Metallic Materials - Metal Diffusion

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1 Metals and solutes

Using the diffusion database from *Diffusion Database (Kakusan)* (n.d.) website, three metals were selected along with two solutes. The metals were chosen based on the solutes they had in common as well as the disponibility of data for the systems that wanted to be studied.

To choose the metals and solutes to use, first a few options for commonly used solutes were considered, such as carbon (C), silver (Ag) and aluminum (Al). The different systems of solute-metals was searched using the *Diffusion Database (Kakusan)* (n.d.) website, in order to find which elements were common solutes to all three metals. As a result of this process, the solutes chosen were silver and aluminum, while the metals for which it was possible to find information with the selected solutes were copper, platinum and tittanium.

Metal	Structure	Common 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 from the *Diffusion Database (Kakusan)* (n.d.) by indicating the solute (Ag or Al) and the metal in which it will be diffused.

For the self-diffusion systems, the solute indicated was the same as the metal, however, there was no information available for the self-diffusion of aluminum; the only information found corresponded to systems that also had iron in them. This information was not used because the systems considered for self-diffusion were only those who did not have other species in them.

The information corresponding to the systems is presented in the following tables:

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 all diffusion systems.
*Source: Adapted from (*Diffusion Database (Kakusan)*, n.d.) database.*

2 Diffusion coefficient

The diffusion coefficient can be calculated with the Arrhenius relation:

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

where D is the Diffusion coefficient, D_0 is a pre-exponential factor, ΔH is the activation entalphy of diffusion in J/mol (which is also represented as Q), R is the ideal gas constant ($8,314\ J/K \cdot mol$) 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:

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

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, 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).

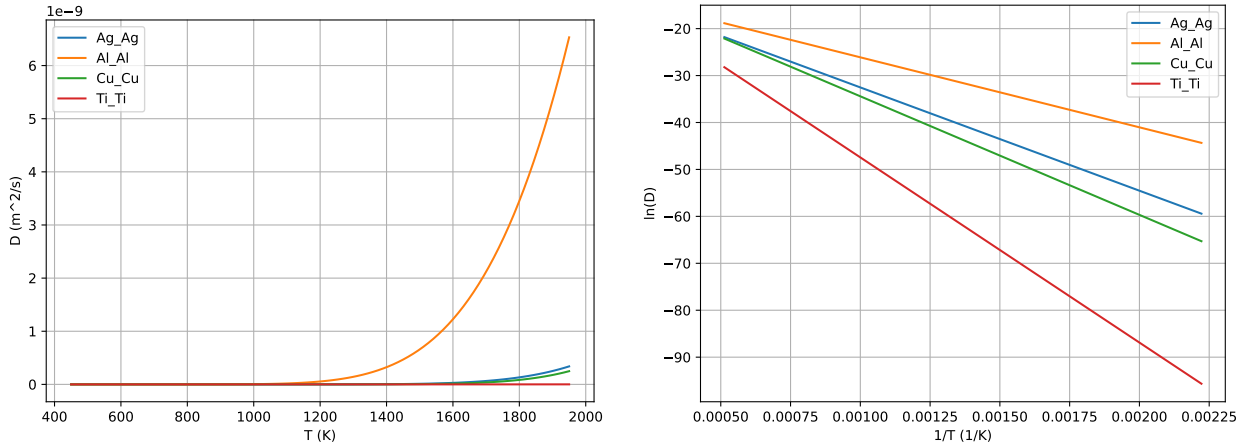
After calculating the diffusion coefficient for the systems, the lorgarithm of the diffusion coefficients and the inverse of the temperature were also calculateded, in order to present the results in the linearized form of equation (3).

2.1 Self diffusion

The self-diffusing systems are Ag-Ag, Al-Al, Cu-Cu and Ti-Ti. Figure 1 presents the graphs of the diffusion coefficient for the self-diffusion systems, where 1a shows the diffusion coefficient as a function of time and 1b shows the logarithm of the diffusion coefficient.

Figure 1a shows that the diffusion coefficient increases with the temperature, for all self-diffusion systems. It can also be noted from this plot, that the increase of the diffusion coefficient is higher for aluminum, than it is for the other systems, which indicates that there is faster self-diffusion for aluminum.

