International Journal of Advances in Materials Science and Engineering (IJAMSE) Vol.14, No.1/2/3, July 2025

DEVELOPMENT OF A STATISTICAL THERMODYNAMIC MODEL FOR CALCULATION OF SELF-DIFFUSION PARAMETERS IN METALS

Serhii Bobyr [1], Joakim Odqvist [2]

[1] Uppsala University, Ångström Laboratory, Lägerhyddsvägen 1, Box 538, SE 751 21, Uppsala, Sweden,
[2] KTH Royal Institute of Technology, Department of Materials Science and Engineering, Brinellvägen 23, SE-100 44, Stockholm, Sweden,

ABSTRACT

The theory of diffusion in metals is based on the fundamental concepts of physical kinetics and is very important branch in Material Science. Vacancy migration is the dominant mechanism of self-diffusion, in most elemental crystals, and is of fundamental importance in processes like solid phase transformations, nucleation and defect migration.

The purpose of this project is to develop a statistical thermodynamic model for the self-diffusion in metals and to apply it for calculating the diffusion coefficients of atoms in metals and alloys. The direct relationship between the diffusion flux of vacancies and the gradient of their chemical potential in this model has been established. For a solid solution of vacancies in a metal, an expression for the self-diffusion coefficient has been found. To calculate the activation energy of self-diffusion in metals and simple alloys, the statistical calculation model (SCM) has been developed. The SCM-calculations are compared with the known experimental data on the diffusion in iron and other metals with a good agreement between the results. Based on the processing of experimental results on diffusion in metals using SCM, thermodynamic parameters of self-diffusion in α- and γ-Fe, Ti, V, Mo, W, Ag, Cu and other metals were established. For calculation self-diffusion in metals and simple alloys the SCM-model was implemented.

KEYWORDS

Metals; statistical thermodynamics; self-diffusion; vacancies; pre-exponential factor; activation energy

1. INTRODUCTION

The theory of diffusion in metals is based on the fundamental concepts of physical kinetics, statistical and non-equilibrium thermodynamics, and is closely related to the study of defects in crystals [1–3]. Description of the vacancy mechanism of self-diffusion in metals has a significant meaning for this theory [3–12].

Vacancy migration is the dominant mechanism behind atomic transport, e.g., self-diffusion, in most metals and alloys, and is of *a fundamental mechanism of solid phase transformations, nucleation and defect migration* [5–14]. Vacancies also play an important role for surface morphology, as shown in [14]. In the atomistic theory of diffusion in metals, vacancies, created at the surface or at defects, exist at a certain concentration in all materials [7–12].

The equilibrium concentration C^0_V of vacancies is determined by the formation energy E_f,

DOI:10.14810/ijamse.2023.14401

$$C_V = C_V^0 \mathrm{e}^{-\mathrm{E}_f/\mathrm{kT}} \quad , \qquad (1)$$

where T is the temperature and k is Boltzmann’s constant. The self diffusion coefficient is given by a similar expression

$$D_V = D_V^0 \mathrm{e}^{-(\mathrm{E}_f+\mathrm{E}_m)/\mathrm{kT}} \quad , \qquad (2)$$

where E_m is the migration energy (or diffusion barrier). The entropy of formation, as well as that of migration, also enters these expressions but the most important term, in particular at low temperature, is the energy.

The atomic theory of diffusion an expression for the pre-exponential factor of self-diffusion has been established that dependence from the square of the distance between two atomic positions [4–7]. Einstein's well-known diffusion equation consists of the same ratios [7].

However, the main driving force in the theory of diffusion are the gradients of chemical potentials μ_i of the components of the system [7]. This should be considered when finding equations for the self-diffusion coefficients in metals.

In statistical thermodynamics, equations describing diffusion of carbon in metals have been known [15, 16]. Similarly, it is of undoubted scientific and methodological interest to also derive the corresponding diffusion equations for the self-diffusion of atoms in metals.

To quantify the effect of elemental and vacancy diffusion *on* phase transformation, multi-scale modeling is required [17]. The numerical tools that are applied include thermodynamics and phase-field modeling [18 - 24], atomistic dynamics simulation [25, 26], Monte Carlo simulation [27, 28], quasicontinuum rate theory [29], calculations based on density functional theory [30 - 32].

It has been shown that the quantitative agreement between the local density approximation (LDA), the generalized gradient approximation (GGA) and experimental data for self-diffusion of Pt and Pd is a result of two unrelated effects. The calculated vacancy formation energies are, for both the LDA and GGA, close to measured positron annihilation data [30, 31].

Using the calculated enthalpy and entropy of vacancy formation, the first-principles calculated equilibrium vacancy concentration versus experiment as a function of temperature were compared. The agreement was excellent, particularly for the GGA calculations [31]. Inclusion of the entropic contribution to vacancy formation (which increases the vacancy concentration by a factor of 3) is crucial for obtaining this quantitative agreement with experiment [32].

These methods are often very complex and have their limits when applied for modeling steels and alloys [26, 33]. It has been established that the entropy of vacancy formation is not constant and the highly nonlinear temperature dependence in the Gibbs vacancy formation energy naturally explains the differences between positron annihilation spectroscopy and differential dilatometry data [33].

It was established that a number of elements show a remarkable “curvature” and thus deviation from Arrhenius equation in their diffusion. Although such an anomaly is rare for non-bcc metals, it has been found to be especially strong in the group IV metals Ti, Zr, and Hf [34]. It was demonstrated that the nonlinear Arrhenius self-diffusion behavior in bcc metals e.g. Mo and β-Ti can be largely attributed to the thermal expansion effect, using the framework of quasiharmonic transition state theory [34].

First principles calculations have been used to study the structure and self-diffusion energy in the case of face-centered cubic (FCC) metals in several papers [34-40].

Thus, first-principles calculations provide a good description of the geometry of interaction and activation energy of self-diffusion in metals and metallic systems. However, there is no systematic derivation of the self-diffusion coefficients in metals for which the statistical distribution ***is*** *t*aken into account in a wide temperature range. The use of such calculations is important for understanding the possible mechanisms of self-diffusion in metals and clarification of diffusion effects.

