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-Tu	$3,4e-4$	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:

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

where D is the Diffusion coefficient, D_0 is a pre-exponential factor, ΔH is the activation entalphy of diffusion in kJ/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).

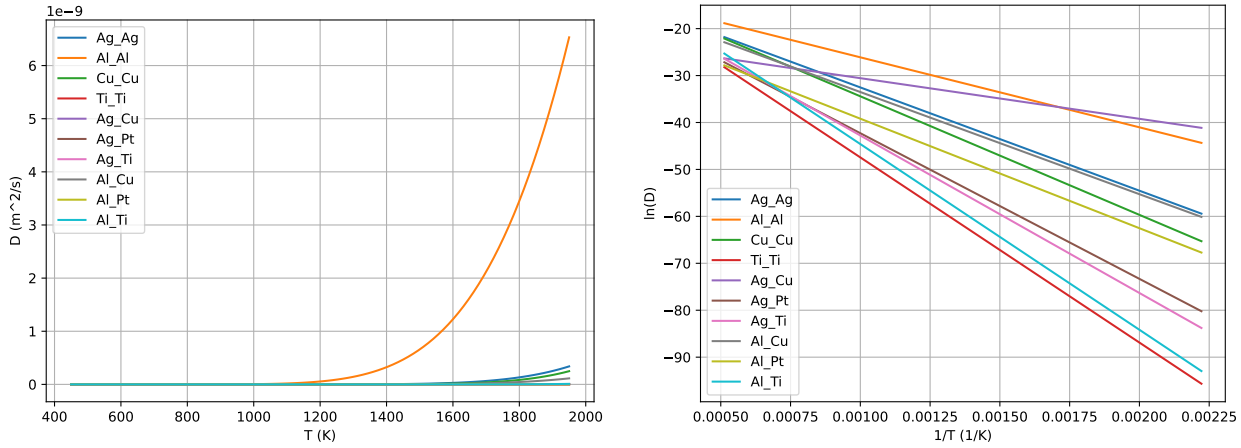
The linearization of Arrhenius relation can be made by taking the logarithm on both sides of equation (1), which yields:

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

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 (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 1. Figure 1a 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 1b, where the logarithm of the diffusion coefficient is plotted as a function of the inverse of the temperature.



(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)).*

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 5. 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).

