1. Mobility Database of Mg-Alloys

PanMg2020_MB is an atomic mobility database for Mg-based alloys, which is compatible with the PanMg2020_TH thermodynamic database and suitable for the simulation of diffusion controlled phenomena using the ***PanDiffusion*** module, ***PanPrecipitation*** module, and/or ***PanSolidification*** module.

1.1 Components (27)

Ag	Al	Bi	C	Ca	Ce	Cu	Dy	Fe	Gd
La	Li	Mg	Mn	Nd	Ni	O	P	Pr	Sc
Se	Si	Sn	Sr	Y	Zn	Zr			

1.2 Phases

The atomic mobility within the Liquid, Bcc, Fcc, and Hcp solution phases are assessed in this database.

1.3 Self-diffusivity of Pure Elements

The color represents the following meaning:

: Validated

: Estimated

: No data

Table 1.1: Assessed self-diffusivity of pure elements with different crystal structures

	Ag	Al	Bi	Ca	Ce	Cu	Dy	Fe	Gd	La	Li	Mg	Mn	Nd	Ni	Pr	Sc	Se
Bcc																		
Fcc																		
Hcp																		

	Si	Sn	Sr	Y	Zn	Zr
Bcc						
Fcc						
Hcp						

1.4 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all included elements in the current PanMg2019_MB database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the Fcc, and Hcp phases are listed, respectively.

Fcc phase

Ag-Al	Ag-Cu	Ag-Sn	Ag-Zn	Al-Cu	Al-Mg	Al-Ni	Al-Si	Al-Zn	Cu-Fe
Cu-Mg	Cu-Si	Cu-Sn	Cu-Zn	Fe-Mn	Fe-Ni	Fe-Si	Mn-Ni	Ni-Zn	

Ag-Al-Zn	Al-Cu-Mg	Al-Cu-Si	Al-Cu-Zn	Al-Mg-Zn	Al-Mn-Ni
Cu-Fe-Mn	Cu-Fe-Ni	Cu-Mn-Ni	Cu-Ni-Zn	Fe-Mn-Si	

Hcp phase

Al-Mg	Mg-Zn	Al-Mg-Zn

1.5 Database Validation

The simulated concentration profiles of a series of magnesium alloys are used to validate the current mobility database for Mg-based alloys. A few examples of such simulation are shown below.

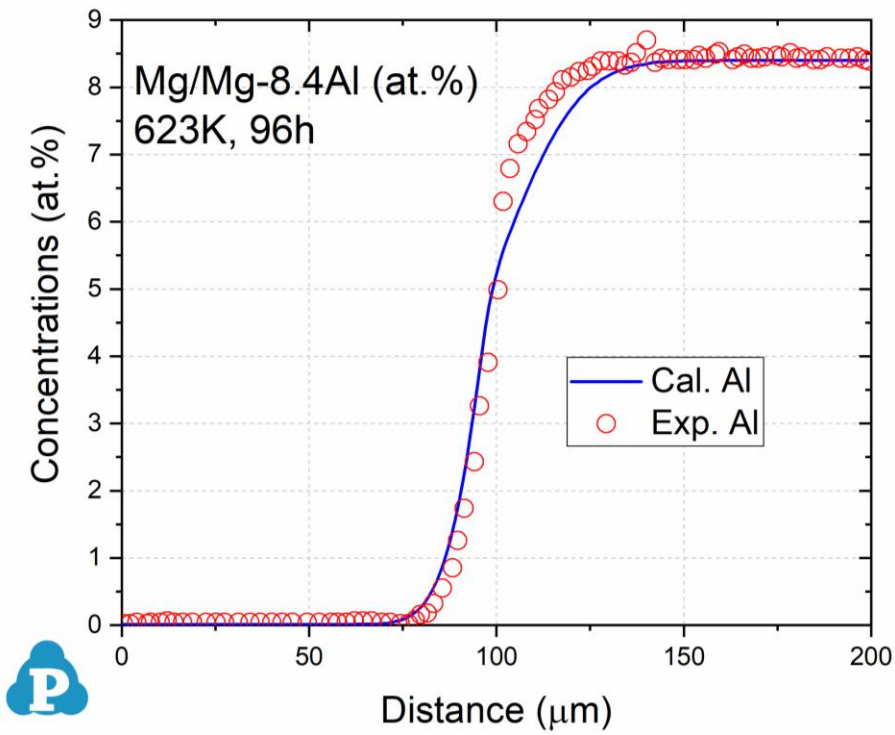

Figure 1.1: Concentration profile of Mg/Mg-8.4Al (at.%) annealed at 623K for 96h with data [1]