Figure 1b presents the logarithm of the self-diffusion coefficient as a function of the inverse of temperature, where the straight lines correspond to the linear behaviour expected from equation 2. The plot shows that the titanium system has a steeper slope, which corresponds to a higher activation energy, meaning that it requires more energy for the diffusion to occur. On the other hand, the aluminum system has the less steep slope, which indicates a lower activation energy, requiring less energy for the diffusion to occur.



(a) (b)

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 the temperature $1/T$ (K^{-1}) for self-diffusion systems.
*Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at (Cap Morales, 2025)).*

2.2 Solute diffusion

The plot for the diffusion systems with aluminum and silver as solutes in copper, platinum and titanium are shown in figure 2.

Figure 2a presents the diffusion coefficient as a funciton of the temperature for all systems. It shows that for the system of Al-Cu (aluminum as a solute in copper) the diffusion coefficient increase is higher than for the other systems, indicating that aluminum can diffuse easier in copper.

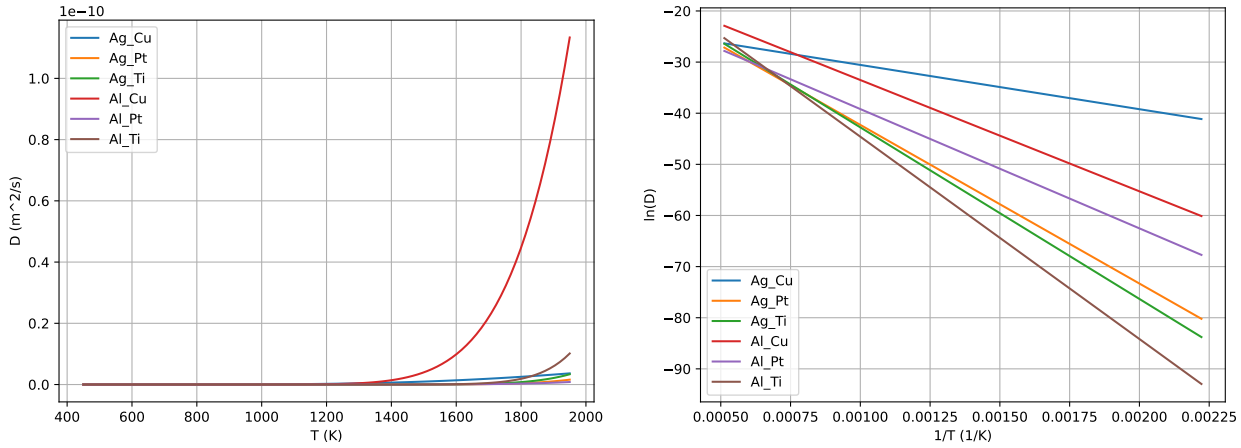
Figure 2b shows the logarithm of the diffusion coefficient as a function of the inverse of the temperature. The plot presents straight lines that correspond to the beharivour expected from Arrhenius relation (equation 2).

For silver as solute, figure 2b shows that the system Ag-Ti has a steeper slope that the other two systems (Ag-Cu and Ag-Pt), this indicates that the activation energy for the Ag-Ti system is lower that it is for the other two systems, meaning that silver requieres more energy to diffuse in titanium that to diffuse on copper and platinum. It can also be seen that the system Ag-Cu has the less steep slope, which means a lower activation energy, indicating that silver requires less energy to diffuse in copper than in platinum and titanium. It can also be seen that both lines for Ag-Pt and Ag-Ti are close to each other, which corresponds to close values of activation energy.

In the case of aluminum as solute, in figure 2b it can be seen that the system Al-Cu has the less steep slope, corresponding to a lower activation energy. Meanwhile, the system Al-Ti has the steeper slope of these systems, which indicates that more energy is required

for aluminum to diffue in tintanium than what it is required for it to diffuse in copper and platinum.

Overall, the Al-Ti system has a more steep slope than the other systems, indicating tha this system requires a higher energy for diffusion to occur. On the other hand, the system Ag-Cu presents the less steep slope, which indicates a lower activation energy, meaning that less energy is required for diffusion to occur in this system.