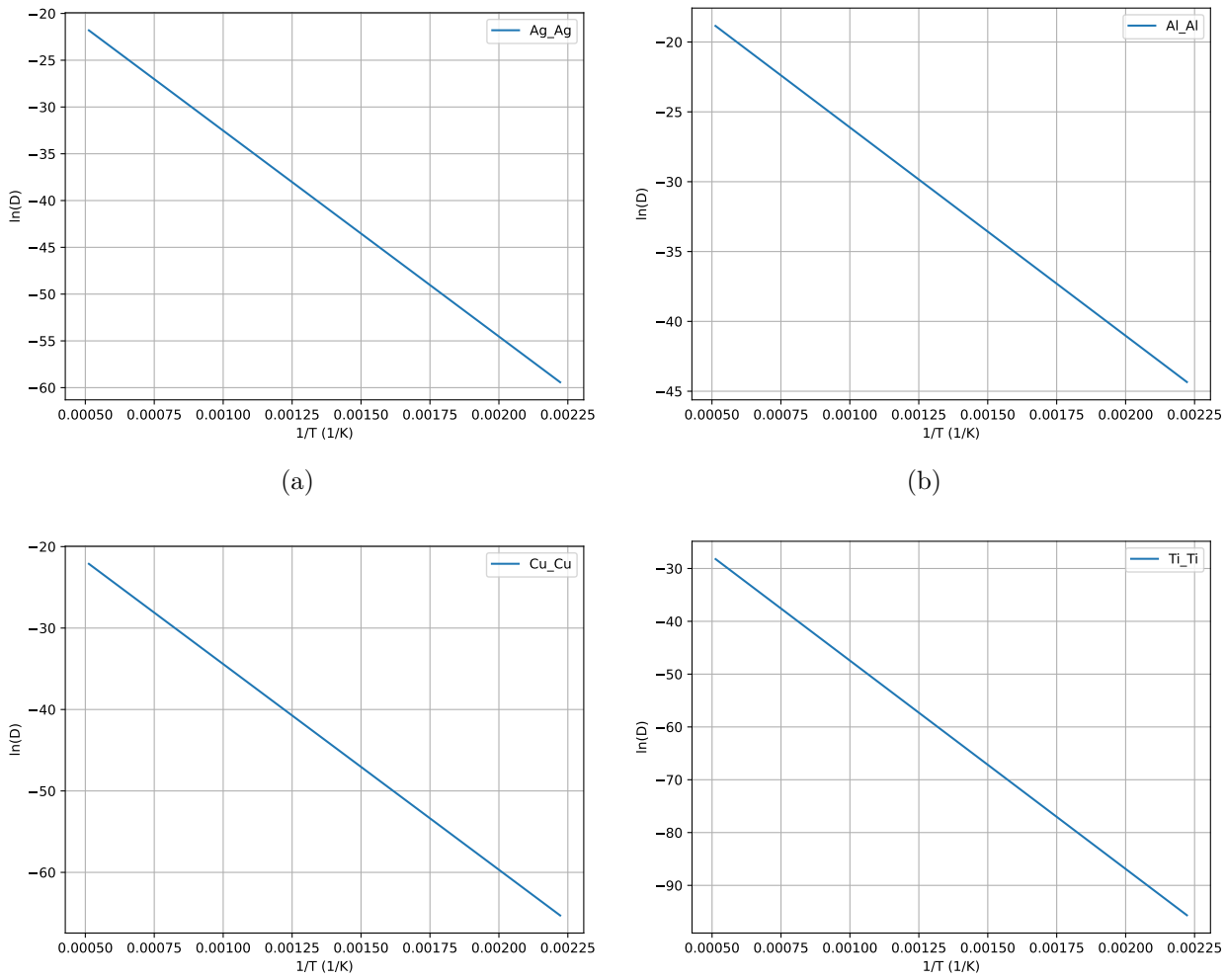


Figure 2: Logarithm of the diffusion coefficient for self-diffusing systems: a) silver, b) aluminum, c) copper and d) titanium.
*Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at (Cap Morales, 2025)).*

2.2 Solute diffusion

The plots for diffusing systems using are shown in figure 3, 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

