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 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

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).

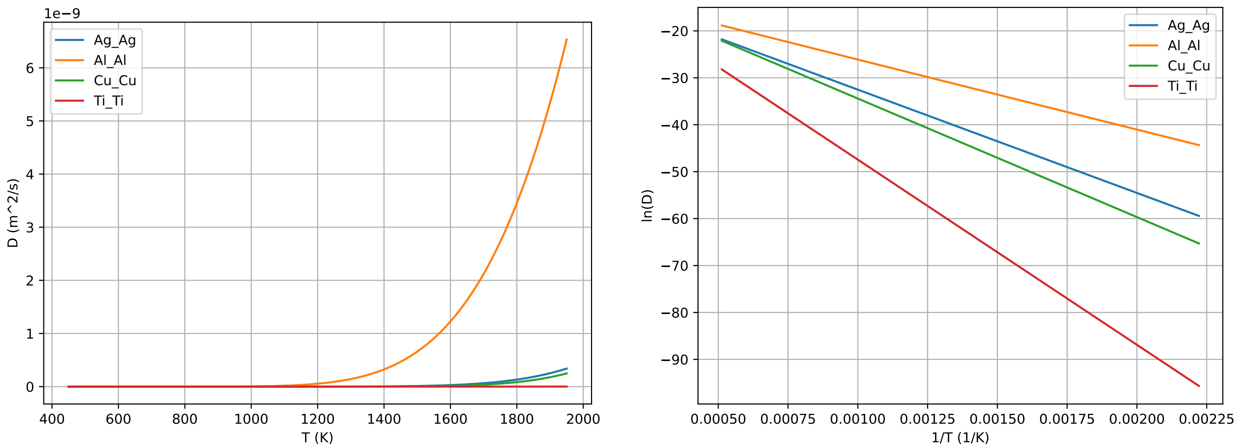
2.1 Self diffusion

The self-diffusing systems are Ag-Ag, Al-Al, Cu-Cu and Ti-Ti. The plots for the logarithm of the diffusion coefficient as a function of the inverse of the temperature are shown in figure **??**. As seen on all four plots, all the systems show a linear behaviour which is consistent of what is expected for systems that follow the Arrhenius relation (2).

2.2 Solute diffusion

The plots for the diffusion systems are shown in figure **??**, where each graph corresponds to a different system in which copper, platinum and titatium were solutes in silver and aluminum. All the plots show a linear behaviour that corresponds to the Arrhenius relation 2.

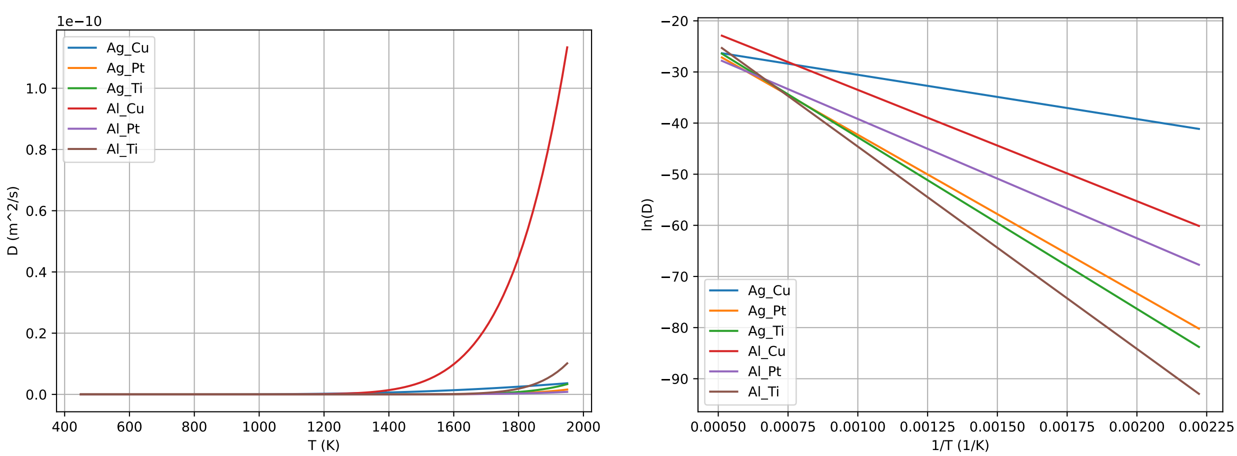
(Which shows that the systems follow blalbalbalbla, agregar la parte del anaisis)



(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 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)

