

Metallic Materials - Metal Diffusion

Cap Morales, Shannon Nazareth
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1 Metals and solutes

Using the diffusion database from DICE website three metals were selected along with two solutes. The way the metals were chosen was based on the solutes they had in common, for systems of only two different species. In this case, the metals chosen were: copper, platinum and titanium because there was available data for aluminum and silver as solutes for those three metals. However, as it is shown on table 2 data for a self-diffusion system for platinum was not found, the only available data were for systems in which iron is also present.

| Metal | Structure | Solute |
|-------|-----------|--------|
| Cu | fcc | Al, Ag |
| Pt | hexagonal | Al, Ag |
| Ti | hexagonal | Al, Ag |

Table 1: Elements chosen for calculations.

Source: Adapted from (Diffusion Database (Kakusan), n.d.) database.

After establishing the metals and solutes to be used, the information related to the diffusion coefficient was obtained by indicating the solute (Ag or Al) and the metal in which it will be diffused. The information corresponding to the systems is presented in the following table:

| System | D_0 (m^2/s) | Q (kJ/mol) | T_{min} (K) | T_{max} (K) |
|--------|-------------------|--------------|---------------|---------------|
| Ag-Ag | $2,70e-5$ | 182,96 | 980 | 1250 |
| Al-Al | $1,37e-5$ | 124 | 583 | 953 |
| Cu-Cu | $1,05e-4$ | 210 | 845 | 1111 |
| Ti-Ti | $3,4e-4$ | 328 | 1393 | 1941 |
| Ag-Cu | $3,10e-10$ | 72 | 498 | 573 |
| Ag-Pt | $1,30e-5$ | 258 | 1473 | 1873 |
| Ag-Ti | $1,00e-4$ | 279 | 823 | 1073 |
| Al-Cu | $8,00e-6$ | 181 | 973 | 1348 |
| Al-Pt | $1,30e-7$ | 194 | 1373 | 1873 |
| Al-Ti | $6,60e-3$ | 329 | 930 | 1140 |

Table 2: Diffusion coefficient data for each system.

Source: Adapted from (Diffusion Database (Kakusan), n.d.) database.

2 Diffusion coefficient

Using the data from table 2, the diffusion coefficient was calculated with the Arrhenius relation:

$$D = D_0 \exp\left(-\frac{\Delta H}{RT}\right), \quad (1)$$

where D is the Diffusion coefficient, D_0 is a pre-exponential factor, ΔH is the activation enthalpy of diffusion in kJ/mol (which is also represented as Q), R is the ideal gas constant ($8,314J/K \cdot mol$) and T is the temperature in Kelvin (Heitjans & Kärger, 2006).

The linearization of Arrhenius relation can be made by taking the logarithm on both sides of equation (1), which yields:

$$\ln(D) = -\frac{\Delta H}{R} \frac{1}{T} + \ln(D_0), \quad (2)$$

which is a linear equation where the slope is given by $-\Delta H/R$ and the intercept in the y-axis is given by $\ln(D_0)$.

Considering that all systems have different temperature ranges (2), to proceed with the calculations, a new temperature range was chosen, from 450 to 1950 K, so that all systems use the same temperature range and can be compared with each other. The new temperature range was used to calculate D for all systems, with a sample of 100 points evenly spaced, and the parameters of D_0 , Q and R using equation (1).

The results for the diffusion coefficient for all systems are presented in figure 4. Figure 4a shows the diffusion coefficient for all systems as a function of temperature, from 450 to 1950K; the linearization of Arrhenius relation is shown in figure 4b, where the logarithm of the diffusion coefficient is plotted as a function of the inverse of the temperature.