(a) (b)

Figure 2: 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)).*

3 Diffusion Distance

The diffusion distance is given by $\sqrt{Dt}$, which is found in the equation that is used to describe the concentration after a time t in a thin layer of the diffusing species is concentrated at $x = 0$ of a semi-infinte sample Heitjans and Kärger (2006):

$$c(x,t) = \frac{M}{\sqrt{\pi Dt}\exp\left(-\frac{x^2}{4DT}\right)}. \tag{3}$$

The diffusion distance at room temperature was calculated for all systems. First, the diffusion coefficient at room temperature was calculated using equation 1 with the values of activation energy from table 3. The results are shown in the following table:

System	D_0 (m^2/s)	Q (kJ/mol)	D_{278K} (m^2/s)
Ag-Ag	$2,70e-5$	$182,96$	$2,29e-37$
Al-Al	$1,37e-5$	124	$2,52e-27$
Cu-Cu	$1,05e-4$	210	$1,62e-41$
Ti-Ti	$3,4e-4$	328	$1,08e-61$
Ag-Cu	$3,10e-10$	72	$7,42e-23$
Ag-Pt	$1,30e-5$	258	$7,75e-51$
Ag-Ti	$1,00e-4$	279	$1,24e-53$
Al-Cu	$8,00e-6$	181	$1,50e-37$
Al-Pt	$1,30e-7$	194	$1,28e-41$
Al-Ti	$6,60e-3$	329	$1,41e-60$

Table 3: Diffusion coefficient data calculated for room temperature (278 K)
*Source: Adapted from (*Diffusion Database (Kakusan)*, n.d.) database.*

With the diffusion coefficient calculated at toom temperature, the diffusion distance was calculated for all systems for time range from 0 to $2e3$ seconds, using the expresion for diffusion distance from equation 3

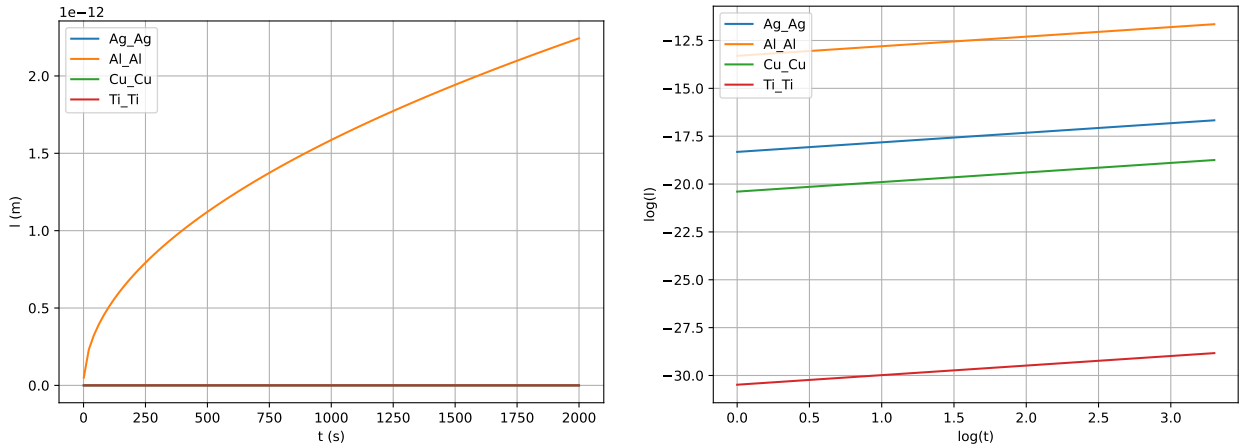
3.1 Self-diffusion

Distance as a fuction of time for self-diffusing systems is plotted in 3a. This plot, shows that for the aluminum self-diffusion system, the diffusion distance is higher than for the other self-diffusing systems.

Because of the scales, it is difficult to properly see the behaviour of the distance for all systems, in order to observe the change of the diffusion distance with time the logarithmic scale is used. Figure 3b shows the logarithm of the diuffusion distance as a function of the logarithm of time. In this graph the system of aluminum self-diffusion shows the highest diffusion didstance,meaning that the aluminum atoms move the farthes in the same time, which also corresponds to the higher diffusivity as it is shown on figure 1b, which corresponds

to the low activation value of 124 kJ/mol with respect to the activation energy values of the other systems.

