

Conference Paper

Simulation of Atomic Structure Near Nanovoids in BCC Iron

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Abstract

Generally, displacement fields near voids are determined by the equations of elasticity theory. Such a description has its disadvantages as it does not take into account the discrete atomic structure of materials. In this work, we use a new variant of Molecular Static method for investigation of the atomic structure near nanovoids. In our model an iterative procedure is employed, in which the atomic structure in the void vicinity and the parameter determining the displacement of atoms embedded into an elastic continuum are obtained in a self-consistent manner. Results show that the displacements are significantly different for varies crystallographic directions.

Keywords: voids; iron; simulation; atomic structure; vacancies

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1. Introduction

Voids are commonly generated in irradiated metals [1] and also in quenched metals after ageing. The voids play significant part in the processes of material structure forming, diffusion phase transformations, swelling, etc. Therefore, it is necessary to develop the methods of determining the voids characteristics. Also, it's obvious that defect characteristics are determined by the atomic structure. Atoms surrounding defect shift from the sites of ideal lattice, e.g. defect atomic structure changes with respect to an ideal one, that in turn leads to changes in interaction energy of neighbour atoms and results in modification of defect energy characteristics and other features. Generally, displacement fields in the vicinity of spherical voids were determined by the solution of equations from the classical theory of elasticity [2], were displacement field has a form:

$$u_{xi} = C_0 x_i + C_1 \frac{x_i}{r^3}, \quad C_0 = \frac{1-2\nu}{E} \frac{2\gamma R^2}{R_G^3 - R^3}, \quad C_1 = -\frac{1+\nu}{E} \frac{\gamma R^2 R_G^3}{R_G^3 - R^3}, \quad (1)$$

where r is a distance from a void center, x_i are coordinates, R is a radius of void, R_G is a radius of district containing the void, ν is the Poisson ratio and E is the Young modulus,

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γ is the surface energy. Such a description has its disadvantages as it doesn't take into account the discrete atomic structure of materials. Results of classical elasticity theory are expected to be valid at distances from a defect that are much larger than the lattice parameter which is a characteristic feature of discreteness, therefore the quantities of atom displacements in the vicinity of such defects as vacancies, vacancy complexes and nanovoids should significantly differ from the predictions of these displacements obtained by means of theory of elasticity. In our recent works, a new approach was developed [3-5]. In particular, in this approach an iterative procedure was used in which the atomic structure in the vicinity of point defect and the parameter determining the displacement of atoms embedded into an elastic continuum with accordance with asymptotic solution of equations from the classical theory of elasticity, are obtained in a self-consistent manner. The vacancy features (including formation volumes and migration volumes) obtained for a few cubic metals agreed well with experimental values [4, 5]. We also note that the MD simulation results that are concerned the self-diffusion in bcc iron under pressure [6], agree within error of MD experiment with the data of our work [4]. We used our model for simulations of the di-vacancy features [7] and later for simulations of the vacancy complexes [8]. In this work, we use our approach for direct investigation of the atomic structure in the vicinity of nanovoids in bcc iron.

2. Model

Now we describe main points of the approach. Equilibrium positions of atoms in computation cell are simulated by using a variational procedure analogous to the one, which is usually used in Molecular Static Method [9]. Computation cell is rounded by atoms embedded in an elastic continuum and displacements of these atoms \mathbf{u} concerned with perturbations, which are induced by defect, are calculated using solutions of static isotropic elastic equation [2]:

$$(\lambda + 2\mu) \nabla (\nabla \cdot \mathbf{u}) - \mu \nabla \times (\nabla \times \mathbf{u}) = 0, \quad (2)$$

where λ is Lamé modulus, μ is shear modulus. Solution of this equation can be expressed in term of spherical harmonics and thus there are an infinite number of solutions to displacement of each atom \mathbf{u} as a function of its position \mathbf{r} (i.e. function of its distance from a defect). We use the first two terms of series for atomic displacements calculation in an elastic matrix. First term has spherical symmetry and can be written like Eq. 1 and has only second term when $R_G \gg R$ [2, 9]:

$$u_1 = C_1 r/r^3. \quad (3)$$

Next term of series has cubic symmetry and usually written in the form [9]:

$$u_2 = C_2 \nabla \left[\frac{1}{r^5} \left(\frac{x^4 + y^4 + z^4}{r^4} - \frac{3}{5} \right) \right], \quad (4)$$

where C_2 is a constant.