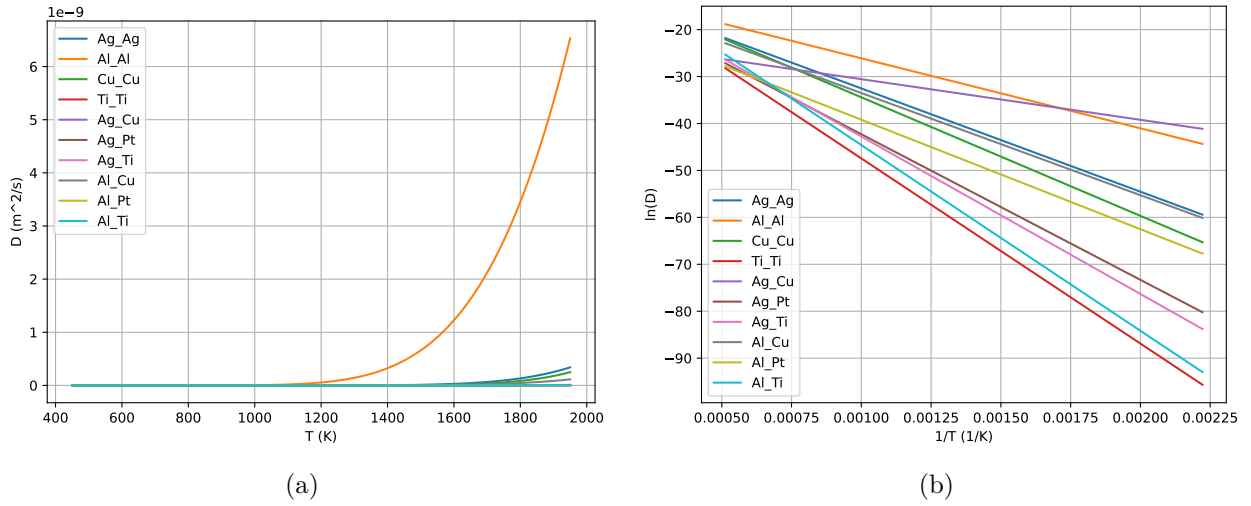


Figure 1: a) Diffusion coefficient D (m^2/s) as a function of temperature T (K) and b) logarithm of the diffusion coefficient $\ln(D)$ as a function of the inverse of temperature $1/T$ (K^{-1}).

Source: Data from (Diffusion Database (Kakusan), n.d.), visualization by the author (code available at (Cap Morales, 2025)).

2.1 Self diffusion

The self-diffusing systems are Ag-Ag, Al-Al, Cu-Cu and Ti-Ti. The plot for the logarithm of the diffusion coefficient as a function of the inverse of the temperature are shown in figure 5.

2.2 Solute diffusion

3 Diffusion Distance

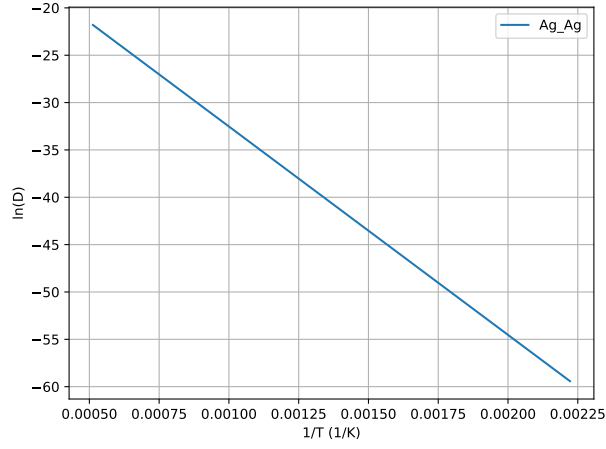
3.1 Self-diffusion

3.2 Solute diffusion

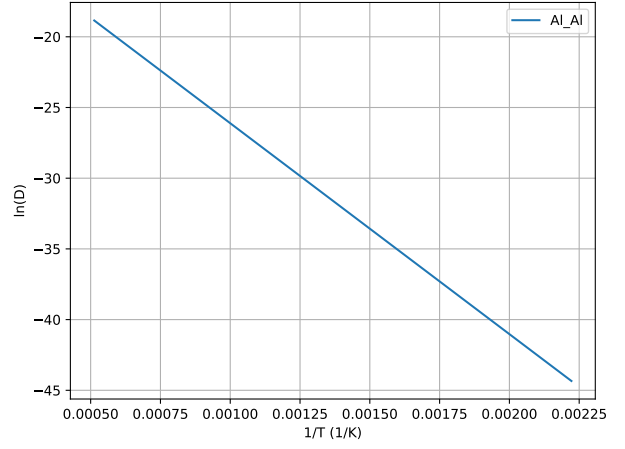
(c) For the metals and solute atoms covered in question (a), assuming a sufficiently large sample size, graph the self-diffusion distance (logarithm) and the solute atom diffusion distance at room temperature against time (logarithm).