The purpose of this work is to develop a statistical thermodynamic model for calculating the parameters of self-diffusion of atoms in metals and to apply it for calculating the diffusion coefficients of atoms in metals and alloys.

2. METHODS

2.1. Theoretical Method

To describe the diffusion of atoms in the crystal lattice of a metal in work a statistical model of diffusion of impurity atoms in metals has been developed [41].

In this article, a statistical thermodynamic model will be used to substantiate the parameters of self-diffusion of vacancies in metals. For this, we apply the Boltzmann distribution to describe the energy of the vacancies.

Atoms in the crystal lattice of a metal are held by different attractive forces. Consequently, the potential energy of moving vacancies, i.e. diffusing atoms, is greater than the potential energy of the atoms of the crystal lattice by the value U - the activation energy of vacancy diffusion.

In a unit volume of metal, we can identify a single surface perpendicular to the x axis (Figure 1), and calculate the total flow of vacancies.

The number of vacancies and equal number of diffusive atoms in each state is determined by the Boltzmann distribution [41, 42]:

$$N_i = \frac{1}{\exp((\varepsilon_i - \mu)/kT)}, \qquad (3)$$

T is the temperature, μ is the chemical potential of atoms, ε_i is the energy of state i and k is Boltzmann's constant.

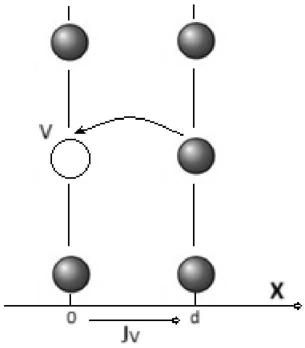

Figure 1. Schematic illustration of diffusion of vacancies in a statistical thermodynamic model. Gray spheres symbolize metal atoms, an empty circle symbolizes a vacancy

Performing calculations for the diffusion flux of vacancies, similar to the calculations of carbon diffusion [15, 16], taking into account Eq. (3), it was found that the total diffusion flux of vacancies in the positive direction of the x-axis is given by:

$$J_V = -\frac{2\pi mkTd}{h^3} \mathrm{e}^{-W/kT} \frac{\partial \mu_V}{\partial x} \quad , \tag{4}$$

where $W = U - \mu_{V0}$;
μ_V is the chemical potential of vacancies;
d is the interplanar distance;
h is the Planck constant;
m is the atomic mass of the element.

Eq. (4) is the statistical thermodynamics equation of vacancy diffusion in a metal. It explicitly shows that the diffusion flow of vacancies directly depends on the gradient of the chemical potential, as it should be in a consistent thermodynamic theory [7, 23, 24].

Using equation (4) we can calculate ab initio the pre-exponential factor of vacancy diffusion in a crystal lattice of a metal [15,16].

If we further consider the ideal solid solution of vacancies in the bulk of a metal, then we can write the following expression for the chemical potential of vacancies [7]:

$$\mu_V = \mu^0_V + kT \ln C_V, \tag{5}$$

and

$$\frac{\partial \mu_V}{\partial x} = \frac{kT}{C_V} \frac{\partial C_V}{\partial x} \quad . \tag{6}$$

Substituting the expression (5) and (6) in (4), we find the diffusion flow of vacancies in a solid solution:

$$J_V = -\frac{2\pi C_V m_e k^2 T^2 d}{N h^3} \mathrm{e}^{-\frac{U-\mu_V^0}{\mathrm{kT}}} \frac{\partial C_V}{\partial x} \quad , \tag{7}$$

where U is the activation energy of the diffusion of vacancies in a solid solution (or the activation energy of the diffusion of an atom close to vacancy).
Using the expression (1) for the concentration of vacancies we finally get:

$$J_V = -\frac{2\pi C_V^0 m_e k^2 T^2 d}{N h^3} \mathrm{e}^{-\frac{U+E_f-\mu_V^0}{\mathrm{kT}}} \frac{\partial C_V}{\partial x} . \qquad (8)$$

Then the expression for the vacancy diffusion coefficient in the metal (or self-diffusion) can be identified:

$$D_0 = \frac{2\pi C_V^0 m_a k^2 d}{h^3 N \rho} \cdot N_e \cdot M_e \cdot T^2 , \qquad (9)$$

where N_e is the atomic number of the element; N is the Avogadro number;
m_a is the atomic mass unit; ρ is the metal density;
M_e is the atomic mass of a metal (or an alloy with interstitial elements such as Fe–C).

Expression (9) of the developed statistical thermodynamic model of self-diffusion significantly differs from the *classical expressions* [4-12]. *The interplanar distance d in this expression is to the first degree, but it assumes the dependence of* D_0 *on the atomic number and atomic mass of the metal and the square of the diffusion temperature.*

For practical calculations of self-diffusion the statistical calculation model (SCM) *has been developed. The* diffusion coefficient D can be calculated by the expression, obtained by combining (8) and (9):

$$D^i = D^i_0 \exp\,(-\,Q_i\,/\mathrm{RT}), \qquad (10)$$

where $Q_i = U+E_f - \mu^0{}_V$ for every i-metal,

$$D^i_0 = A^i_0 T^2, \qquad (11)$$

A^i_0 is the coefficient, followed from Eq. (9) for every i-metal.

2.2. Calculation of Activation Energy and Coefficient of Self-Diffusion in Metals

In the literature many diffusion parameters are known, constructed from experimental data [32 - 43] that can be used to construct the distribution of experimental values of coefficients and activation energies of self-diffusion in metals together with calculated values.

The activation energies of self-diffusion in some metals, primarily in iron, were calculated from first principles using DFT calculations [21- 31] and included in the *SCM-model* database.
However, reliable experimental or computational data are known only for a limited number of metals [7-13, 43, 44]. Therefore, to estimate the activation energy of self-diffusion in metals we propose to use physicochemical methods for establishing correlations.

From works on diffusion in metals, the correlation between the activation energy of self-diffusion in metals and the heat and melting point of the metal is well known [7, 38, 44].

