CALCULATION OF ACTIVATION ENERGY OF DIFFUSION
AND SELF-DIFFUSION

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The methodology is given for the evaluation of activation energy of diffusion and self-diffusion based on the application of spatial-energy parameter (P-parameter). The corresponding calculations are made for 57 structures. The calculation results are in accordance with the experimental data.

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Introduction

Activation energy is one of the basic characteristics of diffusion processes. A lot of works are dedicated to theoretical calculations and experimental evaluations of this value. However the comparison of reference data reveals rather contradictory results on many systems. For instance, a significant discrepancy between theoretical and experimental data of activation energy was obtained even for such well-investigated process as silicon self-diffusion (3.2 eV and 4.76 eV, respectively).

It is customary to distinguish between several types of main diffusion mechanisms in crystals viz., diffusion by internodes, vacancy mechanism, replacement mechanism, etc. The diffusion activation energy equals the value of the potential barrier that has to be overcome by the atom to take a new balanced position in the neighboring node or internode.

Theoretical calculations of activation energy are very difficult. Therefore different authors tried to correlate it with some other values that can be calculated or defined theoretically. Thus according to Frenkel during self-diffusion process the activation energy should be close to the value of crystal evaporation heat. However, as a rule, lower values are experimentally observed. Braune tried to correlate the activation energy with melting temperature of crystals. However the correlation proposed by him is useful only for rough estimation of activation energy since the criterion for selecting the empirical constant of initial equation is missing.

A well-known Arrhenius equation is widely used for energy estimation of diffusion processes.

\[ A = A_0 \exp \left( - \frac{E_a}{RT} \right) \]  (1)

where

\( A = \text{coefficient of diffusion,} \)

\( A_0 = \text{pre-exponential factor,} \)

\( E_a = \text{activation energy of diffusion,} \)

\( R = \text{gas constant and} \)

\( T = \text{thermodynamic temperature.} \)

The dependence of initial parameters upon the temperature and pressure, the presence of pre-exponential factor in the equation rather complicate the issue of rational objectivity of data being obtained, in particular, when comparing diffusion mechanisms near the surface and inside the crystal.

In this research there is an attempt to numerically calculate the activation energy of diffusion based on initial spatial-energy characteristics of free atoms (methodology of P-parameter).

Spatial-energy parameter

The comparison between multiple regularities of physical and chemical processes allows assuming that in many cases the principle of adding inverse values of volume energies or kinetic parameters of interacting structures is fulfilled. Some examples are ambipolar diffusion, total rate of topochemical reaction, change in the light velocity when moving from vacuum to the given medium, resulting constant of chemical reaction rate (initial product – intermediary activated complex – final product).

Lagrangian equation for relative motion of isolated system of two interacting points with masses \( m_1 \) and \( m_2 \) in coordinate \( x \) with acceleration \( a \) can look as follows:

\[ \frac{1}{m_1} \frac{\Delta x}{\Delta t} \approx -\Delta U \]  (2)

\[ \frac{1}{\Delta U} \approx \frac{1}{\Delta U_1} + \frac{1}{\Delta U_2} \]  (3)

where

\( \Delta U_1 \) and \( \Delta U_2 \) are the potential energies of material points on elementary portion of interactions and \( \Delta U \) is the resulting (mutual) potential energy of these interactions.
Calculation of activation energy of diffusion and self-diffusion

The atom system is formed of differently charged masses of nucleus and electrons. In this system the energy characteristics of sub-systems are orbital energy of electrons and effective energy of nucleus taking into consideration the screening effects. At the same time the bond energy of electrons or ionization energy of atom \((E_i)\) can be used as orbital energy. Therefore, assuming that the resulting interaction energy in the system orbital-nucleus (responsible for inter-atom interactions) can be calculated following the principle of adding inverse values of some initial energy components, the introduction of P-parameter\(^{12}\) as an averaged energy characteristics of valence electrons based on the following equations can be substantiated.