References

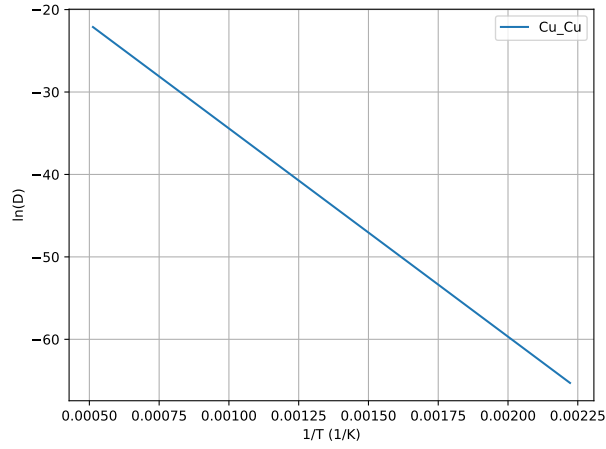
- Cap Morales, S. N. (2025). *Github repository: Metallic materials*. https://github.com/ShannonNCM/Metallic_materials.git. (Source code for data processing and visualization)
- Diffusion database (kakusan)*. (n.d.). <https://diffusion.nims.go.jp/>.
- Heitjans, P., & Kärger, J. (2006). *Diffusion in condensed matter: methods, materials, models*. Springer Science & Business Media. Retrieved from <https://link.springer.com/book/10.1007/3-540-30970-5>



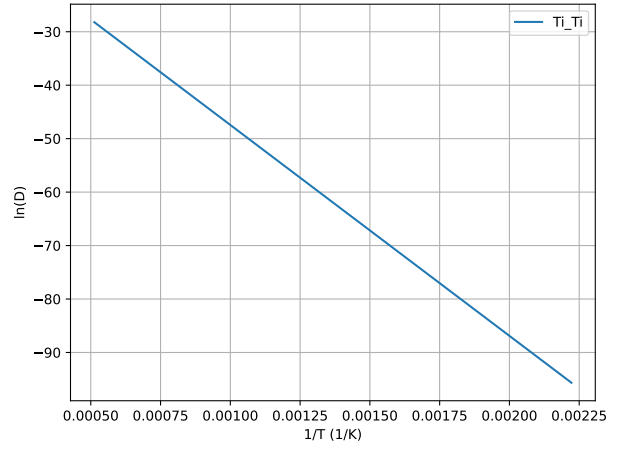
(a)



(b)

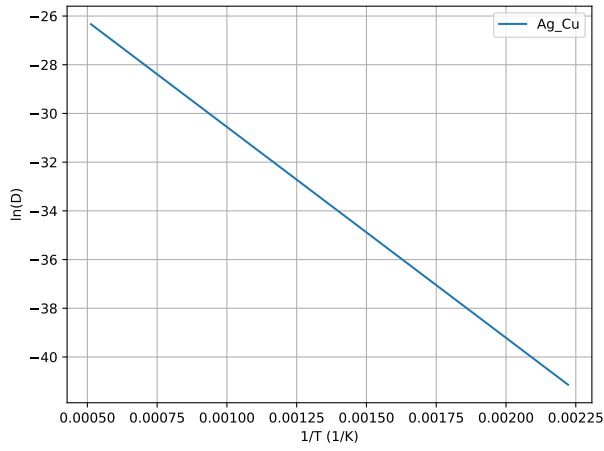


(c)

