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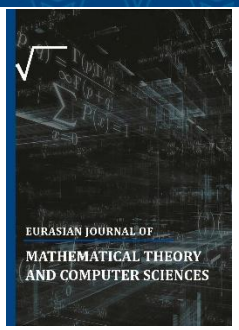

MATHEMATICAL MODELING OF DIFFUSION IN SOLIDS USING ARRHENIUS' LAW

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ABSTRACT

In this article, Arrhenius' law was used in the study of the diffusion process in solids. The reason is that this law is one of the most fundamental laws. Data were obtained that the Arrhenius law depends on temperature, a change in which also leads to a change in the diffusion coefficient of a solid. At the same time, a software product was developed using the Python programming language.

For many years, work on modeling the atoms of matter has been developing at a rapid pace. This is explained by the connection with the development of computers and the proliferation of modeling methods. Due to the constant development of atomic modeling today, modeling is not only an auxiliary tool but also a fundamental component of research methods. It is widely used in many areas of research, such as finding new materials during experimental research or studying the properties of materials.

The study of the diffusion process is very important. Because the phenomenon of diffusion performs a transport function on atomic scales and characterizes the speed of several physical processes. Information about diffusion properties is studied, for example, to explain the thermal decomposition of substances, sorption processes, and ionic conductors [1].

To find the relationship between temperature and diffusion coefficient, let's consider what diffusion jumps are like. For most of the time, the atom oscillates around its equilibrium position (at the nodes of the crystal lattice). At this time, its energy decreases approximately by kT (k is the Boltzmann constant). But for an atom to jump into another neighboring vacancy (hole), it needed more energy. This is because when a vacant space is leaped over, it approaches other atoms and, as a result, performs work. The energy of the work done for the atom's diffusion jump (Gibbs potential difference) is called the atom's migration energy and is denoted as ΔG_m or simply G_m. According to the law of particle distribution, the probability of finding a particle with this energy is proportional to exp (-Gm/kT). Correspondingly, the temperature dependence of diffusion jump

$$\nu = \nu_0 \exp\left(-\frac{G_m}{kT}\right) \quad (1)$$

is written as. In this case, ν0 is the frequency of the diffuse jump, and this value is usually taken as the Debye frequency. Relation (1) is called the Arrhenius dependence [2].

From this dependence, the known value ln (ν) is a linear function of 1/T, and this is useful in the temperature analysis of diffusion velocity. The corresponding coordinate system is called the Arrhenius system.

During diffusion (according to the porosity mechanism), the correlation factor is approximately 0.721 for a centrally centered cubic lattice, 0.781 for a laterally centered cubic lattice, and 0.655 for a simple cubic lattice. Considering the correlation effect, the diffusion coefficient takes the following form:

$$D = f\nu\frac{\Delta^2}{6} \tag{2}$$

when calculating the pore diffusion coefficient using expression (2), it should be noted that the correlation factor should be considered equal to 1. This is because the probability of a cavity jumping in any direction is the same [3].

Substituting expression (1) into expression (2), we obtain the equation where the diffusion coefficient depends on temperature:

$$D = f\nu_0\frac{\Delta^2}{6}\exp\left(-\frac{G_m}{kT}\right) \tag{3}$$

In expression (3), it should be noted that the diffusion jumps of the diffusant's atoms (or molecules) occur independently. Therefore, expression (3) yields a good result when applied to the vacancy diffusion coefficient (e.g., carbon). Expression (3) is not suitable for evaluating the self-diffusion coefficient because when this phenomenon occurs, atoms involved in the migration of crystal lattice defects, often vacancies, disperse. In this case, the self-diffusion coefficient

$$D_{self} = fD_v c_v \tag{4}$$

will be in the form of. In this expression, the vacancy diffusion coefficient (for the case f=1) is written as expression (3) [4].

We substitute expression (3) into expression (4):

$$D_{self} = f\nu_0\frac{\Delta^2}{6}\exp\left(-\frac{G_m}{kT}\right)c_v \tag{5}$$

In expression (5), the diffusion of atoms, not vacancies, is considered, therefore the correlation factor is equal to 1. The concentration of vacancies also depends on the temperature:

$$c_v = \exp\left(-\frac{G_f}{kT}\right) \tag{6}$$

G_f – vacancy energy (Gibbs). If we substitute expression (6) into expression (5),

$$D_{self} = f\nu_0\frac{\Delta^2}{6}\exp\left(-\frac{G_m + G_f}{kT}\right) \tag{7}$$

the expression appears.

As can be seen from expression (7), the self-diffusion coefficient also depends on temperature according to Arrhenius' law. The symbol G_a, which replaces the numerator of expression (7), is called the activation energy of self-diffusion and takes the following form:

$$D_{self} = D_0\exp\left(-\frac{G_a}{kT}\right) \tag{8}$$

In this expression, G_a is called the activation enthalpy of self-diffusion, and $D_0$is called the pre-exponential factor. G_a and D_0 in expression (8) are frequently used in obtaining experimental data.