On the other hand, the titanium self diffusion system has the lowest diffusion ditance, this also corresponds to this system having the highest activation energy as is obseverved in figure 1b, where this system has the steepest slope indicating that it requires more energy for the diffusion to occur, which also translates in a lower value for the distance that the atoms can move on the same period of time compared to a system that requires less energy for the diffusion to occur.



(a) (b)

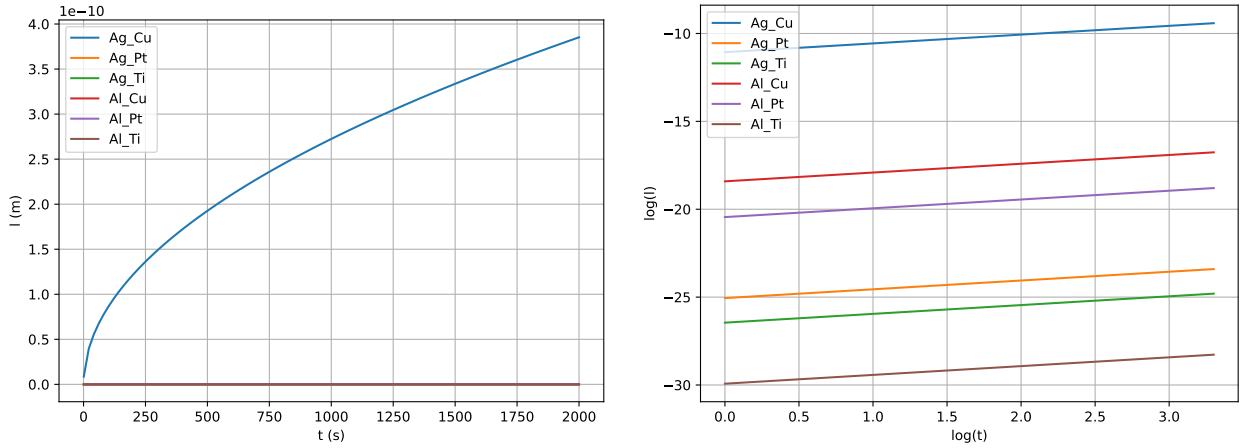
Figure 3: a) Diffusion distance l (m) as a function of time t (s) and b) logarithm of the diffusion distance as a function of the logarithm of time for selft-diffusion systems.
*Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at (Cap Morales, 2025)).*

3.2 Solute diffusion

Figure 4 presents the graphs for the diffusion distance for systems with aluminum and silver as solutes in copper, platinum and titanium. The plots in figure 4a show the diffusion distance as a function of time for all systems, where the system Ag-Cu (silver diffusing in copper) shows the highest diffusion distance than the other systems. The behaviour of all systems can be observed better in figure 4b, where the logarithm of the diffusion distance is plotted as a funcion of the logarithm of time.

For the systems with silver as solute, figure 4b shows that the highest distance is for the Ag-Cu silver, while the lowest distance is for the Ag-Ti system. This shows that silver atoms can diffuse a higher distance in copper than they can diffuse in platinum; which is consistent with the results obtained for the diffusion coefficient in figure 2b. It can also be seen that the diffusioin distancees for silver in platinum and titanium are in closer, which could be due to both metals having an hexagonal crystal structre; as well as having close values for activation energies: 258 and 279 kJ/mol for Ag-Pt and Ag-Ti respectively.

For the systems where aluminum is a solute, from figure 4b, it can be seen that the Al-Cu systems has the highest diffusion distance, as a contrast with Al-Pt and Al-Ti systems. Which indicates that aluminum can diffuse more easily in copper than in platinum or titanium. It can also be seen that systems Al-Cu and Al-Pt have closer values of diffusion distance, even though the crystal structures for copper and platinum are different, they do have close values of activation energy, 181 and 194 kJ/mol for Al-Cu and Al-Pt respectively. In the case of the Al-Ti system, the diffusion distance is the lowest, which corresponds to the higher value of activation energy for this systeem (329 kJ/mol), meaning that it requires more energy for the aluminum atoms to diffuse in titanium than it does for diffusion in copper and platinum.



(a) (b)

Figure 4: a) Diffusion distance l (m) as a function of time t (s) and b) logarithm of the diffusion distance as a function of the logarithm of time.
*Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at (Cap Morales, 2025)).*

References

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