Prior calculations carried out for vacancy in bcc iron using Johnson's potential [9] have shown that atomic displacements calculated with only first spherically symmetric term of the series, don't agree with results of variation computations even for sufficiently large systems [4, 5]. This circumstance becomes apparent when the formation and migration volumes are estimated. Taking into account the second term of series (Eq. 4) allows us to define atomic displacements in an elastic matrix and, consequently, equilibrium positions of all atoms in the vicinity of a defect more precisely. Other terms of series have symmetry, which is differ from atomic structure symmetry in the vicinity of a defect, or they very fast decrease with r and their contributions in \mathbf{u} are negligible at distances corresponding to atom locations in an elastic continuum. Self-consistent iteration procedure to calculate the constants C_1 , C_2 and simulate atomic structure in defect crystal is realized in our model. Stable convergence upon constants C_1 and C_2 has been received. This procedure and our model in all have been described in detail [4, 5].

3. Results and discussion

The simulation is done for voids of different sizes. The atoms in the centre of the computational cell are deleted to create a nanovoid. The void radius, R , was between 8.72 and 20.06 Å. We used N-body potentials developed in [10] for bcc iron.

The results of simulation are presented on Figure 1 and in Table 1. In particular, there give typical atom displacement dependencies on the distance from the void centre and the calculation results on the equations for the single isolated void (Eq. 1 and Eq. 3). Dashed vertical lines indicate the radii of the void and the computational cell respectively.

The displacement dependences of atoms on the distance from the center of the voids for pores of other sizes have a similar appearance. The highest values of the atom displacements near the void surface and values of constant C_1 for voids of different sizes are presented in Table 1.

Results show that the fields of displacements near nanovoids are significantly more complicated and with much bigger magnitudes of atom displacements than near vacancies [3-5]. In addition, the displacement significantly different for variant crystallographic directions. The highest value of the atom displacements near the void

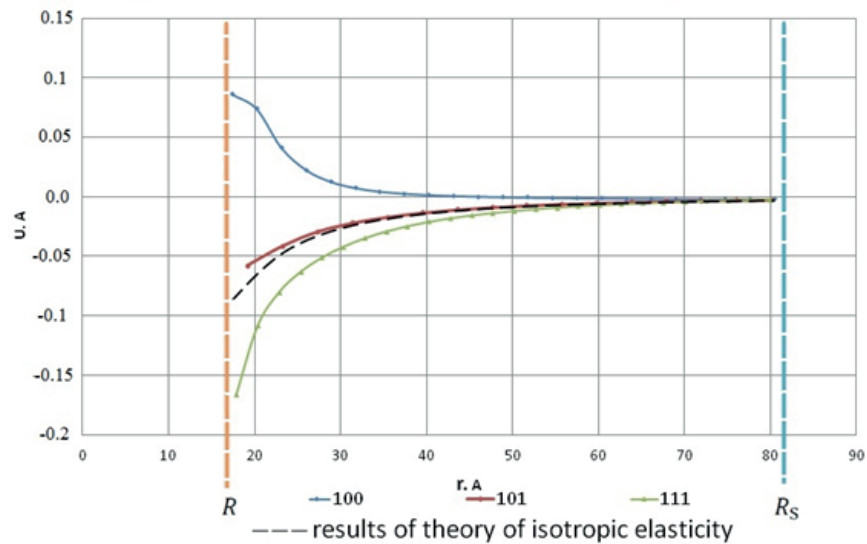


Figure 1: The atom displacements for variant crystallographic directions in bcc iron for nanovoid ($R = 17.46 \text{ \AA}$).