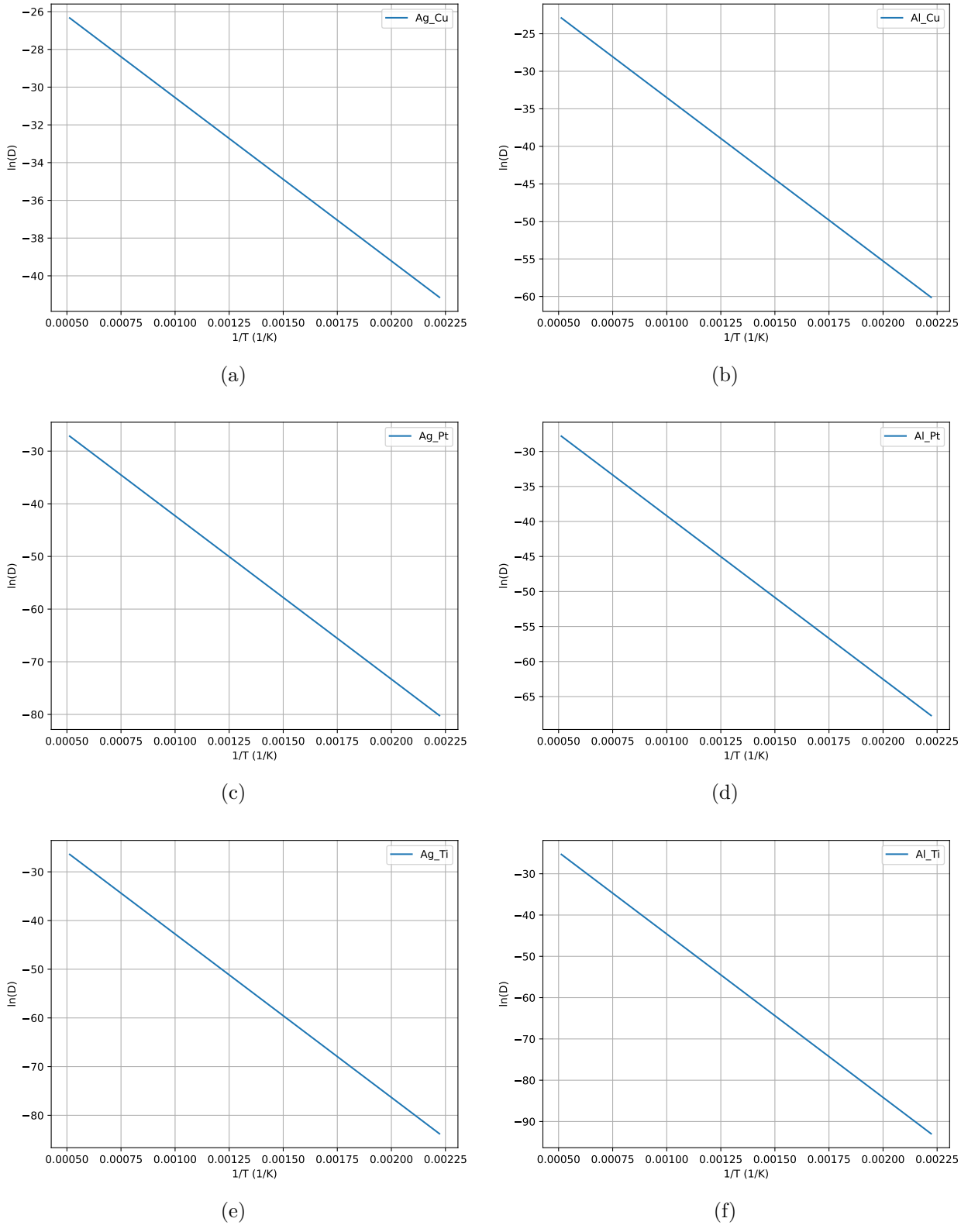


Figure 3: Logarithm of the diffusion coefficient for the systems: copper diffusing in a) silver and b) aluminum; platinum diffusing in c) silver and d) aluminum; and platinum diffusing in f) silver and g) aluminum.

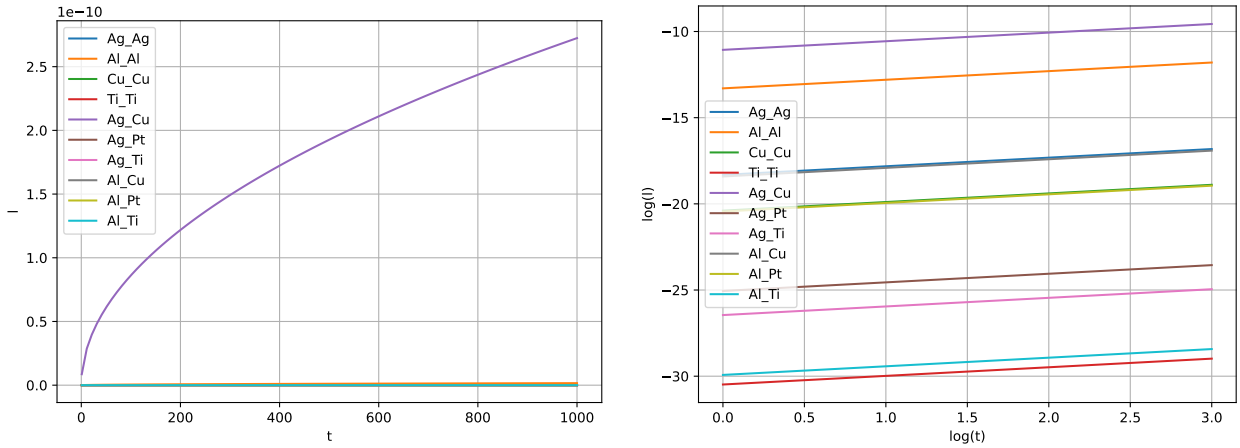
*Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at Cap*Morales *(2025)).*

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):

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

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 4.



