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Atomic mechanisms and energetics of thermally activated processes of helium redistribution in vanadium

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Abstract

Semi-empirical potentials of helium–helium and helium–vanadium interactions in vanadium are calculated based on the earlier developed theoretical model of a metal crystal which includes contributions of two-body components of atomic interactions and the s- and d-electrons into the binding energy of transition metals. Using the molecular dynamics (MD)-method the equilibrium properties (energies, entropies, relaxation volumes and others) are calculated and the atomic configurations of helium-vacancy clusters (He_nV_m, $n \leqslant 15$, $m \leqslant 3$) with the minimum free energy of formation are determined. The most probable mechanisms of helium clustering and diffusion are defined. Energetic criteria for realization of the main processes which contribute to the experimental helium thermal desorption spectra are investigated with reference to the experiments on thermal helium desorption spectroscopy (THDS).

1. Introduction

Study of energetics and kinetics of interaction processes for self and impurity defects in vanadium crystal matrix and understanding on these basis of the physical mechanisms responsible for evolution of the vanadium microstructure is an important task during the development of theoretical models for predicting performance of vanadium-based structural materials under fusion reactor conditions. Until now major characteristics controlling the processes of phase formation and diffusional redistribution of radiation defects, helium atoms and interstitial impurities in vanadium and its alloys have practically not been investigated. This is connected in a large extent, to the lack of a theoretically consistent model for vanadium base crystal. The development of the model is a difficult problem due to the specific nature of atom interaction in vanadium. The features of the interactions are mostly determined by many-body effects and localized non-central forces.

Investigations of atomic configurations, energetic and other characteristics of helium-containing defects in vanadium were done by the molecular dynamics (MD)-method based on: (a) the theoretical model for a transition metal and (b) the potential of vanadium atom interaction in a vanadium crystal, both of which were obtained in Ref. [1]. In these calculations, a new analytical form is proposed for the ‘helium–helium’ and ‘vanadium–helium’ potentials. The V–He potential parameters were optimized using the empirical data on the thermodynamically stable helium solutions in metals, obtained in Ref. [2]. They are also calculated in Ref. [3] and the present work based on the energetic process characteristic of the experimentally observed [4] helium thermal desorption spectra.

2. Helium–helium and helium–vanadium interaction potentials

The form of the He–He potential has been extensively studied by both experimental and theoretical methods [3,5,6,8,9]. In this work a two-body potential was used [3]:

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$$\varphi(r) = \frac{Z^2e^2}{r}\psi(r) - f(r)\left\{\frac{C_6}{r^6} + \frac{C_8}{r^8} + \frac{C_{10}}{r^{10}}\right\}, \tag{1}$$

$$f(r) = \exp\left\{-\beta\left[\left(\frac{D}{r} - 1\right)^m - 1\right]\right\}, \quad m \geqslant 2, \ Z = 2, \tag{2}$$

where C_6, C_8, C_{10} are the dispersion constants [8]; $\psi(r)$ is a function of Coulomb interaction screening calculated in this work by the analytical approximation used in data calculations of the work [10]. Parameters β and D in Eq. (2) were determined by fitting the calculated data to the experimental data, given in Ref. [7], accounting for the quantum effects in the values of the second virial coefficient.

Simple estimates show that in metals, the average distances between helium atoms in helium-containing clusters correspond to rather high helium densities in the macroscopic sense. On the other side, some works (for example in Ref. [6] theoretically and in Ref. [5] experimentally) show that in dense systems, the helium atom interaction potential is significantly modified due to many-body effects. In order to account for this circumstance, the potential He–He was developed in Ref. [3] to describe properties of crystal helium in a super high pressure range. The He–He potential was obtained by a polynomial joint of potential from Ref. [1] and the effective pair potential calculated in Ref. [6].

A more difficult problem is calculation of the potential describing interactions of helium atoms with the atoms of vanadium crystal. It has been shown in Refs. [2,3] that:

- The thermally activated helium dissolution in metals takes place probably by a vacancy mechanism and is characterized by the dissolution energy $E_S = E_V^F + E_{He,V}^F$, where $E_{He,V}^F$ is the energy of helium location in a vacancy;
- The energies of helium dissolution in metals are probably close to the vacancy formation energies;
- The properties of helium in vanadium calculated by the MD-method are in better agreement with the experimental data when availability of a small negative minimum in V–He interaction potential is considered and the range of values, $E_S = E_{He,V}^F = 2.2 \pm 0.2$ eV, is adopted for dissolution energy.