\[
\frac{1}{q^3} + \frac{1}{E_i} = \frac{1}{P_E}\tag{4}
\]

\[
P_E = \frac{P_0}{r_i}\tag{5}
\]

\[
\frac{1}{P_0} = \frac{1}{q^2} + \frac{1}{(Er)}\tag{6}
\]

\[
q = Z^* \frac{1}{n^*}\tag{7}
\]

where

\(E_i\) is the atom ionization energy,\(^{13}\)

\(r_i\) is the orbital radius of \(i\)-orbital,\(^{14}\)

and \(Z^*\) and \(n^*\) are effective charge of nucleus and effective main quantum number, respectively.\(^{15,16}\)

\(P_0\) will be called a spatial-energy parameter and \(P_E\) an effective P-parameter. Effective \(P_E\) parameter has a physical sense of some averaged energy of valence electrons in an atom and is measured in energy units, e.g. in electron-volts (eV).

According to the calculations\(^{12}\) the values of \(P_E\) parameters are numerically equal (in the range of \(\pm 2\%\)) to the total energy of valence electrons \((U)\) by atom statistic model. Using the known relation between the electron density \((\beta)\) and intra-atomic potential by atom statistic model, it is possible to obtain the direct dependence of \(P_E\) parameter on the electron density at the distance \(r_i\) from nucleus by Eqn. (8).

\[
\beta_i^2 = \frac{Ap_0}{r_i} = AP_E\tag{8}
\]

where \(A\) is a constant.

The reliability of this equation was confirmed experimentally by determining the electron density using wave functions by Clementi and comparing it with the value of electron density calculated via the value of \(P_0\)-parameter.

Modifying the rules of adding inverse values of energy magnitudes of subsystems as applied to complex structures, the equation (Eqn. 9) for calculating \(P_S\)-parameter of complex structure can be obtained

\[
\frac{1}{P_S} = \left(\frac{1}{NP_{E_1}}\right)_1 + \left(\frac{1}{NP_{E_2}}\right)_2 + \cdots \tag{9}
\]

where \(N_1\) and \(N_2\) are a number of homogeneous atoms in the subsystem.

The same electron density should be fixed during the formation of solution and other structural interactions in the spots of contact between atoms-components. This process is followed by the redistribution of electron density between valence zones of both particles and transition of part of electrons from one external sphere to adjoining ones. Apparently, the frame electrons of atoms do not participate in such an exchange.

Obviously, the proximity of electron densities in free atoms-components results in the minimization of transition processes between boundary atoms of particles, thus favouring the formation of a new structure. Therefore, the task of estimating the degree of structural interactions in many cases means a comparative estimation of electron density of valence electrons in free atoms (on averaged orbitals) participating in the process.

The less is the difference \((P'S'/r'_i - P'S/r_i)\), the more energetically favourable is the formation of a new structure or solid solution.

The estimation of mutual solubility for structural interactions of isomorphic type in many (over one thousand) simple and complex systems\(^{12}\) was carried out based on this technique. Isomorphism as a phenomenon is considered as applied to crystalline structures. But, apparently, analogous processes can also proceed between molecular compounds where their role and value are none the less than in purely Coulomb interactions. It seems diffusion processes, replacement in particular, can also be estimated via the methodology of \(P\)-parameter.

**Calculation methodology**

It is established that during self-diffusion the activation energy often equals the total of enthalpies of formation and transition of vacancies. Obviously, in any actual situation different diffusion mechanisms can act simultaneously, but the activation energy must always be defined by inter-atom interactions in structures.

Thus, the task of estimating the activation energy is to define the actual energy of paired inter-atom interaction of diffusion atom and atoms of diffusion medium, for each specific type of interactions.

Earlier the diffusion coefficients of some refractory oxides were calculated using initial spatial-energy notions\(^{17}\) via total \(P\)-parameter of interacting diffusion atoms and diffusion medium.