TABLE 1: Atom displacements for variant crystallographic directions in bcc iron for voids of different sizes.

R, Å	8.72	10.49	12.17	15.37	17.46	20.06
$U_{\langle 100 \rangle}$, Å	0.029	0.034	0.05	0.066	0.086	0.091
$U_{\langle 101 \rangle}$, Å	-0.021	-0.026	-0.031	-0.04	-0.057	-0.044
$U_{\langle 111 \rangle}$, Å	-0.083	-0.081	-0.1	-0.113	-0.166	-0.17
C_1 , Å ³	-1.6	-3.76	-4.25	-8.91	-13.66	-28.63
Simulation						
C_1 , Å ³ Theory, Eq.(1)	-4.84	-7	-9.42	-15.03	-19.4	-25.61

surface increases with increasing void size (Table 1). It should be emphasized that the positive displacement of the atoms located near the surface in the $\langle 100 \rangle$ direction increase with the size of the voids, instead of decreasing as one would expect. In addition, it is interesting that the trend is continued, although the void radius value exceeds 20 \AA in the simulation (Table 1). Thus, discreteness of structures plays an important role in the formation of the atom displacements near the void surface.

It should be noted an important consequence of the results. Usually, the equation of vacancy diffusion in the presence of stress field has the following form [11]:

$$\vec{J} = -D_V \left[\nabla c + c \frac{V_{Rel}}{kT} \nabla (Sp\sigma) \right], \tag{5}$$

were c is the vacancy concentration, σ is a tensor of stress, V_{Rel} is a relaxation volume.

A similar expression we have obtained in the zero approximation in the framework of the microscopic approach proposed by us to describe the effect of the elastic fields on the diffusion fluxes of vacancies [12]:

$$J_x = -\frac{1}{\Omega} \left[D_V \frac{\partial c}{\partial x} - c \frac{K^V}{kT} \left(D_V \frac{\partial Sp\epsilon}{\partial x} \right) \right], \quad (6)$$

where Ω is the volume per lattice site, D_V is the vacancy diffusion coefficient in the perfect system and $\epsilon_{ij} = (1/2) (\partial u_i / \partial x_j + \partial u_j / \partial x_i)$ is the strain tensor ($i, j = 1, 2, 3$).

$$K^V = \frac{1}{2} \sum_s \sum_{k \neq s} \frac{(x_{ks}^V)^2}{R_{ks}^V} \frac{\partial E_{Sys}}{\partial R_{ks}} \Big|_{R_{ks}^V} \quad (7)$$

x_k, y_k, z_k are the coordinates of the atom k of a system, E_{Sys} is the system energy, $x_{ks} = x_k - x_s, y_{ks} = y_k - y_s, z_{ks} = z_k - z_s, k \neq s, R_{ks} = |\mathbf{r}_k - \mathbf{r}_s| = \sqrt{x_{ks}^2 + y_{ks}^2 + z_{ks}^2}$ for all atoms, $x_{ks}^V, y_{ks}^V, z_{ks}^V, R_{ks}^V$ are the coordinate differences between the atoms k and s and spacing's between them in system with the vacancy.

It is known that the vacancy flux density on the void surface determines growth rate of the voids [1]. If we use the solution of equations from the classical theory of elasticity in the vicinity of the void (1), then:

$$Sp\epsilon = 3C_0, \nabla Sp\epsilon = 0, \text{ and } \vec{J} = -D_V \nabla c. \quad (8)$$

There is no stress influence on flux of vacancies [1, 13].

Obtained results show that $\nabla Sp\epsilon \neq 0$, and a kinetics equation for the growth rate of voids must contain the additional terms conditioned by strains, arising from voids. Thus, these factors, together with the factors which change the diffusion coefficients [13], affect the kinetics of pore growth under different conditions. It should be taken into account that in many cases the growing and dissolving pores pass through the stage of nanometers.