Expression (8) gives us the following form of code written using the Python programming language.

First, we will call the necessary libraries:

```
import numpy as np
import matplotlib.pyplot as plt
```

After the import, we will determine the constants:

```
R = 8.314  # Gaz turaqlısı J/(mol*K)
D0 = 1.0  # Exponencial aldı faktor
Ea = 50.0  # Activaciya enegiyası kJ/mol
```

We choose the desired temperature range:

```
T = np.linspace(200, 600, 100)  # Temperatura 200 den 600 K ge shekem ózgeredi
```

We write the formula for Arranius's law:

```
D = D0 * np.exp(-Ea / (R * T))  # Tezlik turaqlısı
```

Commands are written to display on the screen:

```
plt.figure(figsize=(10, 6))
plt.plot(T, D, label='Tezlik turaqlısı')
plt.xlabel('Temperatura (K)')
plt.ylabel('Tezlik turaqlısı (s^-1)')
plt.title('Arrenius nızamı')
plt.legend()
plt.grid(True)
plt.show()
```

The program ends.

When this program is launched, an image appears in the following form:

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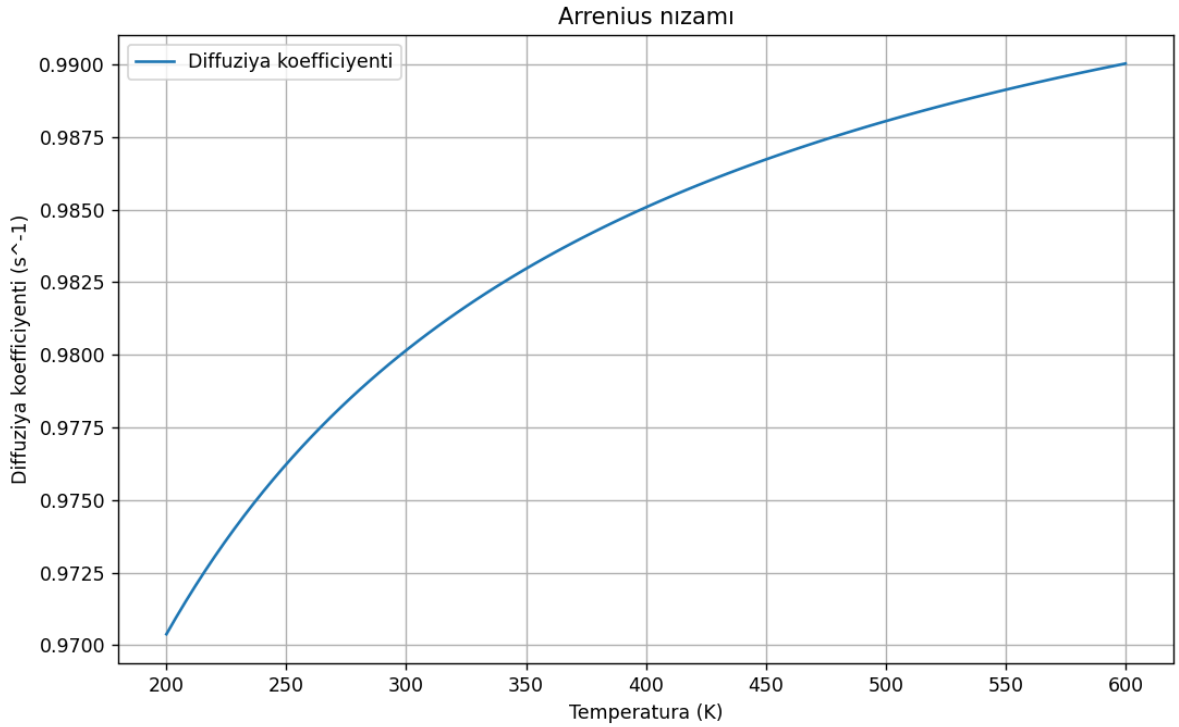

Figure 1 Figure taken in the range from 200 K to 600 K at an activation energy of 50 kJ/mol.

The increase in the diffusion coefficient with increasing temperature is related to the thermal motion of the element's particles. When the temperature rises, their kinetic energy increases, which leads to even stronger chaotic motion. This, in turn, helps particles move faster between regions of different concentrations.

This proposed graph allows for a deeper understanding of the effect of temperature on the diffusion coefficient according to Arrhenius' law. A graph depicting the temperature dependence of the diffusion coefficient is a primary tool for studying physical processes such as diffusion in solids. A graph is a curve that shows the temperature-dependent change in the diffusion coefficient. The OX axis represents the temperature measured in kelvins, while the OY axis represents the diffusion coefficient in s^{-1}. The graph shows the exponential dependence of the diffusion coefficient on temperature. With increasing temperature, the rate of change of the diffusion coefficient decreases. This, in turn, corresponds to Arrhenius's law. Thus, when the temperature rises, the molecules of the material possess more energy, which contributes to their greater mobility and, consequently, faster dispersion.

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