Let us now demonstrate that with the help of \(P\)-parameter it is possible to rather reliably and easily estimate the activation energy during the transfer of atoms in solids.

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For this we use the tabulated values of \( P_0 \)-parameters calculated via the ionization energy (Table 1) based on the Eqns. 4-7. In diffusion processes, with the prevalence of ionic structures, it is preferable to use the energy of atom ionization \( E_0 \) as the orbital energy.

Now, with the help of \( P_0 \)-parameter, we can determine the averaged effective energy of paired inter-atom interaction in the system \( M^+M^- \). Having summed up \( P_0 \) by valence electrons and divided the value of \( P_0/2n \) by a number of effective valence electrons \( n \), we obtain some effective energy of atom falling at one valence electron (Eqn. 10).

\[
Q = \frac{P_0}{2r_in} \quad (10)
\]

Applying the previously stated principle of adding inverse values of \( P_0 \)-parameters (Eqn. 9), we obtain the resulting value of effective energy of paired interaction of atoms 1 and 2 during diffusion and self-diffusion.

\[
\frac{1}{E_a} = \frac{1}{Q_1} + \frac{1}{Q_2} \quad (11a)
\]

or

\[
\frac{1}{E_a} = 2 \left[ \left( \frac{r_{in}}{P_0} \right)_1 + \left( \frac{r_{in}}{P_0} \right)_2 \right] \quad (11b)
\]

where \( E_a \) = activation energy.

If during self-diffusion \( n_1 = n_2 \) and \( Q_1 = Q_2 = Q \), then

\[
E_a = \frac{P_0}{2} \frac{1}{4r_in} \quad (12)
\]

Table 1. \( P_0 \)-parameters of valence orbitals of neutral atoms in basic state (calculated via the ionization energy of atoms).

| Atom | Valence orbitals | \( E_0 \) (eV) | \( n_i \) (Å) | \( q^2 \) (eVÅ) | \( P_0 \) (eVÅ) | \( \Sigma P_0 \) (eVÅ) |
|------|-----------------|----------------|---------------|----------------|----------------|---------------------|
| H    | 1s              | 13.595         | 0.5295        | 14.394         | 4.7985         | 4.7985              |
| Li   | 2s              | 5.390          | 1.586         | 5.890          | 3.487          | 3.487               |
| Be   | 2s              | 9.323          | 1.040         | 13.159         | 5.583          | 13.347              |
|      | 2p              | 18.211         | 1.040         | 13.158         | 7.764          |                     |
| C    | 2p              | 11.260         | 0.596         | 35.395         | 5.641          |                     |
|      | 2p              | 24.383         | 0.596         | 35.395         | 10.302         |                     |
|      | 2s              | 47.86          | 0.620         | 37.243         | 16.515         |                     |
|      | 2p              | 64.48          | 0.620         | 37.243         | 19.281         |                     |
| O    | 2p              | 13.618         | 0.414         | 71.380         | 5.225          | 17.304              |
|      | 2p              | 35.118         | 0.414         | 71.380         | 12.079         |                     |
| Na   | 3s              | 5.138          | 1.713         | 10.058         | 4.694          | 4.694               |
| Mg   | 3s              | 7.469          | 1.279         | 17.501         | 6.274          | 15.436              |
|      | 3s              | 15.035         | 1.279         | 17.501         | 9.162          |                     |

Section E Research Paper
Calculation of activation energy of diffusion and self-diffusion

The results of calculations based on Eqn. 11 and 12 are given in Table 2. An example of calculations for self-diffusion of carbon atom (as shown in Table 2) is given below.

\[
\frac{1}{E_a} = 2 \times \left( \frac{0.596 \times 2}{51.739} + \frac{0.596 \times 4}{51.739} \right) = 7.23 \text{eV} \quad (13)
\]