The nature of attractive forces in 'V–He' potential is not clear. Therefore, an analytical form for their description should be refined on the basis of empirical data. 'He–V' interaction potential was calculated in this work in the form

$$\varphi(r) = \frac{Z_1Z_2e^2}{r}\psi(r) + \frac{B\exp\left[-\left(\frac{\beta}{r}\right)^n\right]}{r^m}, \quad n \geqslant 2, \ m = 6, \tag{3}$$

where Z_1 and Z_2 are the nuclei charges of helium and vanadium atoms; $\psi(r)$ is the function of Coulomb interaction screening; and B and β are empirical parameters.

The calculation of $\psi(r)$ was performed by an analytical approximation of V^0–He potential given in Ref. [11]. In the interval $[r_m,r_c]$,($[r_m,\epsilon]$ are coordinates of the potential minimum, r_c is the cut-off radius), potential (3) is modified by a polynomial satisfying the conjugancy conditions with an accuracy of up to the second-order derivative at the point of minimum and $\varphi(r_c) = \varphi'(r_c) = \varphi''(r_c) = 0$. Parameters of the potential (3) were determined under the conditions that the characteristics of helium in a substitutional position, as calculated by the MD-method are in the range of probable values of energy and entropy of helium dissolution in vanadium calculated in Ref. [2]. The selection of the optimal parameter values was carried out by the adjustment of experimental and calculated (by the method described below) helium thermodesorption spectra. The V–He effective pair potential, calculated on the basis of the algorithm described above, is shown in Fig. 1.

3. Properties of helium-containing defects and cluster formation mechanisms

Using the method of defect study in metals described in Ref. [1] and the He–He ([3]) and the V–He (Fig. 1)

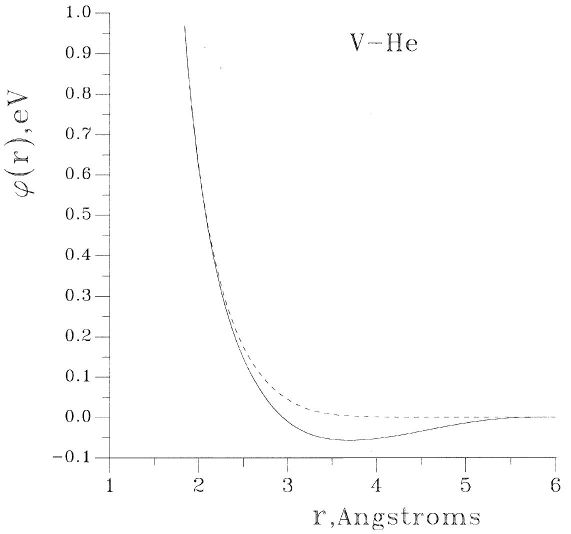

Fig. 1. Optimized pair potential of helium interaction with vanadium crystal atoms (V–He potential). (- - - -) Two-body interatomic potential of helium and vanadium atom interaction calculated in the free-electron approximation of work [11].

interaction potentials, properties of helium atoms in the interstitial positions and He combined in complexes with vacancies and self-interstitials atoms were calculated. The main characteristics of the simplest helium-containing defects in vanadium are presented in Table 1.

As applicable to thermal helium desorption spectroscopy (THDS)-experiments, investigations of a number of metastable states of He_nV_m type helium-containing clusters (at $n \leqslant 15$, $m \leqslant 3$) were carried out in vanadium lattice. The equilibrium properties were calculated (energies, entropies, relaxation volumes, etc) and atomic configurations of clusters with the minimal free energy of formation in a vanadium crystal were determined. The probable schemes and energy criteria of growth processes and cluster thermal decomposition were also determined.

The results of calculation of the cluster-binding energies relative to the dissociation processes

$$\mathrm{He}_n\mathrm{V}_m \to \mathrm{He}_{n-1}\mathrm{V}_m + \mathrm{He}^{\mathrm{mobile}}, \tag{4}$$

$$\begin{gathered}\mathrm{He}_n\mathrm{V}_m \to \mathrm{He}_n\mathrm{V}_{m+1} + \mathrm{I}^{\mathrm{mobile}},\\ \text{at}\, n \leqslant 15,\ m = 0,1,2,3\end{gathered} \tag{5}$$

are presented in Fig. 2.