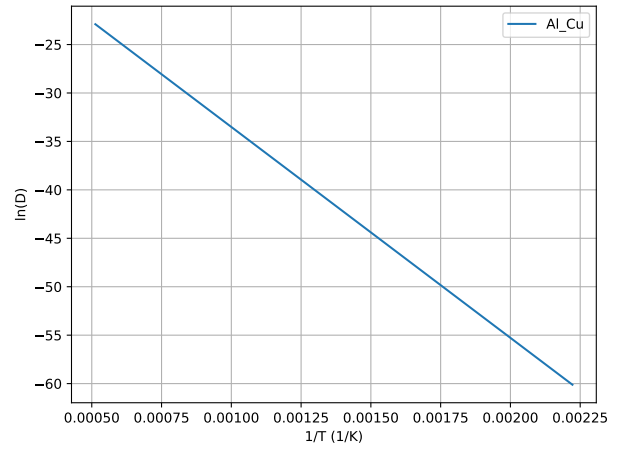


(d)

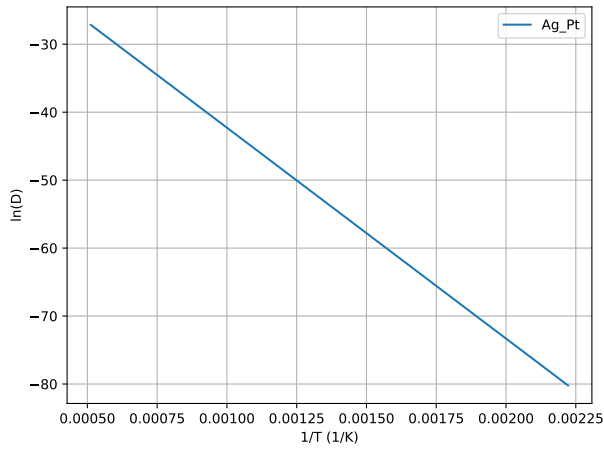
Figure 2: Logarithm of the diffusion coefficient for self-diffusing systems: a) silver, b) aluminum, c) copper and d) titanium.
Source: Data from (Diffusion Database (Kakusan), *n.d.*), visualization by the author (code available at (Cap Morales, 2025)).



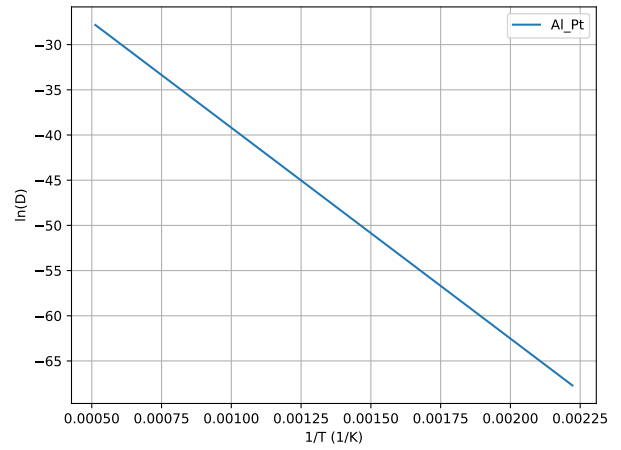
(a)



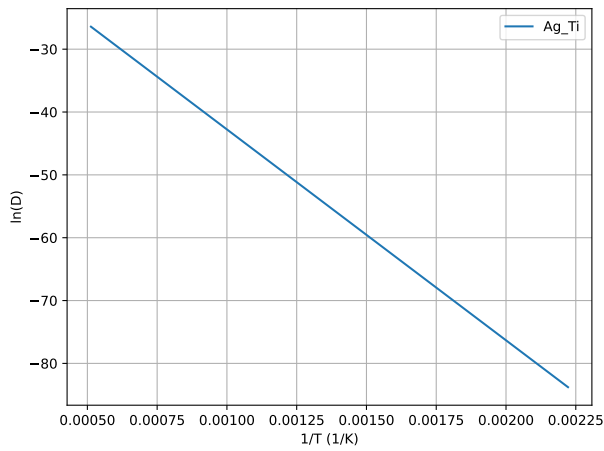
(b)