Askill [45] briefly reviewed various correlations between activation energy for self-diffusion and the physical properties of materials, including melting point, heats of fusion and vaporization, elastic module, compressibility, and coefficients of linear expansion. Among these relations, the correlation between the activation energy and the melting temperature may be the most widely used one. The original form of such a correlation reads

$$Q = AT_m, \tag{12}$$

where A is a constant (38 for fcc and 32.5 for bcc) and T_m is the melting temperature in Kelvin.

By taking the effects of the valence V, and crystal structure factor K_0 into account, Sherby and Simnad [18] proposed another correlation as,

$$Q = RT_m (K_0 + V), \tag{13}$$

with R being the gas constant. In this correlation, K_0 is 14 for bcc metals, 17 for fcc and hcp metals, and 21 for metals of diamond structure, while V is 1.5 for Group IVB (Ti, Zr, Hf), 3.0 for Group VB (V, Nb, Ta), 2.8 for Group VIB (Cr, Mo, W), 2.6 for Group VIIB (Mn, Re), and 2.5 for other transition elements.

Besides, another similar equation was derived by Le Claire [19]:

$$Q = RT_m (K+1.5V) \tag{14}$$

with K = 13 for bcc metals, 15.5 for fcc and hcp metals, and 20 for diamond structure.

Similarly, Cahoon [20] also proposed a correlation between activation energy of liquid metals and the melting temperature:

$$Q = 0.17\, RT_m (K_0+16) \tag{15}$$

where K_0 is 1 for bcc, 2 for hcp and 3 for fcc. In addition to the above correlations between the activation energy and the melting temperature, some other correlations were also proposed in the literature.

For instance, Gòrecki [21] found that there exists a simple correlation for the activation energy of self-diffusion and impurity diffusion coefficients in metals on passing through the melting point. The statistical analysis in paper [21] shows that the mean value of the ratio for the self diffusion coefficient in the solid phase to that for the liquid phase is 5 with a standard deviation of 0.31, and that for rare gases is 5.03 with a deviation of 0.36.

Therefore, for metals for which the activation energy is still unknown, we propose to use the correlation relationship between the activation energy of self-diffusion and the melting temperature of the i-element T^i_{melt}:

$$Q_i = K_0 K_i k T^i_{melt}, \tag{16}$$

k is the Boltzmann constant;
K_0 is the constant coefficient (~ 15.07 for self-diffusion), was selected from the correspondence of the activation energy calculated using formula (16) with reliable data from works [39, 43, 46] on the self-diffusion in iron;

K_i is the coefficient, considering amendments for element i, made on the base of experimental data from work [39, 43, 46] on the self-diffusion in metals. This coefficient for known experimental data is close to 1.0 (0.7-1.3) and equal to 1.0 for unknown parameters of self-diffusion in metals.

The statistical calculation model (SCM) for self-diffusion in metals and alloys was implemented in the corresponding database, including 43 base metals and silicon.

3. RESULTS

3.1. A Comparison of Experimental and Calculated Data on the Values of the Diffusion Parameters for Metals

The self-diffusion coefficients for metals were calculated according to the formula (10) and given in Figure 2 along with experimental data.

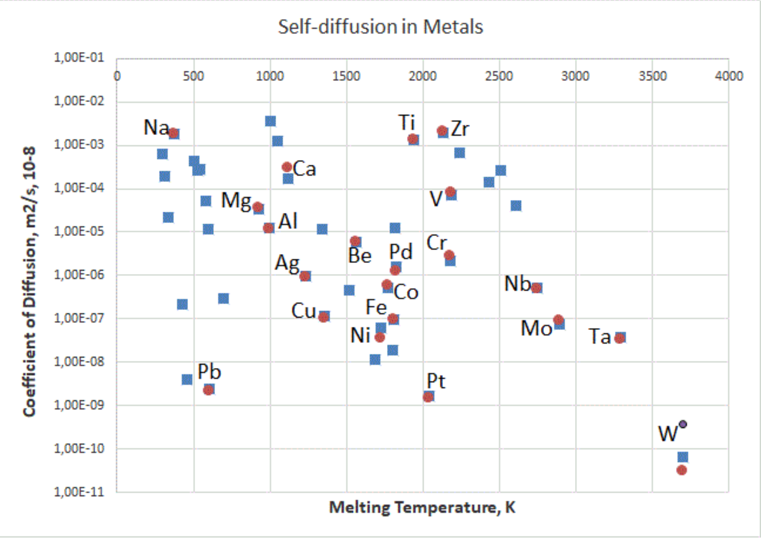

Figure 2. Calculated data on the values of the self-diffusion coefficient in metals, in comparison with the experimental data. Blue squares show calculated values of D^i according to formula (10) with T = 1000 K, brown circles are experimental values. Violet sircle shows calculated value of D for W with T = 2000 K.

Figure 2 shows that the calculated values of the self-diffusion coefficient for metals agree well with the experimental values that would be expected.

3.2. A Comparison of Experimental and Calculated Data on the Values of Diffusion Coefficients for Some Selected Metals

In this section, a comparison is made of the SCM-calculated data and the experimental data of the diffusion coefficients obtained earlier in the corresponding works and represented by the Arrhenius equation. The values of the self-diffusion parameters for these metals are presented in Table 1.

The SCM model provides a smaller **deviation** from the pre-exponential values of the coefficients for metals than the experimental values of Arrhenius equation.

Table 1. Calculated values for an activation energy (E_a) and a pre-exponential factor (D_0) of self-diffusion in α-Fe, γ-Fe, Ti and V together with experimental values

Metals	**α-Fe**	**γ-Fe**	**Ti**	**V**
Calc. SCM at 1000 K, D_0 10^{-7} (m^2/s)	10.9	14.3	14.3	12.3
Calc. SCM, E_a (kJ)	212,3	265,3	227,5	255,9
Expt., D_0 10^{-7} (m^2/s)	2750 [47] 1900 [48]	180 [49] 490 [50]	30 [51] 3000 [52]	360 [53] 288 [53]
Expt., E_a (kJ)	254 [47] 239 [48]	273 [49] 284 [50]	188 [51] 230 [52]	308 [53] 309 [54]

The values of the self-diffusion coefficients in α- and γ-iron are shown in Fig. 3 and Fig. 4 respectively.