The activation energy of diffusion of various elements in germanium has been calculated (Table 3). Here for hydrogen atom the ion radius equal to 1.36Å has been used. As an example the calculation of activation energy of diffusion of aluminium in germanium is shown. \( 1/E_a = 1/Q_i + 1/Q_s \); \( Q = (2 \times 1.312 \times 3)/31.24 + (2 \times 1.90 \times 4)/61.76 \), \( E_s = 2.55 \text{eV}, E_s(\text{exp}) = 2.70 \text{eV}. \)

### Table 2. Calculation of activation energy of volume self-diffusion.

| Atom | Orbitals | \( P_0(\text{eVÅ}) \) | \( r_0(\text{Å}) \) | \( n_1-n_2 \) | \( E_s(\text{eV}) \) (calc.) | \( E_s(\text{eV}) \) (Exp.) |
|------|----------|----------------|---------------|----------------|----------------|----------------|
| Li   | 2s\(^1\) | 3.487          | 1.586         | 1 – 1          | 0.55           | 0.57          |
| Be   | 2s\(^2\) | 13.347         | 1.04          | 2 – 2          | 1.60           | 1.70 – 1.63  |
| C\(_1\) | 2p\(^3\) + 2s\(^2\) | 51.739 | 0.596 | 4 | 7.23 | 7.07 |
| C\(_2\) | 2p\(^2\) + 2s\(^2\) | 51.739 | 0.596 | 2 | | |
| Mg   | 3s\(^2\) | 15.436         | 1.279         | 2 – 2          | 1.51           | 1.40          |
| Al\(_1\) | 3p\(^1\) + 3s\(^2\) | 31.624 | 1.312 | 3 | 1.47 | 1.47 |
| Al\(_2\) | 3p\(^1\) | 6.055          | 1.312         | 1              |               |               |
| Na   | 3s\(^1\) | 4.694          | 1.713         | 1 – 2          | 0.457          | 0.45          |
| Si\(_1\) | 3p\(^3\) + 3s\(^2\) | 54.394 | 1.068 | 4 | 4.24 | 4.76 |
| Si\(_2\) | 3p\(^3\) + 3s\(^2\) | 54.394 | 1.066 | 2 | | |
| P    | 3p\(^1\) | 7.696          | 0.919         | 5 – 5          | 0.419          | 0.408         |
| K    | 4s\(^1\) | 5.062          | 2.162         | 1 – 2          | 0.390          | 0.406         |
| Cl   | 3p\(^1\) | 8.125          | 0.728         | 7 – 7          | 0.399          | –             |
| Ca   | 4s\(^2\) | 15.803         | 1.690         | 1 – 2          | 1.56           | 1.67          |
| Sr\(_1\) | 3p\(^2\) | 20.682         | 0.808         | 4              | 2.13           | 2.03          |
| Sr\(_2\) | 3p\(^2\) | 20.682         | 0.808         | 2              | (monocrystal)  |               |
| Zn   | 4s\(^1\) | 7.623          | 1.065         | 2 – 2          | 0.896          | 0.885         |
| Zn\(_1\) | 4s\(^1\) + 3d\(^1\) | 12.798 | 1.065 | 2 – 2 | 1.50 | 1.34 |
| Cd\(_1\) | 5s\(^1\) | 8.349          | 1.184         | 2 – 2          | 0.881          | 0.83          |
| Ge\(_1\) | 4p\(^3\) + 4s\(^2\) | 61.175 | 1.090 | 4 – 4 | 3.508 | 3.15 |
| Ge\(_2\) | 4p\(^3\) + 4s\(^2\) | 61.175 | 1.09 | 4 | 3.37 | 3.15 |
| Ge\(_2\) | 4p\(^3\) | 19.361         | 1.09          | 2              |               |               |
| Se\(_1\) | 4p\(^3\) | 22.614         | 0.918         | 6              | 1.2 – 1.4      |               |
| Se\(_2\) | 4p\(^3\) | 22.614         | 0.918         | 2              | 1.54           |               |
| α-Zr | 5s\(^2\) + 4d\(^2\) | 58.773 | 1.593 | 4 – 4 | 2.30 | 2.25 |
| β-Zr | 5s\(^2\) + 4d\(^2\) | 17.055 | 1.593 | 2 – 2 | 1.338 | 1.17 |
| β-Ti | 4s\(^2\) | 17.026         | 1.435         | 2 – 2          | 1.48           | 1.52          |
| V\(_1\) | 4s\(^2\) + 3d\(^1\) | 71.579 | 1.401 | 5 | 4.26 | 4.08 |
| V\(_2\) | 4s\(^2\) + 3d\(^1\) | 71.579 | 1.401 | 1 | 4.26 | |
| In\(_1\) | 5p\(^1\) | 6.999          | 1.382         | 3              | 0.606          | 0.810         |
| In\(_2\) | 5p\(^1\) | 6.999          | 1.382         | 1              |               |               |
| Sn\(_1\) | 5p\(^2\) | 20.761         | 1.240         | 4 – 4          | 1.05           | 1.01          |
| Sn\(_2\) | 5p\(^2\) | 20.761         | 1.240         | 5 – 5          | 1.76           | 1.55 – 2.08   |
| Te\(_1\) | 5p\(^3\) | 50.542         | 1.111         | 6 – 6          | 1.896          | 1.75 – 2.03   |
| Hf\(_6\) | 6s\(^2\) | 19.828         | 1.476         | 2 – 2          | 1.68           | 1.68; 1.804   |