As clusters are filled by helium atoms, the calculations show that for some critical numbers of He_nV_m, the accumulated elastic energy is sufficient to cause spontaneous cluster restructuring. In this process a Frenkel pair (VI^*) connected with the initial cluster is created. This process is a major source of helium-vacancy clusters in metals irradiated by helium ions with subthreshold energy.

Depending on the irradiation temperature and He^+ ion energy nucleation and growth of helium-containing clusters is described by one of the following reaction chains:

$$\begin{cases}\mathrm{He}_{n-1} + \mathrm{He} \xrightarrow{2 \leqslant n < n_c(0,0)} \mathrm{He}_n\\ \mathrm{He}_{j-1} + \mathrm{He} \xrightarrow{j = n_c(0,0)} \mathrm{He}_j\mathrm{VI}^*\\ \dots\\ \mathrm{He}_{n-1}\mathrm{V}_m\mathrm{I}_k^* + \mathrm{He} \xrightarrow{n_c(m-1,k-1) \leqslant n < n_c(m,k)} \mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^*\\ \mathrm{He}_{i-1}\mathrm{V}_m\mathrm{I}_k^* + \mathrm{He} \xrightarrow{i = n_c(m,k)} \mathrm{He}_i\mathrm{V}_{m+1}\mathrm{I}_{k+1}^*\end{cases} \tag{6}$$

In the case of subthreshold irradiation $m = k$, and under conditions of damaging irradiation $m \geqslant k$ (m is number of vacancies, k is number of SIAs connected with the cluster). During reactions (6), for some critical number of helium atoms $n = n_c(m, k)$, cluster $He_nV_mI_k^*$ spontaneously transforms into $He_nV_{m+1}I_{k+1}^*$ cluster. Further filling of the new cluster by helium, for the next critical number of helium atoms $n_c(m + 1, k + 1)$, leads to the spontaneous formation of a Frenkel pair. In such a case, the vacancy is formed at the nearest lattice site so that the next stable configuration of a core-cluster is created. Numbers $n_c(m,k)$ were determined here by the MD-method. For the small helium-vacancy clusters the following values of $n_c(m,k)$ were obtained for which the processes described by reaction chains (6) take place in vanadium:

$$\begin{aligned}&n_c(0,0) = 5\text{–}6,\\ &n_c(1,0) = n_c(1,1) = 9\text{–}11,\\ &n_c(2,0) = n_c(2,1) = n_c(2,2) = 14\text{–}15,\\ &n_c(3,0) = n_c(3,1) = n_c(3,2) = n_c(3,3) = 19\text{–}21.\end{aligned}$$

The uncertainty in $n_c(m,k)$ values can be explained since in investigations of clusters by the MD-method the $n_c(m,k)$ depends on the determination of how the crystal atom nearest to the cluster should shift when the cluster is filled by helium due to reduction in the strain energy in order for it to be considered as an SIA.

Table 1
The main parameters of some helium-containing defects in vanadium calculated by the molecular dynamics method

Interstitial He	HeV	HeV_2
$P_{11} = 8.756$ eV	$E^F_{HeV} = 2.21$ eV	$E^F_{HeV_2} = 3.97$ eV
$P_{22} = P_{33} = 4.524$ eV	$E^B_{HeV} = 3.04$ eV	$V^R_{HeV_2} = -0.35\ \Omega$
$E^F_{He,Oct} = 3.17$ eV	$V^R_{HeV} = -0.085\ \Omega$	$E^B_{HeV_2} = 2.95$ eV
$V^R_{He,Oct} = 0.43\ \Omega$	$\nu_{He,V} = 1.109 \times 10^{13}\ s^{-1}$	$E^B_{V,HeV} = 0.32$ eV
$\nu^{Mean}_{He,Oct} = 1.9 \times 10^{13}\ s^{-1}$	$\theta_{He,V} = 532$ K	$E^B_{HeV_2} = 0.65$ eV
$\theta^{Mean}_{He,Oct} = 848$ K	$\Delta S^F_{HeV}/k_B = 2.4$	$\theta_{HeV_2} = 505$ K
$E^M_{He,O \to T \to O} = 0.22$ eV		
$E^{M(*)}_{He} = 0.23 \pm 0.02$ eV		