One more consequence: it is to be expected that the displacement fields around nano-sized precipitates will also significantly differ from the predictions of the elasticity theory. Therefore, the existing theories and models for nucleation and growth of pores and phase inclusions need a significant revision, taking into account the results of the simulation. The above-mentioned consequences are especially relevant for the swelling models of materials [1] and Frenkel's effects (Kirkendal of the second kind) [14, 15] with interdiffusion.

4. Conclusion

1. New model is presented for determining atomic structure near nanovoids. The main points of the model are the following. First, we allow for displacements of

atoms embedded in an elastic continuum around computation cell. Second, we consider the influence of discreteness of the atomic structure in the vicinity of a defect on the values and directions of atomic displacements in elastic matrix. The third point is that the atomic structure in the vicinity of the void and the displacement of atoms in the elastic medium are calculated in a self-consistent manner using a convergent iterative procedure.

2. The model permits us to find qualitatively new peculiarities of the atomic structure in the void vicinity that cannot be correctly obtained with the use of the elasticity theory because it cannot be applied to the atomic scale.
3. In addition, the displacement significantly different for various crystallographic directions.
4. The obtained atom positions give us the possibility to provide the following more advanced level simulation of nanovoid growth in materials supersaturated with vacancies.

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References

- [1] G. S. Was, *Fundamentals of Radiation Materials Science: Metals and Alloys*, Springer, New York, 2007.
- [2] L. D. Landau, E. M. Lifshitz, *Theory of Elasticity*, Elsevier, 1986.
- [3] I. V. Valikova, A. V. Nazarov, *Defect Diffus. Forum* 277 (2008) 125.
- [4] I. V. Valikova, A. V. Nazarov, *Phys. Met. Metallogr.*105 (2008) 544.
- [5] I. V. Valikova, A. V. Nazarov, *Phys. Met. Metallogr.* 109 (2010) 220.
- [6] J.-W. Jang, J. Kwon, B.-J.Lee, *Scripta Mat.* 63 Issue:1 (2010) 39.
- [7] I. V. Valikova, A. V. Nazarov, *Solid State Phenomena* 172-174 (2011) 1222.
- [8] A. B. Germanov, I. V.Ershova, E. V. Kislitskaya,A. V. Nazarov, A. G. Zaluzhnyi, *Metal Physics and Advanced Technologies*, 35 (2013) 1391.
- [9] R. A. Johnson, *Phys. Rev. A* 134 (1964) 1329.
- [10] G.J. Ackland, D.J. Bacon, A.F. Calder, T. Harry, *Philos. Mag. A* 75 (1997) 713.

- [11] B. Ya. Lyubov, *The Kinetic Theory of Phase Transformations*. Metallurgiya, Moscow, 1969. (in Russian). There is translation: B. Y. Lyubov, *Kinetic Theory of Phase Transformation* ~National Bureau of Standards, Amerind, New Delhi, 1978.
- [12] A.V.Nazarov, A.A. Mikheev, *Defect Diffus. Forum* 363 (2015) 112.
- [13] A.A. Mikheev, A.V. Nazarov, I.V. Ershova, A.G. Zaluzhnyi, *Defect Diffus. Forum* 363 (2015) 91.
- [14] A. M. Gusak, T. V. Zaporozhets, Y. O. Lyashenko, S. V. Kornienko, M. O. Pasichnyy, and A. S. Shirinyan, *Diffusion-Controlled Solid State Reactions: in Alloys, Thin-Films, and Nanosystems*, New York, John Wiley and Sons, 2010.
- [15] A. Paul, T. Laurila, V. Vuorinen, S.V. Divinski, *Thermodynamics, Diffusion and the Kirkendall Effect in Solids*, Springer, 2014.