(a) (b)

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

3.1 Self-diffusion

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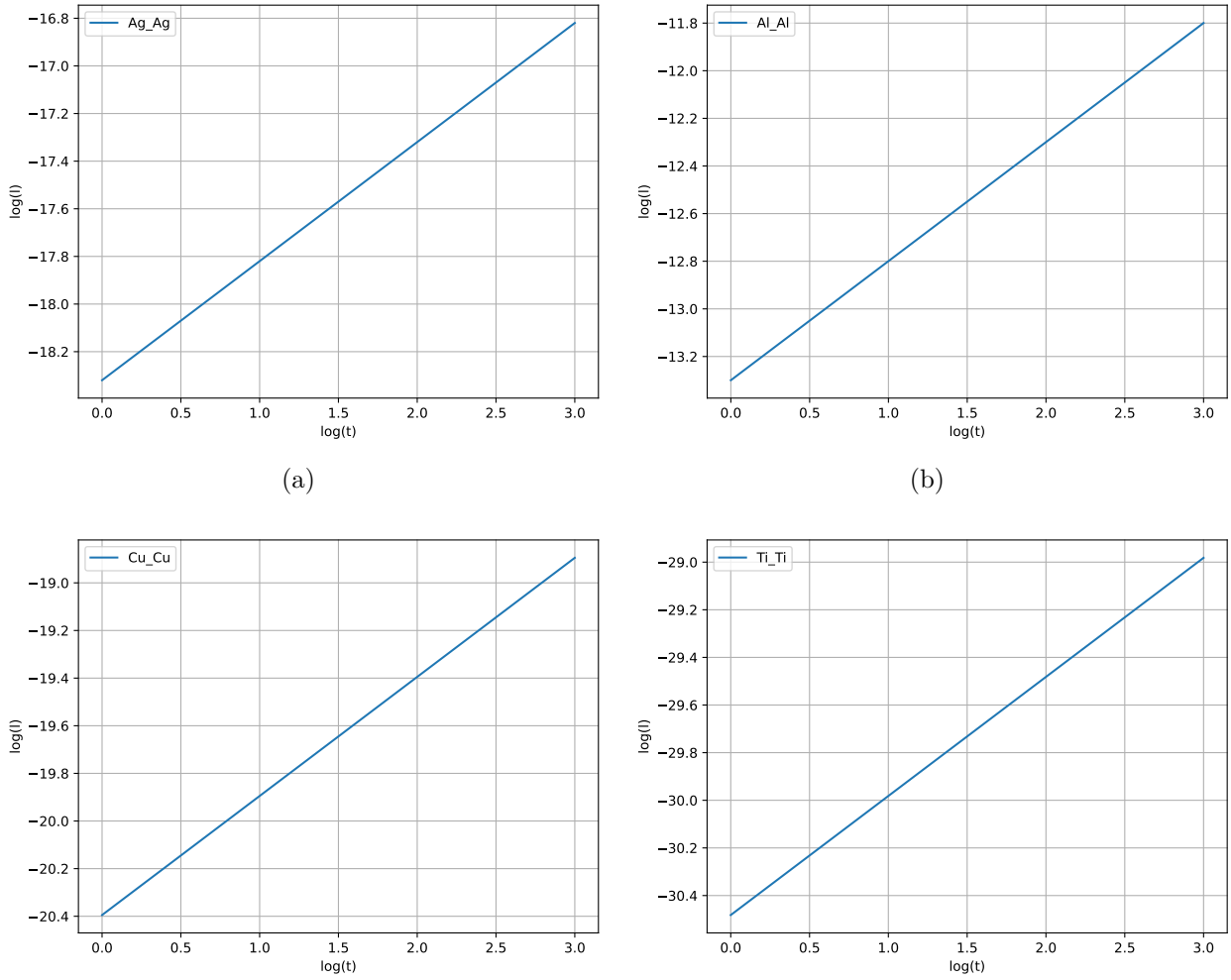

Figure 5: Distance of diffusion : a) silver, b) aluminum, c) copper and d) titanium. *Source: Data from (*Diffusion Database (Kakusan)*, n.d.), visualization by the author (code available at (Cap Morales, 2025)).*

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`