E^F, E^M are the energies of defect formation and migration; E^B the defect binding energies by definition: ($E^B_{HeV} = E^F_{He} + E^F_V - E^F_{HeV}$; $E^B_{He,V_2} = E^F_{He} + E^F_{V_2} - E_{HeV_2}$; $E^B_{V,HeV} = E^F_V + E^F_{HeV} - E^F_{HeV_2}$); $\Delta S^F_{HeV}/k_B$ the change in crystal vibrational entropy due to formation of defect (not including the helium atom oscillations); (*) the energy of helium migration over lattice interstitial position, calculated in present work; P_{ij} the defect force-dipole tensor in crystal coordinate system; V^R the relaxation volumes; Ω the atomic volume; ν, θ the frequencies of helium atom oscillation in a lattice, in s^{-1} and K, correspondingly; V_2 the stable configuration of divacancy (vacancy locations at a distance of the second coordinating sphere); k_B the Boltzman constant.

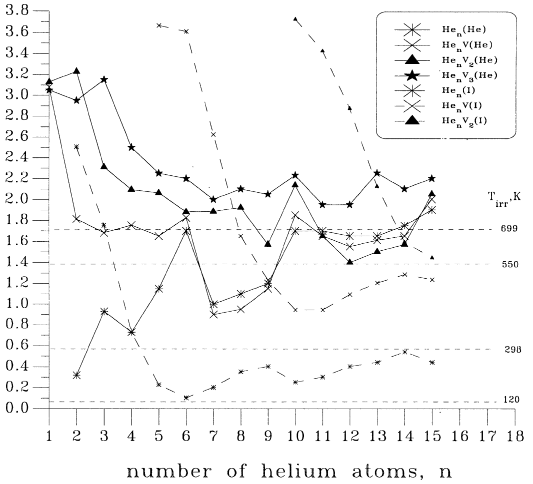

Fig. 2. Binding energies of interstitial helium atoms and SIAs with clusters $\mathrm{He}_n\mathrm{V}_m$ ($n \leqslant 15$, $0 \leqslant m \leqslant 3$) calculated by the MD-method relating to: helium atoms release processes (continuous curves $\mathrm{He}_n\mathrm{V}_m(\mathrm{He})$ – reactions of type (4); free SIA formation processes (dotted curves $\mathrm{He}_n\mathrm{V}_m(\mathrm{I})$ – reactions of type (5). The horizontal dotted lines correspond to the upper boundary of the cluster-binding energy, clusters are thermally unstable at the irradiation temperatures indicated. This calculation was performed with optimal parameters of the gas release dissociation-diffusion model for the experiment [4].

In this work the following definition was adopted: in a cluster containing m vacancies and connected to k SIAs, number of helium atoms $n_c(m,k)$ is a critical number for one of the processes described by reaction chains (6) if, as a result of the minimization of the strain energy by the system, an additional SIA connected to the cluster is created. This new SIA has the minimum energy configuration for the lattice symmetry. In this case, the formed core-cluster has a structure close to the structure of the most energetically favorable cluster configuration $\mathrm{He}_n\mathrm{V}_{m+1}$. Under this determination, the numbers $n_c(m,k)$ in the first approximation do not depend on k, i.e. they are determined only by the vacancy content in the cluster and form rows: 6, 10, 15, 20 for $m \leqslant 3$.

4. Mechanisms of helium thermodesorption for small implantation doses

In the recent years, the THDS became one of the most efficient experimental methods to study cluster formation processes in helium-irradiated metals. The reasons for gas release are the thermal decomposition processes of helium-containing complexes and subsequent diffusion of the new mobile interstitial helium atoms to sample surface. With the increasing irradiation dose, number of the thermoactivated processes in which helium atoms participate sharply increases, and consequently, the complexity of the spectral curves (number of peaks in the spectra).

In this work, we carried out analysis of the results from experiments [4], in which kinetics of helium release from vanadium samples was investigated. In Ref. [4], specimens were irradiated by 1 keV helium ions to implantation doses of 5×10^{15}–1×10^{18} m^{-2} in the irradiation temperature range of 120–700 K.