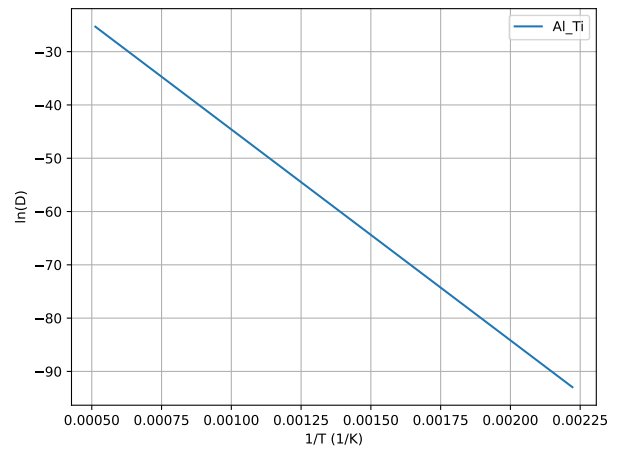
(c)



(d)



(e)



(f)

Figure 3: Logarithm of the diffusion coefficient for the systems: copper diffusing in a) silver and b) aluminum; platinum diffusing in c) silver and d) aluminum; and platinum diffusing in f) silver and g) aluminum.

Source: Data from (Diffusion Database (Kakusan), *n.d.*), visualization by the author (code available at Cap⁶Morales (2025)).

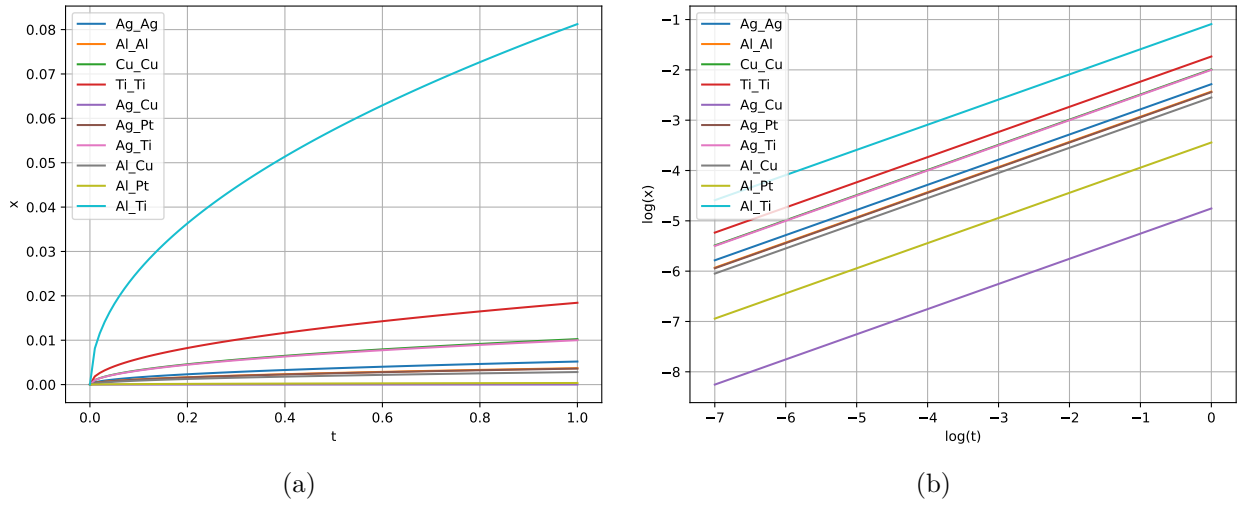
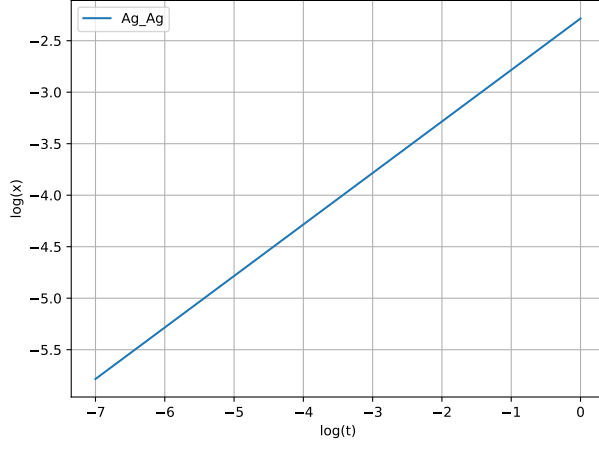
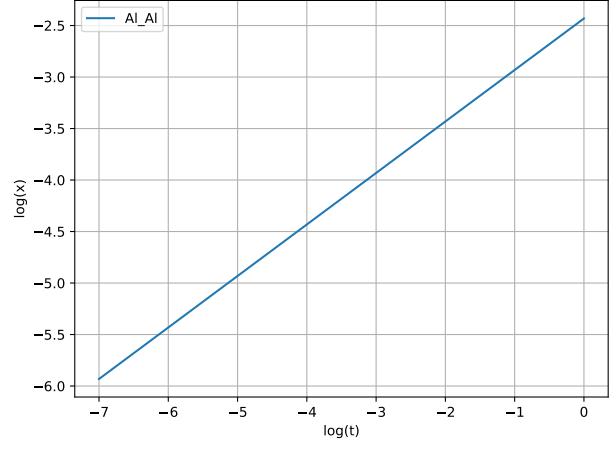