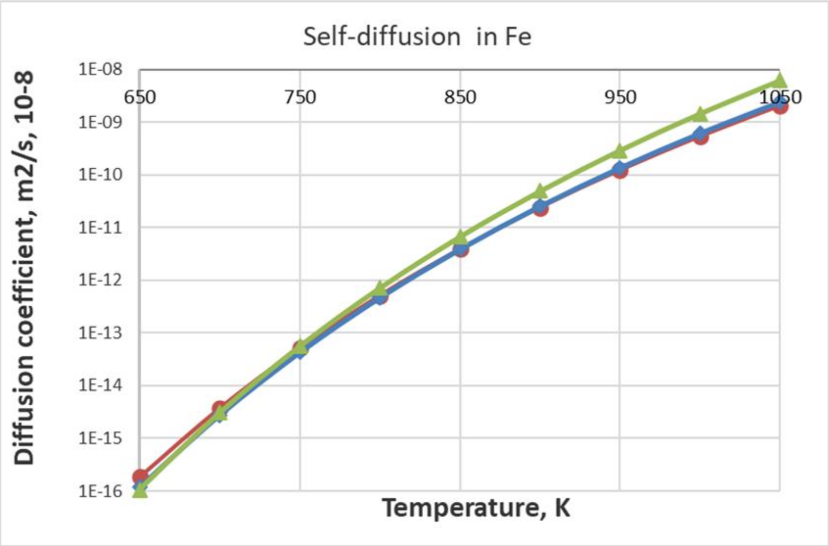

Figure 3. Comparison of calculated data on self-diffusion coefficient values in α-Fe, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 2.75\times10^{-3}$ m^2/s and Ea = 254 kJ from [47], blue rhombs represent calculated values with $D_0 = 1.9\times10^{-4}$ m^2/s and Ea = 239 kJ from [48] respectively.

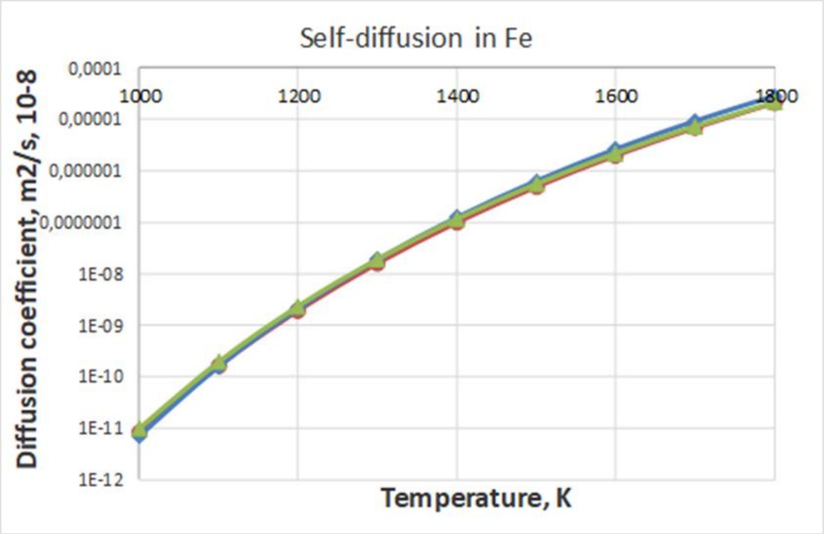

Figure 4. Comparison of calculated data on self-diffusion coefficient values in γ-Fe, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 1.8\times10^{-5}$ m^2/s and *Ea* = 273 kJ from [49], blue rhombs represent calculated values with $D_0 = 4.9\times10^{-5}$ m^2/s and *Ea* = 284 kJ from [50] respectively.

From Figures 3 and 4 we can see a good agreement between the values calculated using the Arrhenius equation and the SCM model. For γ-Fe, the values of all three equations, used for the analysis, were practically identical over a wide temperature range. The SCM model is quite efficient for estimating self-diffusion coefficients in iron.

Similar calculations were performed for two metals with average melting temperature - Ti and V. Comparison of calculated data on diffusion coefficient values in Ti and V represents on the Figures 5 and 6 respectively.

For Ti almost complete agreement with the experimental results and SCM-calculated is observed in the low-temperature region (Figure 5). For V very good agreement with the experimental results and SCM-calculated have a place in the high-temperature region (Figure 6).

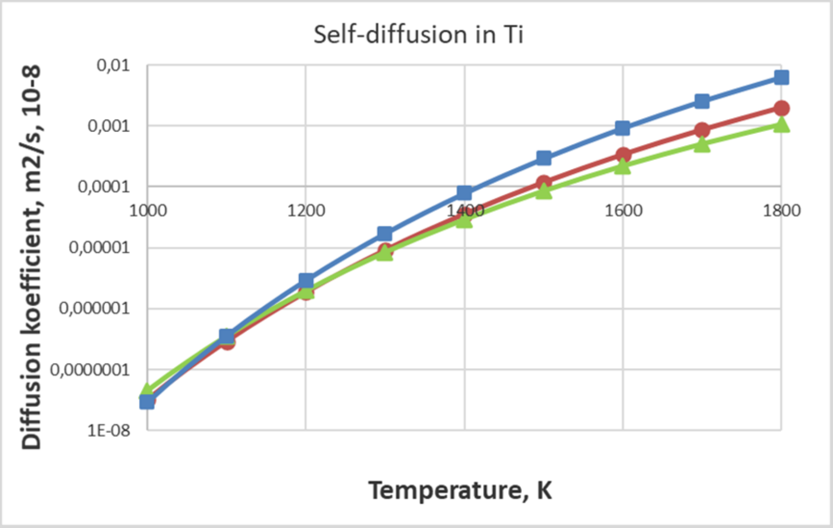

Figure 5. Comparison of calculated data on self-diffusion coefficient values in Ti, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 3.0\times10^{-6}$ m^2/s and Ea = 188 kJ from [51], blue squares represent calculated values with $D_0 = 3.0\times10^{-4}$ m^2/s and Ea = 230 kJ from [52] respectively.