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Table 3. Calculation of activation energy of volume self-diffusion in germanium. Initial data for germanium: Orbital 4p: $P_0 = 7.128$, n = 1, $r_1 = 1.090 \AA$. Orbital 4p: $P_0 = 19.361$ eVÅ, $r_1 = 1.090 \AA$, n = 2. For $4p^2 + 4s^2$: $P_0 = 61.17$ eVÅ, $r_1 = 4$, $r_{max} 1.090$ Å.

| Diffusing element | $E_a$ (eV) | Calculated | Experimental |
|-------------------|------------|------------|--------------|
| Li 2s | 3.487 | 1.586 | 1 | 4p | 7.128 | 1 | 0.469 | 0.46 |
| Zn 4s² | 19.599 | 1.065 | 2 | 4p² + 4s² | 61.176 | 4 | 2.78 | 2.80 |
| Al 3p³ + 3s² | 31.624 | 1.312 | 3 | 4p² + 4s² | 61.176 | 4 | 2.55 | 2.70 |
| In 3p³ + 5s² | 40.749 | 1.328 | 3 | 4p² + 4s² | 61.176 | 4 | 2.96 | 3.2 |
| Sn 5p² | 20.761 | 1.240 | 2 | 4p² | 19.361 | 2 | 2.15 | 1.90 |
| Pb 6p³ + 6s² | 71.221 | 1.215 | 4 | 4p² + 4s² | 61.176 | 4 | 3.58 | 3.60 |
| H 1s¹ | 4.794 | R_H = 1.36 | 2 | 4p¹ | 7.128 | 4 | 0.44 | 0.38 |
| As 4p³ | 39.448 | 1.001 | 5 | 4p² + 4s² | 61.176 | 4 | 2.52 | 2.51 |
| B 2p² + 2s² | 26.753 | 0.776 | 1 | 4p² + 4s² | 61.176 | 4 | 5.09 | 4.54 |
| La 4p³ + 4s² | 37.678 | 1.254 | 3 | 4p² + 4s² | 61.176 | 4 | 2.95 | 2.5 - 3.14 |
| P 3p³ | 35.996 | 0.919 | 5 | 4p² + 4s² | 61.176 | 4 | 2.51 | 2.49 |
| Sb 5p³ | 41.870 | 1.193 | 5 | 4p² + 4s² | 61.176 | 4 | 2.34 | 2.42 |
| Be 2s² | 13.347 | 1.040 | 2 | 4p² + 4s² | 61.176 | 4 | 2.20 | 2.50 |
| N 2p³ | 33.664 | 1.578 | 3 | 4p² + 4s² | 61.176 | 4 | 2.36 | 2.58 |
| Bi 6p³ | 48.483 | 1.295 | 5 | 4p² + 4s² | 61.176 | 4 | 2.44 | 2.42 |