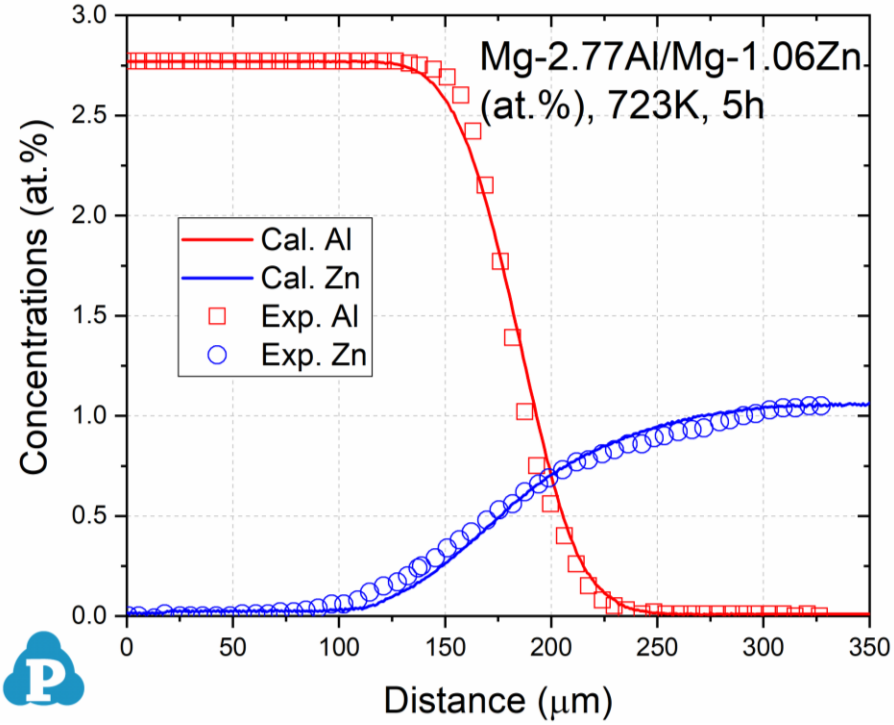

Figure 1.2: Concentration profile of Mg-2.77Al/Mg-1.06Zn (at.%) annealed at 723K for 5h [2]

1.6 Applications

This mobility database is combined with the thermodynamic database for Mg-based alloys, ***PanMg_TH***, to simulate the diffusion-controlled precipitation kinetics and solidification process of Mg-based alloys. A few examples are given below.

1.6.1: Precipitation kinetics of magnesium alloys

The ***PanPrecipitation*** module was developed for the simulation of precipitation kinetics of multi-component alloys. It has been seamlessly integrated with the thermodynamic calculation engine of the ***Pandat*** software, and has been used to simulate the evolution of microstructure and the corresponding mechanical property responses to heat treatment magnesium alloys [3]. Below shows an example simulation performed for the AZ91 alloy. Figure 1.3 shows the simulated particle size evolution with time of the γ-$Mg_{17}Al_{12}$ precipitate aged at 200°C compared with the experimental data of [4]. Figure 1.4 shows yield strength evolution with time. As is seen, the particles grow and coarsen with ageing time, while the yield strength reaches peak at a time varies with heat treatment temperature. The database used to do this simulation is the combined thermodynamic and mobility database of Mg-based alloys: ***PanMg_TH+MB***. More information regading to precipitation simulation can be found in ***PanPrecipitation*** module under the **Software** section.

