5] A.V.Nazarov and A.A. Miheev, Physica Scripta, T108, (2004) 90–94.
[6] A.V.Nazarov, M,G,Ganchenkova and A.A. Miheev, Defect and Diffusion Forum, **194-199,** (2001) 49-54.