Table 4. Estimation of activation energy of diffusion and self-diffusion in metal systems

| Atoms | $P_0$, eVÅ | $R_1$, Å | n | $P_0/Rn$ | Atoms | $P_0$, eVÅ | $R_1$, Å | n | $P_0/Rn$ | Calcd.(eq.11, 12) | Expt. |
|-------|-------------|-----------|---|-----------|-------|-------------|-----------|---|----------|-----------------|-------|
| γ-Fe (4s³ 3d¹) | 29.026 | 0.67 | 3 | 14.441 | γ-Fe (4s³) | 18.462 | 0.80 | 2 | 11.539 | 3.207 | 2.8–3.2 |
| γ-Fe (4s³ 3d¹) | 29.026 | 0.67 | 3 | 14.441 | Cr (4s³) | 25.835 | 0.64 | 3 | 13.456 | 3.483 | 3.468 |
| γ-Fe (4s³ 3d¹) | 29.026 | 0.67 | 3 | 14.441 | C (4s³ 3d²) | 32.458 | 2.60 | 3 | 4.1613 | 1.615 | 1.586 |
| γ-Fe (4s³ 3d¹) | 29.026 | 0.67 | 3 | 14.441 | Mn (4s³) | 18.025 | 0.91 | 2 | 9.9038 | 2.937 | 2.71±0.04 |
| γ-Fe (4s³ 3d¹) | 18.462 | 0.80 | 2 | 11.539 | Mn (4s³) | 18.025 | 0.91 | 2 | 9.9038 | 2.665 | 2.419 |
| γ-Fe (4s³) | 18.462 | 0.80 | 2 | 11.539 | Ni (4s³) | 18.838 | 0.74 | 2 | 12.728 | 3.026 | 2.905 |
| γ-Fe (4s³ 3d¹) | 18.462 | 0.80 | 2 | 11.539 | Mo (5s³ 4d¹) | 17.475 | 0.915 | 2 | 9.5492 | 2.613 | 2.557 |
| γ-Fe (4s³) | 18.462 | 0.80 | 2 | 11.539 | W (6s³ 5d¹) | 20.689 | 0.98 | 2 | 10.821 | 2.792 | 2.709 |
| γ-Fe (4s³ 3d¹) | 29.026 | 0.80 | 3 | 14.441 | Cu(I) (4s³) | 7.081 | 0.98 | 1 | 7.2255 | 2.408 | 2.309 |
| γ-Fe (4s³ 3d¹) | 29.026 | 0.80 | 3 | 14.441 | Cu(II) (4s³ 3d³) | 13.272 | 0.80 | 2 | 8.295 | 2.634 | 2.644 |
| α-Fe (4s³ 3d³) | 23.399 | 0.67 | 3 | 11.641 | α-Fe (4s³ 3d³) | 12.835 | 0.80 | 2 | 8.022 | 2.375 | 2.493–2.658 |
| α-Fe (4s³ 3d³) | 23.399 | 0.67 | 3 | 11.641 | Cr (4s³ 3d³) | 25.835 | 0.64 | 3 | 13.456 | 3.121 | 2.904 |
| α-Fe (4s³ 3d³) | 12.835 | 0.80 | 2 | 8.0219 | C (2p³) | 5.641 | 2.60 | 1 | 2.1696 | 0.854 | 0.867 |
| α-Ti (4s³) | 17.026 | 0.78 | 4 | 5.4571 | α-Ti (4s³ 3d³) | 13.044 | 0.78 | 4 | 4.1808 | 1.184 | 1.270 |
| β-Ti (4s³) | 17.026 | 0.78 | 4 | 5.4571 | β-Ti (4s³) | 17.026 | 0.78 | 4 | 5.4571 | 1.304 | 1.303 |
| α-Zr (5s³ 4d³) | 17.055 | 0.92 | 2 | 9.2027 | α-Zr (5s³ 4d³) | 17.055 | 0.925 | 2 | 9.2027 | 2.305 | 2.25 |