Under irradiation doses $<10^{17}$ m^{-2} (as in experiment [4]) only processes with the annealing temperature up to ≈ 1000 K are activated. According to our calculations, this fact indicates that in this dose range helium-containing clusters, $\mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^*$, are created with $m \leqslant 3 - 4$ under irradiation. Taking this into account a study by the MD-method was done to evaluate energetics for some cluster thermal decomposition reactions in accordance to

$$\mathrm{He}_n\mathrm{V}_m \xrightarrow{T=T^{\mathrm{diss}}_{\mathrm{He}_n\mathrm{V}_m}} \mathrm{He}_{n-l}\mathrm{V}_m + l\,\mathrm{He}^{\mathrm{mobile}} \qquad (7)$$

In the course of this reaction (or reaction chain, if at the given temperature after the decomposition $l < n$ and the unstable clusters are again created (Fig. 3)) interstitial helium atoms are created, which then diffuse to the sample's surface leading to thermodesorption peaks.

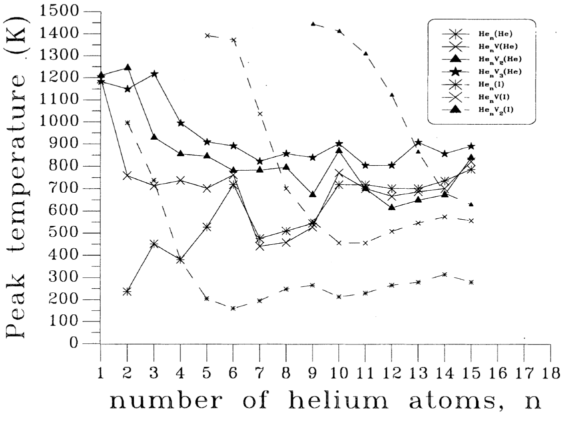

Fig. 3. Peak activation temperatures of helium thermodesorption from vanadium samples, corresponding to energy parameters of the cluster thermal decomposition reactions classified in Fig. 2. These calculations were performed on the basis of Fig. 2 data with use of the dissociation-diffusion relationships for a gas release model at optimal parameters for experiment [4] conditions (irradiation by 1 KeV He^+ ions). Continuous ($\mathrm{He}_n(\mathrm{He})$; $\mathrm{He}_n\mathrm{V}(\mathrm{He})$; $\mathrm{He}_n\mathrm{V}_2(\mathrm{He})$; $\mathrm{He}_n\mathrm{V}_3(\mathrm{He})$) curves correspond to the dissociation reactions of $\mathrm{He}_n\mathrm{V}_m$ ($m \leqslant 3$) clusters with formation of helium mobile atoms of type (7). The dotted ($\mathrm{He}_n(\mathrm{I})$; $\mathrm{He}_n\mathrm{V}(\mathrm{I})$; $\mathrm{He}_n\mathrm{V}_2(\mathrm{I})$) curves correspond to the dissociation processes with formation of free SIA and their subsequent annihilation on helium-vacancy clusters, reactions of type (8) and (9).

The possibility for realization of the following type of reactions was also investigated:

$$\begin{cases} \mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^* \xrightarrow{T=T^{\mathrm{diss}}_{\mathrm{I,He}_n\mathrm{V}_m\mathrm{I}_k^*} < T^{\mathrm{diss}}_{\mathrm{He,He}_n\mathrm{V}_m\mathrm{I}_k^*}} \mathrm{He}_n\mathrm{V}_m\mathrm{I}_{k-l}^* + l\,\mathrm{I}^{\mathrm{mobile}} \\ \mathrm{He}_{n'}\mathrm{V}_{m'} + \mathrm{I} \rightarrow \\ \rightarrow \mathrm{He}_{n'}\mathrm{V}_{m'-1} \xrightarrow{T^{\mathrm{diss}}_{\mathrm{He,He}_{n'}\mathrm{V}_{m'-1}} < T^{\mathrm{diss}}_{\mathrm{I,He}_{n'}\mathrm{V}_{m'-1}}} \mathrm{He}_{n'-1}\mathrm{V}_{m'-1} + \mathrm{He}^{\mathrm{mobile}} \end{cases} \tag{8}$$