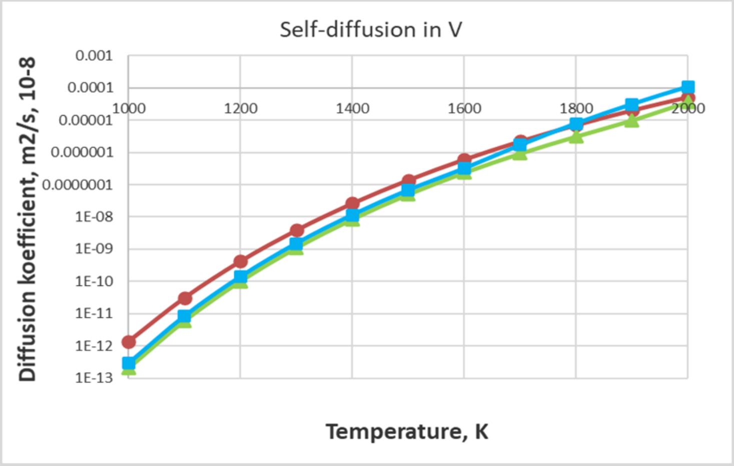

Figure 6. Comparison of calculated data on self-diffusion coefficient values in V, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 3.6\times10^{-5}$ m^2/s and Ea = 308 kJ from [53], blue squares represent calculated values with $D_0 = 2.88\times10^{-5}$ m^2/s and Ea = 309 kJ from [54] respectively.

Deviations from Arrhenius law are also observed in self-diffusion in V and Ti [51, 53], which is quite explainable using the proposed SCM.

Similar calculations were performed for two refractory metals - Mo and W, *and for two low-melting metals, Ag and Cu.* In this case, experimental data from two different sources were also taken into account. The values of the self-diffusion parameters for these metals are represented in Table 2.

Table 2. Calculated values for an activation energy (E_a) and a pre-exponential factor (D_0) of self-diffusion in Mo, W, Ag and Cu together with experimental values

Metals	**Mo**	**W**	**Ag**	**Cu**
Calc. SCM, $D_0 10^{-7}$ (m^2/s)	107 at 2000 K	212 at 2000 K	12.3 at 1000 K	14.3 at 1000 K
Calc. SCM, E_a (kJ)	423.5	606.4	178.1	183.1
Expt. $D_0 10^{-7}$ (m^2/s)	380 [55] 100 [56]	10800 [57] 40 [58]	620 [59] 43 [60]	877 [61] 2320 [62]
Expt. E_a (kJ)	422 [55] 386 [56]	610 [57] 526 [58]	189 [59] 170 [60]	211 [61] 206 [62]

For these metals, we observed a very good correlation between the calculated and experimental activation energy values.

A comparison of the calculated data on the values of the self-diffusion coefficients in Mo and W is presented in Figures 7 and 8, respectively.

From these figures it is clear that the SCM model fits well at least one experimentally obtained Arrhenius equation [55-58]. For Mo and W, almost complete agreement with the experimental results is observed in the high-temperature region (Figure 7, 8).

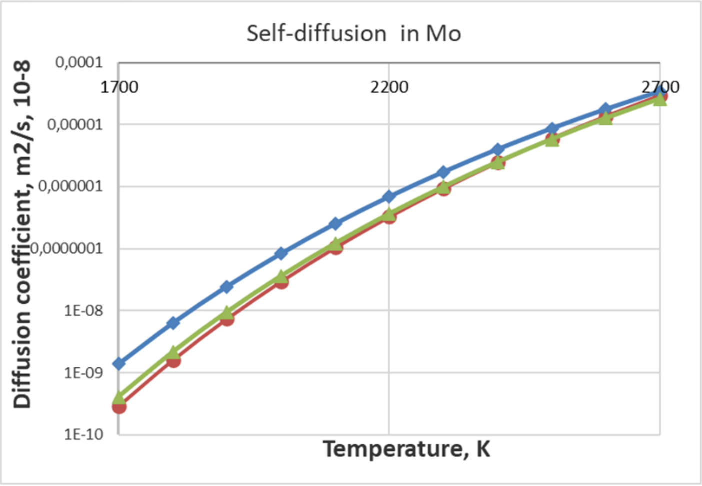

Figure 7. Comparison of calculated data on self-diffusion coefficient values in Mo, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 3.8\times10^{-5}$ m^2/s and Ea = 422 kJ from [55], blue rhombs represent calculated values with $D_0 = 1.0\times10^{-5}$ m^2/s and Ea = 386 kJ from [56] respectively.

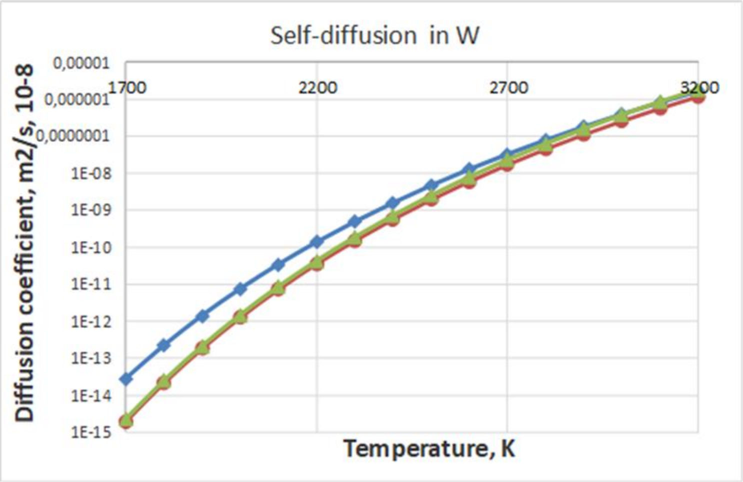

Figure 8. Comparison of calculated data on diffusion coefficient values for W, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 1.08\times10^{-3}$ m^2/s and *Ea* = 610 kJ from [57], blue rhombs represent calculated values with $D_0 = 4.0\times10^{-6}$ m^2/s and *Ea* = 526 kJ plus $D_0 = 4.6\times10^{-4}$ m^2/s and *Ea* = 666 kJ from [58] respectively.