Figure 4: a) Diffusion coefficient D (m^2/s) as a function of temperature T (K) and b) logarithm of the diffusion coefficient $\ln(D)$ as a function of the inverse of temperature $1/T$ (K^{-1}).

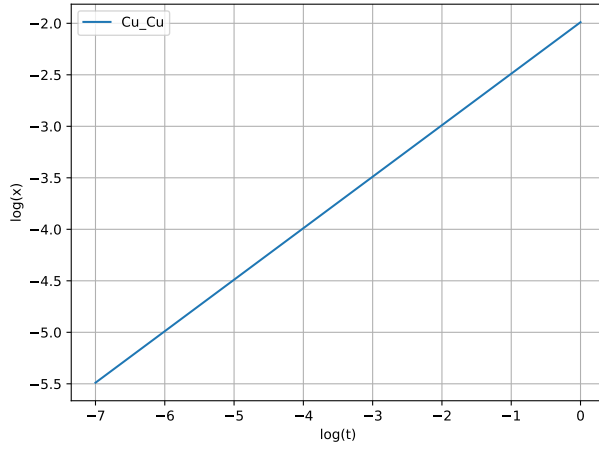
Source: Data from (Diffusion Database (Kakusan), *n.d.*), visualization by the author (code available at (Cap Morales, 2025)).



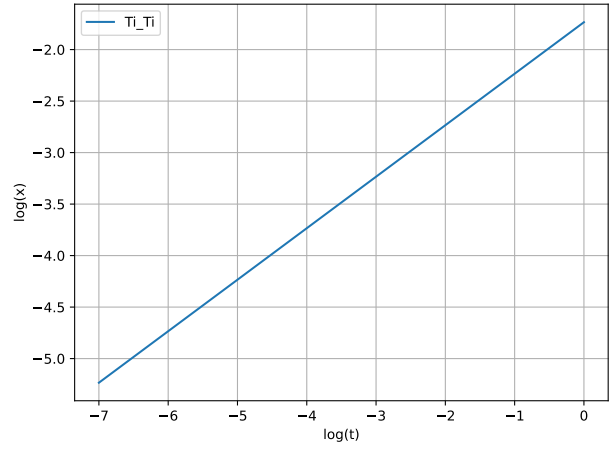
(a)



(b)



(c)



(d)

Figure 5: Logarithm of the diffusion coefficient for self-diffusing systems: a) silver, b) aluminum, c) copper and d) titanium.

Source: Data from (Diffusion Database (Kakusan), n.d.), visualization by the author (code available at (Cap Morales, 2025)).