$$\begin{cases} \mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^* \xrightarrow{T=T^{\mathrm{diss}}_{\mathrm{I,He}_n\mathrm{V}_m\mathrm{I}_k^*} < T^{\mathrm{diss}}_{\mathrm{He,He}_n\mathrm{V}_m\mathrm{I}_k^*}} \mathrm{He}_n\mathrm{V}_m\mathrm{I}_{k-l}^* + l\,\mathrm{I}^{\mathrm{mobile}} \\ \mathrm{He}_n\mathrm{V}_m\mathrm{I}^*{}_{k-l} \xrightarrow{T^{\mathrm{diss}}_{\mathrm{He,He}_n\mathrm{V}_m\mathrm{I}_{k-l}^*} < T^{\mathrm{diss}}_{\mathrm{I,He}_n\mathrm{V}_m\mathrm{I}_{k-l}^*}} \mathrm{He}_{n-1}\mathrm{V}_m\mathrm{I}_{k-l}^* + \mathrm{He}^{\mathrm{mobile}} \end{cases} \tag{9}$$

Reactions (8) and (9) describe dissociation of $\mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^*$ clusters with formation of free SIAs, which either go to traps or annihilate on other helium-vacancy clusters, where this process is not energetically forbidden.

Thus, processes (8) and (9) lead to helium release by the two channels:

Process (8). Unstable clusters, according to reaction (7), are created after SIA annihilation on the simplest helium-vacancy type defects, $\mathrm{He}_{n'}\mathrm{V}_{m'}$

Process (9). In $\mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^*$ clusters dissociation, unstable $\mathrm{He}_n\mathrm{V}_m\mathrm{I}_{k-l}^*$ clusters are formed at a given temperature, again relating to reaction (7).

To analyze and interpret the experimental THDS spectra, in this work the solutions for helium flux obtained for dissociation-diffusion gas release model [3] were used in this work. In [3], a non-stationary diffusion problem was solved. This model describes the kinetics of helium release from helium-irradiated samples as a consequence of helium diffusion to the surface if thermally activated sources of mobile atoms are distributed over the given implantation profile. Here the reactions (7)–(9) were considered as sources of helium atoms. Mobile helium atom generation rate (diffusion problem source function) was calculated, using the solution of a first order thermodesorption equation, describing $\mathrm{He}_n\mathrm{V}_m$ cluster decomposition rate under linear increase of annealing temperature. Features of the solutions obtained for the diffusion problem are such that, in the limiting case of zero depth of helium implantation (low irradiation energies) or in the case $E^{\mathrm{M}} < E^{\mathrm{B}}$ the solution for helium flux transforms to solution of a first-order thermodesorption equation. In the opposite case at $E^{\mathrm{B}} \to 0$ (absence of helium thermal sources) the solution describes a purely diffusional process of helium release from the given implantation profile beyond the sample boundaries. Energetic process characteristics in the model considered (relating to (7), (8) and (9) reactions) are $\mathrm{He}_n\mathrm{V}_m$ cluster dissociation energies, which are determined by expressions

$$E^{\mathrm{D}}_{\mathrm{He,He}_n\mathrm{V}_m\mathrm{I}_k} = E^{\mathrm{B}}_{\mathrm{He,He}_n\mathrm{V}_m\mathrm{I}_k} + E^{\mathrm{M}}_{\mathrm{He}}, \tag{10}$$

$$E^{\mathrm{D,He}}_{\mathrm{I,He}_n\mathrm{V}_m\mathrm{I}_k} = E^{B}_{\mathrm{I,He}_n\mathrm{V}_m\mathrm{I}_k} + E^{\mathrm{M}}_{\mathrm{I}} + E^{\mathrm{M}}_{\mathrm{He}}, \tag{11}$$

where $E^{\mathrm{B}}_{\mathrm{He,He}_n\mathrm{V}_m}$, $E^{\mathrm{B}}_{\mathrm{I,He}_n\mathrm{V}_m}$ are the binding energies of helium atoms and SIA with clusters, $E^{\mathrm{M}}_{\mathrm{He}}$, $E^{\mathrm{M}}_{\mathrm{I}}$ are the corresponding migration energies.

It is assumed that Eq. (11) describes the helium release mechanism by the two possible channels according to reactions (8) and (9).

Fig. 2 presents the binding energies of helium atoms and SIA calculated by the MD method relating to their free state in vanadium lattice with the most stable configurations of $\mathrm{He}_n\mathrm{V}_m\mathrm{I}_k^*$ cluster-bound state. A more detailed picture also includes multiple metastable cluster states. However, the kinetics of the processes observed is defined, mainly, by energetics of the most stable clusters.