In the end, similar calculations were performed for two low-melting metals, Ag and Cu (Figures 9 and 10 respectively).

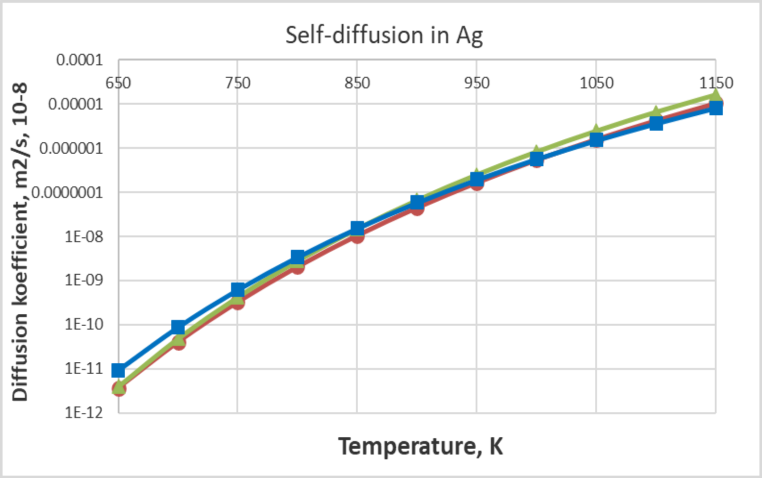

Figure 9. Comparison of calculated data on diffusion coefficient values for Ag, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 6.2\times10^{-5}$ m^2/s and *Ea* = 189 kJ from [59], blue rhombs represent calculated values with $D_0 = 4.3\times10^{-6}$ m^2/s and *Ea* = 170 kJ from [60] respectively.

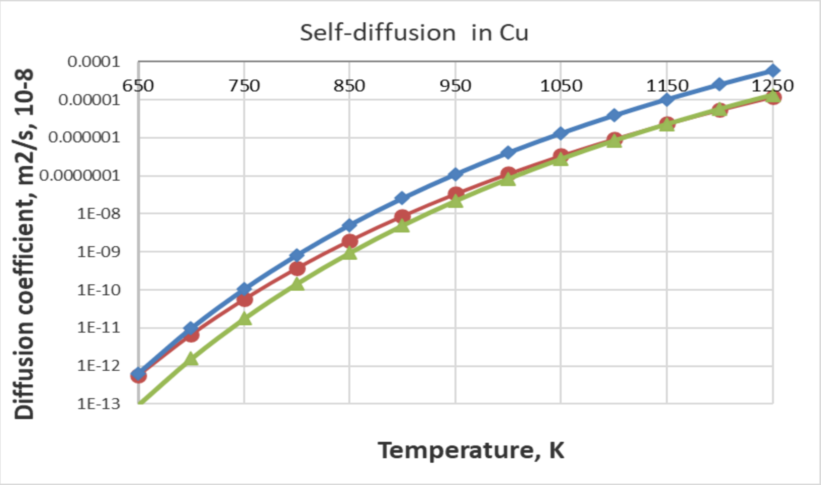

Figure 10. Comparison of calculated data on diffusion coefficient values for Cu, red circles show calculated values from the SCM, green triangles represent values from Arrhenius equation with $D_0 = 8.77\times10^{-5}$ m^2/s and Ea = 211 kJ from [61], blue rhombes represent calculated values with $D_0 = 2.32\times10^{-4}$ m^2/s and Ea = 206 kJ from [62] respectively.

For Ag, there was a very good agreement between the calculated SCM and the empirically validated Arrhenius equations over the entire temperature interval (Figure 9).

For Cu SCM-calculated values of self-diffusion coefficients were between two empirically substantiated Arrhenius equations (Figure 10).

In this case, the accuracy of the values calculated by the SCM was also very satisfactory.

To increase the accuracy of calculations in the SCM model, it is necessary to *consider* the values of the activation energy of diffusion, calculated from first principles, taking into account their dependence on temperature [26-35]. However, in this case, the SCM model ceases to be predictive for other metals.

Undoubtedly, this model does not consider many specific factors affecting the diffusion parameters of atoms in metals, such as the interaction of impurities and vacancies, the presence of lattice defects and stresses, etc. *This model cannot be used to calculate diffusion coefficients for alloying elements in alloys.*

Further development of this model will allow us to take into account the influence of these factors on self-diffusion in iron and metals and to calculate the diffusion coefficients for alloying elements in alloys.

4. CONCLUSIONS

1. Thus, a statistical thermodynamics model of the self-diffusion in the crystal lattice of metals in the article has been developed. *The direct relationship between the diffusion flux of vacancies and the gradient of their chemical potential in the model has been established.*

2. For a solid solution of vacancies in metals, an expression for the diffusion coefficient of self-diffusion from the basic principles of statistical thermodynamics has been found. Its magnitude depends on the physical constants, the atomic weight of the metal, the square of the temperature, and the concentration of vacancies in the solid solution.
3. To calculate the activation energy of self-diffusion in metals and simple alloys, a SCM model was proposed that takes into account energy calculations from first principles, statistical processing of experimental data on self-diffusion of metals, and a physicochemical model using the correlation relationship between the activation energy of self-diffusion and the melting temperature of metals.
4. Based on the processing of experimental results on diffusion in metals using SCM, thermodynamic parameters of self-diffusion in α- and γ-Fe, Ti, V, Mo, W, Ag, Cu and other metals were established. *The calculated values of the self-diffusion coefficient for metals agree well with the experimental values that would be expected.*
5. The calculations from SCM are compared with the known experimental data on the self-diffusion in iron and metals with a good agreement between the results. This agreement for the given special cases of diffusion is higher than in classical atomic diffusion models. Deviations from the Arrhenius law are also observed during the self-diffusion in V and Ti, which can also be explained by the proposed SCM.

The SCM for self-diffusion in metals and simple alloys was implemented in the corresponding database, including 43 base metals and silicon.