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

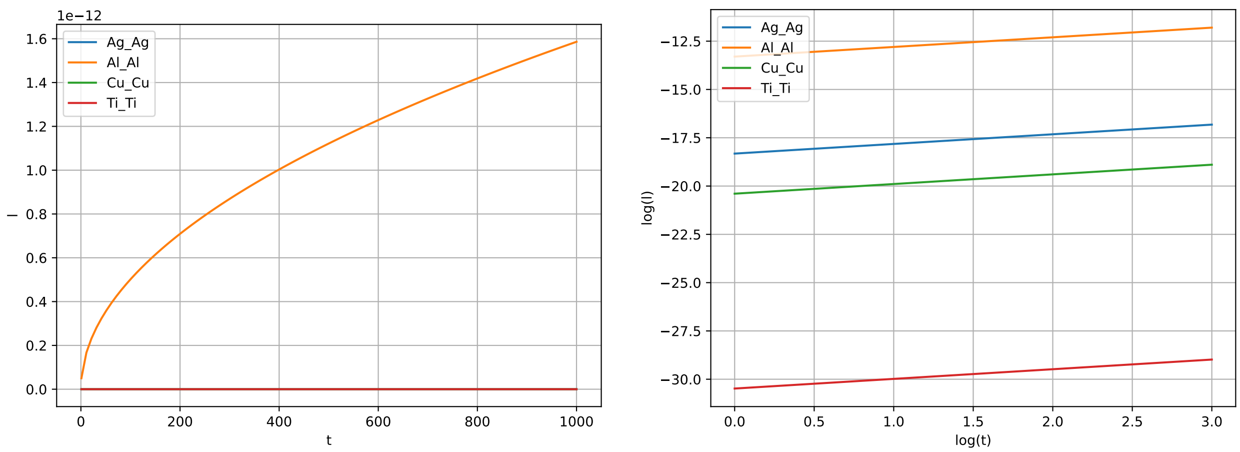
The diffusion distance is given by $\sqrt{Dt}$, which is found in the equation that is used to describe the concentration after a time t in a thin layer of the diffusing species is concentrated at $x = 0$ of a semi-infinte sample Heitjans and Kärger (2006):

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

Using the previous statement, the difussion distance was calculated using a time range from zero to (tengo que arreglar esta parte, porque creo que meti la pata con el calculo del tiempo :c). The plots for the diffusion distance as a function of time and the lilnealization of the diffusion distance are shown in the figure **??**.

3.1 Self-diffusion

The shoshfdos



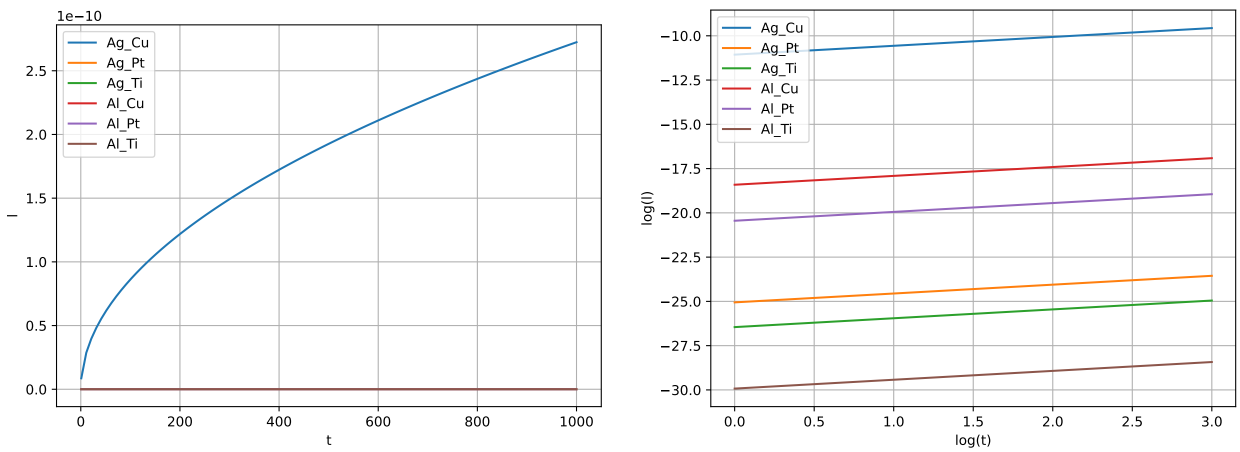
(a) (b)

Figure 3: 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)).*

3.2 Solute diffusion

The fsdfojsofdjsodfs



(a) (b)

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)).*

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`