For the given parameters of the diffusion problem (implantation profile characteristics, helium diffusion coefficient, etc.), the dissociation energies of the processes (7), (8) and (9) are uniquely connected with the corresponding activation temperatures, which by definition, coincide with the maximum temperatures of helium release peaks. Similar relationships also take place for the peaks' widths at half-height. Using the obtained diffusion problem solution, the decomposition of experimental THDS-spectra was performed to individual monoenergetic processes, the activation temperatures for these processes were also determined. Then, for the same diffusion model parameters, using results of MD-calculations on the binding energies of helium-containing clusters (Fig. 2), theoretically expected peak maximum temperatures, in accordance with reactions (7), (8) and (9) were evaluated. They are given in Fig. 3. By comparing calculated and the experimentally obtained peak temperatures, the interpretation was made of the experimental spectra. After identification of the THDS-spectra structure, using MD-calculation data, by an iteration method (from the requirement of maximum full alignment of the calculated and experimental THDS-spectra) optimal values were determined for He–V potential parameters (Fig. 1) and diffusion problem parameters.

The final calculation results for helium-containing cluster-binding energies and process activation temperatures at optimal parameters of the diffusion model are also presented in Fig. 2 and Fig. 3.

5. Conclusions

Justification of the analytical form was performed and parameters were calculated for effective two-body potentials of He–He and V–He atoms interactions.

The characteristics of $\mathrm{He}_n\mathrm{V}_m$ type helium-vacancy clusters (for $n \leqslant 15$, $m \leqslant 3$) and the basic mechanisms of helium diffusion in a vanadium crystal were investigated by the MD-method.

A growth mechanism of the helium-containing clusters due to athermal incorporation of near-by Frenkel pairs was studied.

Based on optimal fitting of calculated and experimental thermodesorption spectra, the dissociation energies and frequency factors were calculated for processes corresponding to the helium-vacancy cluster thermal decomposition reactions. Optimal characteristics were determined for helium distribution profile in vanadium after irradiation by 1 KeV He^+ ions (mean path is 10 nm, width at a half-height of implantation profile is 15 nm). Using the optimal parameters of the diffusion model and the results of MD-calculations on cluster-binding energies presented in Fig. 2 activation temperatures were calculated corresponding to helium release dissociation peaks. The results of these calculations are presented in Fig. 3. In the course of these calculations, under conditions of calculated and experimental spectra adjustment, optimized parameters for V–He interaction potential were obtained (Fig. 1).

The results of experimental thermodesorption spectra modeling on the basis of the diffusion theory are in good agreement with the study by the MD-method of energetics of dissociation and diffusion processes with participation of helium atoms in a vanadium crystal. The calculated He–V interaction potential (Fig. 1) realistically describes energetics of the processes with participation of helium atoms in a vanadium crystal.

The migration energy was calculated for helium interstitial atoms in vanadium by the reconstruction method of experimental THDS-spectra in the framework of the diffusion model using relationship (10), the data of MD-calculations on binding energies (Fig. 3) and the calculation results for activation energies of some dissociation peaks. The value obtained is practically coincident with direct calculations of saddle point parameters in investigating helium migration over the interstitial positions in vanadium by the MD-method (Table 1). It has been found on the basis of kinetics of helium release that the migration of helium interstitial atoms in a vanadium lattice is characterized by a diffusion coefficient:

$$D_{\mathrm{He}} = D^0 \exp\left(-E^{\mathrm{M}}_{\mathrm{He}}/k_{\mathrm{B}}T\right), \tag{12}$$

where $D^0 = (5.2 \pm 0.3)\ 10^{-7}$ m^2/s; $E^{\mathrm{M}}_{\mathrm{He}} = (0.23 \pm 0.02)$ eV, k_{B} – Boltzman constant.

The analysis of irradiation dose and temperature dependence of the experimental THDS-spectra confirmed the theoretically predicted, by the MD-method, decomposition processes of clusters consisting of bound SIA and helium-vacancy complexes. The assessment was made for formation energy of Frenkel pair in vanadium, based on the calculations by the MD-method data on cluster-binding energies and from the data on activation energies of the processes with SIA participation (processes (8) and (9), obtained by the numerical modeling of corresponding experimental peaks, which was found to be equal to (5.5 ± 0.5) eV. A direct calculation by the MD-method agrees with this assessment value: formation energies for vacancies and the most stable SIA configurations are 2.08 and 3.96 eV, respectively [1].

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