ACKNOWLEDGEMENTS

This project was funded by the Swedish Foundation for Strategic Research (SSF), contract UKR24-0017. *I want to thank prof. Martin Sahlberg for supporting this project and critical remarks.*

REFERENCES

[1] B.S. Bokstein.Thermodynamics and Kinetics in Materials Science. A short course. New York: Oxford University Press, 2005. 326 p.
[2] G. Grosso and P. G. Pastori, Solid State Physics (Academic, London, 2003).
[3] J. R. Hook and H. E. Hall, Solid State physics. Introduction to the Theory (Springer, Berlin, 2007).
[4] Ya. I. Frenkel’, Introduction to the Theory of Metals (Fizmatgiz, Moscow, 1948) [in Russian].
[5] S. D. Gerzriken and I. Ya. Dehtyar, Diffusion in Metals and Alloys in Solid Phase (Fizmatgiz, Moscow, 1960) [in Russian].
[6] M. A. Cristal, The Diffusion Mechanism in Iron Alloys (Metallurgy, Moscow, 1972) [in Russian].
[7] B.S. Bokshtein, Diffusion in metals [in Russian]. Metallurgy, M., 1978, 248.
[8] N.L. Peterson. Self-diffusion in pure metals. Journal of Nuclear Materials V. 69–70, February 1978, Pages 3-37.
[9] G. Neumann, C. Tuijn. Chapter 5 - Self-Diffusion and Impurity Diffusion in Group V Metals. Pergamon Materials Series, 2008, V. 14, P. 215-238.
[10] G. Neumann, C. Tuijn. Self-diffusion and Impurity Diffusion in Pure Metals: Handbook of Experimental Data. Elsevier, 19 aug. 2011 – 360p.
[11] Zoltan Balogh, Guido Schmitz. 5 - Diffusion in Metals and Alloys. In Physical Metallurgy (Fifth Edition), 2014, Pages 387-559.
[12] Mehrer H. Diffusion in Solids: Fundamentals, Methods, Materials, Diffusion-Controlled Processes. Berlin, Heidelberg: Springer-Verlag, 2007
[13] Mehrer H, Divinski S. Diffusion in metallic elements and intermetallics. Diffus Defect Data, 2009, 289-292: 15–38
[14] K. F. McCarty, J. A. Nobel, and N. C. Bartelt, Vacancies in solids and the stability of surface morphology. Nature (London) 412, 622. (2001).

[15] S.V. Bobyr, D.V. Loschkarev, S.A. Sharfnadel. Statistical model calculating the carbon diffusion parameters in steels, Material Sci & Eng., 2022, 6(4), 146.

[16] S. Bobyr. Development of a statistical calculation model for the carbon diffusion parameters in metals and alloys. Material Sci & Eng. 2024;8(3):102–107. DOI: 10.15406/mseij.2024.08.00242

[17] C. Tasan, M. Diehl, D. Raabe. Modeling of Materials: Development with Simulation –Discoveries through Simulation. Multiscale materials simulation. Winter school, 2017, German Research Foundation SPP Aachen Germany.

[18] Sherby O. D., Simnad M. T. Prediction of atomic mobility in metallic systems. ASM Trans Q, 1961, 54: 227–240

[19] Le Claire A. D. Diffusion in Body Centre Cubic Metals. Ohio: American Society for Metals, Metals Park, 1962. 10.

[20] Cahoon J R. A modified hole theory for solute impurity diffusion in liquid metals. Metall Mater Trans A, 1997, 28: 583–593

[21] Gòrecki T. Changes in the activation energy for self- and impurity-diffusion in metals on passing through the melting point. J Mater Sci Lett, 1990, 9: 167–169

[22] Engström A, Ågren J. Assessment of diffusional mobilities in face-centered cubic Ni-Cr-Al alloys. Z Metallkd, 1996, 87: 92–97

[23] Fultz B. Vibrational thermodynamics of materials. Prog Mater Sci, 2009, 55: 247–352.

[24] D. Mukherjee, H. Larsson, and J. Odqvist. Phase-field modeling of diffusion induced grain boundary migration in binary alloys, Computational Material Science, 2020, 184, 1-9.

[25] Jang J, Kwon J, Lee B. Effect of stress on self-diffusion in bcc Fe: An atomistic simulation study. Scr Mater, 2010, 63.

[26] A. Ferrari, B. Dutta, K. Gubaev, Y. Ikeda, P. Srinivasan, B. Grabowski, F. Körmann. Frontiers in atomistic simulations of high entropy alloys. Journal of Applied Physics, 2020, 128 (15), 0025310.

[27] J. Betlej, P. Sowa, R. Kozubski, G.E. Murch, I.V. Belova. Self-Diffusion in a Triple-Defect A-B Binary System: Monte Carlo simulation. Materials Science arXiv:1904.11343 [cond-mat.mtrl-sci].

[28] Wai Kin (Victor) Chan (Redactor). Theory and Applications of Monte Carlo Simulations. London: Intech Open, 06 March 2013, 286 p.

[29] A quasi-continuum multi-scale theory for self-diffusion and fluid ordering in nanochannel flows. Article in Microfluidics and Nanofluidics, December 2014 DOI: 10.1007/s10404-014-1390-2

[30] T. R. Mattsson and A. E. Mattsson. Calculating the vacancy formation energy in metals: Pt, Pd, and Mo. Physical Review B 66, 214110 (2002). DOI: 10.1103/PhysRevB.66.214110

[31] K. Carling and G. Wahnström, T. R. Mattsson, A. E. Mattsson, N. Sandberg, and Göran Grimvall. Vacancies in Metals: From First-Principles Calculations to Experimental Data, Phys. Rev. Let. ,85 (18), 3862 (2000). DOI: 10.1103/PhysRevLett.85.3862.

[32] M. Mantina, Y. Wang, R. Arroyave, L. Q. Chen, and Z. K. Liu. First-Principles Calculation of Self-Diffusion Coefficients, Phys. Rev. Let. ,100, 215901 (2008). DOI: 10.1103/PhysRevLett.100.215901

[33] A. Glensk, B. Grabowski, T. Hickel, J. Neugebauer. Breakdown of the Arrhenius law in describing vacancy formation energies: the importance of local anharmonicity revealed by Ab initio thermodynamics. Physical Review, 2014, X4 (1), 011018.