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Table 5. Calculation of activation energy of diffusion of oxygen atoms

| Oxygen | Diffusion medium | $Q_1$(eV) | Atoms | Orbitals | $P_0$(eV) | $n$ | $P_0/2r=Q_2$ (eV) | $E_a$ (eV) Calcd. eq. (8.9) | $E_a$ (eV) Exp. |
|--------|------------------|-----------|-------|----------|-----------|-----|-----------------|--------------------------|----------------|
|        |                  |           |       |          |           |     |                 |                          |                |
| 3.1809 | Si               | 3p$^3$3s$^2$ | 54.394 | 1.068 | 2 | 12.733 | 2.545 | 2.494 |
| 3.1809 | Fe (at T=1900K) | 4s$^2$ | 18.462 | 1.227 | 6 | 1.2539 | 0.899 | 0.846 |
| 3.1809 | Cu (II)         | 4s$^2$ | 20.841 | 1.191 | 2 | 4.4877 | 1.861 | 1.857 |
| 3.1809 | Ge              | 4p$^2$ | 19.361 | 1.090 | 4 | 2.2203 | 1.308 | 1.334 |
| 3.1809 | Zr              | 5s$^4$4d$^1$ | 17.055 | 1.593 | 2 | 2.677 | 1.454 | 1.293 |
| 3.1809 | Nb              | 5s$^1$ | 7.093 | 1.589 | 1 | 2.2319 | 1.312 | 1.249 |
| 1.9210 | Ta              | 6s$^2$ | 22.565 | 1.413 | 2 | 3.992 | 1.297 | 1.258 |
| 1.9210 | W (at T=1973K) | 6s$^2$ | 23.344 | 1.360 | 4 | 2.1455 | 1.014 | 1.041 |

Analogous calculations for oxygen diffusion are shown in Table 5. In this Table for oxygen:

$$Q_1 = \frac{17304}{21363} = 3.1809 \text{ eV}$$  \hspace{1cm} (14) (orbital 2p$^2$)

$$Q_1 = \frac{5215}{21362} = 1.9210 \text{ eV}$$  \hspace{1cm} (15) (orbital 2p$^3$)

In all cases either the number of valence electrons of one sublevel or number of all valence electrons of the given main number of atom was used as the number $n$.

For hydrogen atom $n=2$, this corresponds to the realization number of all its possible bonds. For elements of groups 1 and 2$n$ equals the group number, for groups 3$a$ during self-diffusion $n_1=3$, $n_2=1$. For groups 4-$a$ $n_1=4$, $n_2=2$. For $Na$ and $K$ $n_1=1$ and $n_2=2$, this reflects the possibility of generalizing valence electrons in inter-structural interactions.

The comparison of calculation and experimental values,\(^1\)\(^-\)\(^10\)\(^-\)\(^18\) of activation energy of diffusion (Table 2-5) shows that these values are in satisfactory accordance (in the limits of experiment accuracy). Temperature factor, that can also have values in diffusion processes, was indirectly considered in this approach via selecting the most valence-active orbitals of the atom. Thus, for instance, for trivalent iron 4s$^2$3d$^1$ can usually be valence-active orbitals at lower temperatures, and 4s$^1$3d$^2$ at higher temperatures of the process.

**Conclusion**

Since the resulting value of P-parameter of a complex structure is quite easily calculated, this method can be applied for predicting the activation energy of diffusion and self-diffusion processes not only in simple but also in complex systems, in bio-systems as well.

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