[34] Y. Wang, Z. Chen, W. Windl, and Ji-C. Zhao. Nonlinear Arrhenius behavior of self-diffusion in β-Ti and Mo. Physical Review Materials 6, 063402 (2022).

[35] Du Y, Chang Y A, Huang B, et al. Diffusion coefficients of some solutes in fcc. and liquid Al: Critical evaluation and correlation. Mater Sci Eng, A, 2003, 363: 140–151

[36] R. G. Hennig, T. J. Lenosky, D. R. Trinkle, S. P. Rudin, and J. W. Wilkins. Classical potential describes martensitic phase transformations between the α, β, and ω titanium phases. Phys. Rev. B **78**, 2008, 054121. – Published 27 August 2008

[37] Zhao D, Kong Y, Wang A, et al. Self-diffusion coefficient of fcc Mg: First-principles calculations and semi-empirical predictions. Journal of Phase Equilibria and Diffusion, 2011, 32: 128–137.

[38] D.U. Yong, Z. Li Jun, C. Sen Lin at all. Atomic mobilities and diffusivities in Al alloys. Science China. Technological Sciences. February 2012, Vol.55 No.2: 306–328.

[39] T. Angsten, T. Mayeshiba, H. Wu and D. Morgan. Elemental vacancy diffusion database from high-throughput first-principles calculations for fcc and hcp structures. New J. Phys., 2014, **16**, 015018. DOI 10.1088/1367-2630/16/1/015018

[40] Ch. Z. Hargather, J. M. O'Connell. Systematic First-Principles Study of Computational Parameters Affecting Self-Diffusion Coefficients in FCC Ag, Cu, and Ni. Journal of Phase Equilibria and Diffusion, Volume 43, pages 764–779, (2022).

[41] S.V. Bobyr. Statistical model of impurity atoms diffusion in the crystal lattice of metals and its application for calculating the diffusion coefficients of hydrogen and carbon atoms in iron. Phys. Solid State, 2021, 3, 345.

[42] E.M. Lifshits, L.P. Pitaevskiy. Statistical physics. Part 2. Theory of condensed matter [in Russian]. Fizmatlit, M., 2000, 496.

[43] L.N. Larikov, V.I. Isaychev: Diffusion in metals and alloys, Kiev, Naukova dumka, 1987, 510.

[44] / Diffusion in body-centered cubic metals [in Russian]. M., Metallurgy, 1978, 284.

[45] Askill J. Tracer Diffusion Data for Metals Alloys, and Simple Oxides. New York: IFI/Plenum, 1970. 19–26.

[46] Sheng H, Kramer M, Cadien A, Fujita T and Chen M. Highly optimized embedded-atom-method potentials for fourteen fcc metals. Phys. Rev., 2011, B 83, 134118.

[47] Sparke B., James D.W., Leak G.M. Lattice diffusion in gamma-iron. – JICI, 1965, 203, No2, pt.2, P.152-153.

[48] Buffington F.S., Hirano K.-I., Cohen M. Self-diffusion in iron. Acta met., 1961, V.9, No5, P. 434-439.

[49] Radwan M., Zmija J. Dyfusja zelaza i chromu w stopach Fe-Cr. Arch. hutn., 1965, V.10, No4, P. 337-356.

[50] Heumman Th, Imm R. Self-diffusion and isotope effect in γ-iron. J. phys. And Chem. Solids, 1968, V.29, No9, P. 1613-1621.

[51] Grehem D. Diffusion in body-centered cubic metals [in Russian]. M., Metallurgy, 1969, P.35-43.

[52] Brik V.B., Larikov L.N., Falchenko V.M. Research of self-diffusion in α- and β-Ti [in Russian]. UFG, 1979, V.24, No 7, P. 1037-1040.

[53] Peart R. F. Diffusion in body-centered cubic metals [in Russian]. M., Metallurgy, 1969, P.244-253.

[54] Pelleg J. Diffusion in the vanadium system. Phil. Mag., 1977, V.36, No3, P. 735-732.

[55] Maier K., Mehrer H., Rein G., Self-diffusion in molybdenum. Z. Metallk., 1979, V. 44, No 2, P271-286.

[56] Askill J. Diffusion in body-centered cubic metals [in Russian]. M., Metallur-gy, 1969, P.254-259.

[57] Povarova K.B. Diffusion and stability of strengthening phases in tungsten [in Russian]. Izv. AN SSSR. Metals, 1981, No 2, P. 163-175.

[58] Mundy J.N., Rothman S.J., Lam N.O. et al. Phys. Rev. B., 1978, V. 18, No 12, P. 6566-6575.

[59] Janitskaja M.E., Zhuhovitskiy A.A., Bokshtein S.Z. About influence of impurity on the rate of self-diffusion [in Russian]. DAN SSSR, 1957, V.112, No 4, P. 720-723.

[60] Bihr J., Mehrer H., Maier K. A comparison between microsectioning studies of low-temperature self-diffusion in silver. Ibid., 1978, V. 50, No 1, P.171-178.

[61] Fujikawa Sh., Hirano K.-I. Self-diffusion of ^{67}Cu in copper. Res. Rept. Lab. Nucl. Sci. Tohoku Univ., 1982., V. 15, No 1, P. 127-136.

[62] Smirnov O. A., Ivanov L.I., Abramjan E.A. Influence of small doping of nickel on diffusion parameters of copper [in Russian]. Izv. AN SSSR. Metals., 1967, No 6, P. 168-170.

AUTHOR

Dr. Sc. Serhii Bobyr is a Leading Researcher in Metal Physics and Materials science. From 01.06.2024 is a Visiting Researcher at Uppsala University Department of Chemistry - Ångström Laboratory. 2022-2023 is a Leading Researcher at KTH - Royal Institute of Technology, 2016 – now is a Leading Researcher at Z.I. Nekrasov Iron & Steel Institute of the Nat Science of Ukraine (ISI NASU).

Prof. Joakim Odqvist works as a Head of Material Science and Engineering Department at KTH-Royal Institute of Technology, Stockholm His research interests are phase transformations in metallic alloys and computer design.