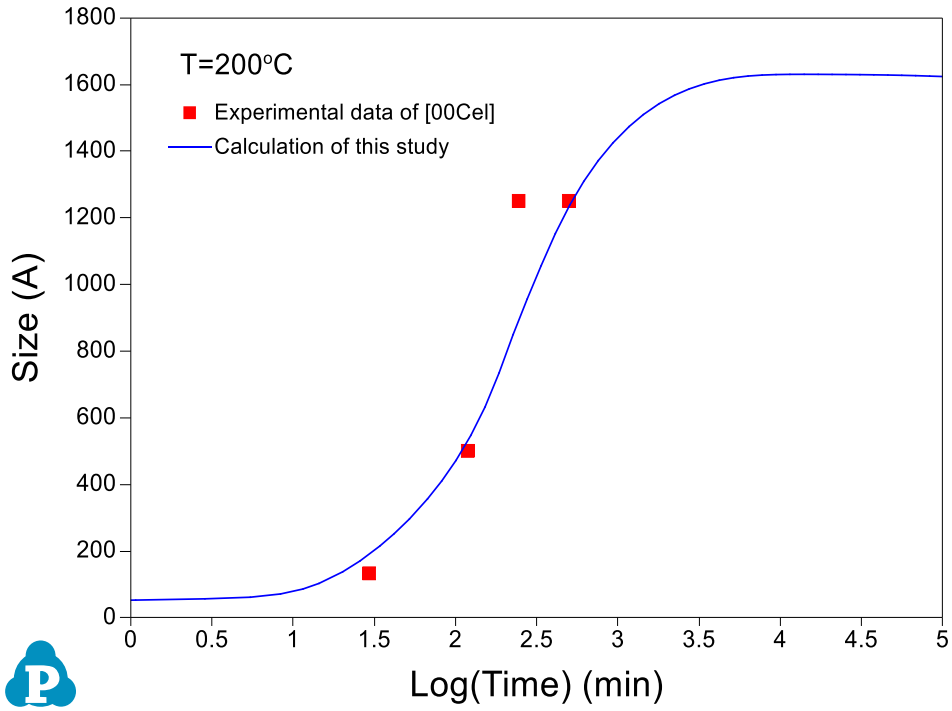

Figure 1.3: Calculated particle size evolution of the γ-Mg17Al12 precipitate aged at 200°C compared with the experimental data of [4].

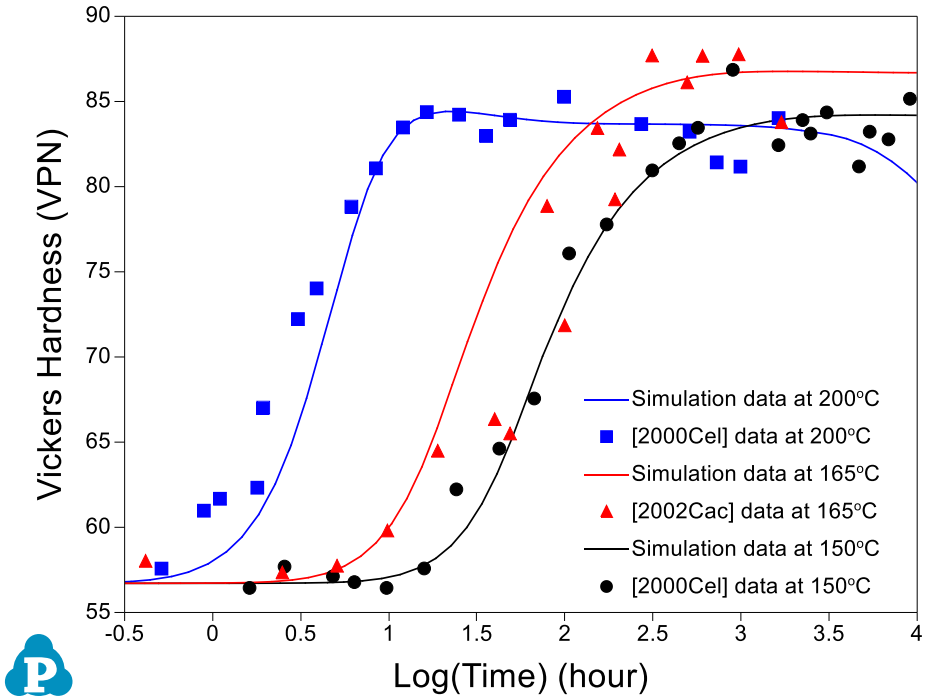

Figure 1.4: Simulated hardness curves of AZ91 alloy aged at 150, 165 and 200°C compared with the experimentally measured data of [4, 5]

1.6.2: Solidification simulation of magnesium alloys

The combined thermodynamic and mobility database of Mg-based alloys: ***PanMg_TH+MB*** is also used to simulate the solidification process considerting back diffusion in the solid phase [6]. Figure 1.5 compares the simulated and measured [7] Al composition profiles in the α(Mg) phase vs. fraction of solid (f_s) for Mg-xAl (x=3, 6 ,9) alloys. Figure 1.6 compares the simulated and measured secondary dendrite arm spacing (SDAS) [8] results of Mg-Al binary alloys. More information regading to solidification simulation can be found in ***PanSolidification*** module under the **Software** section.

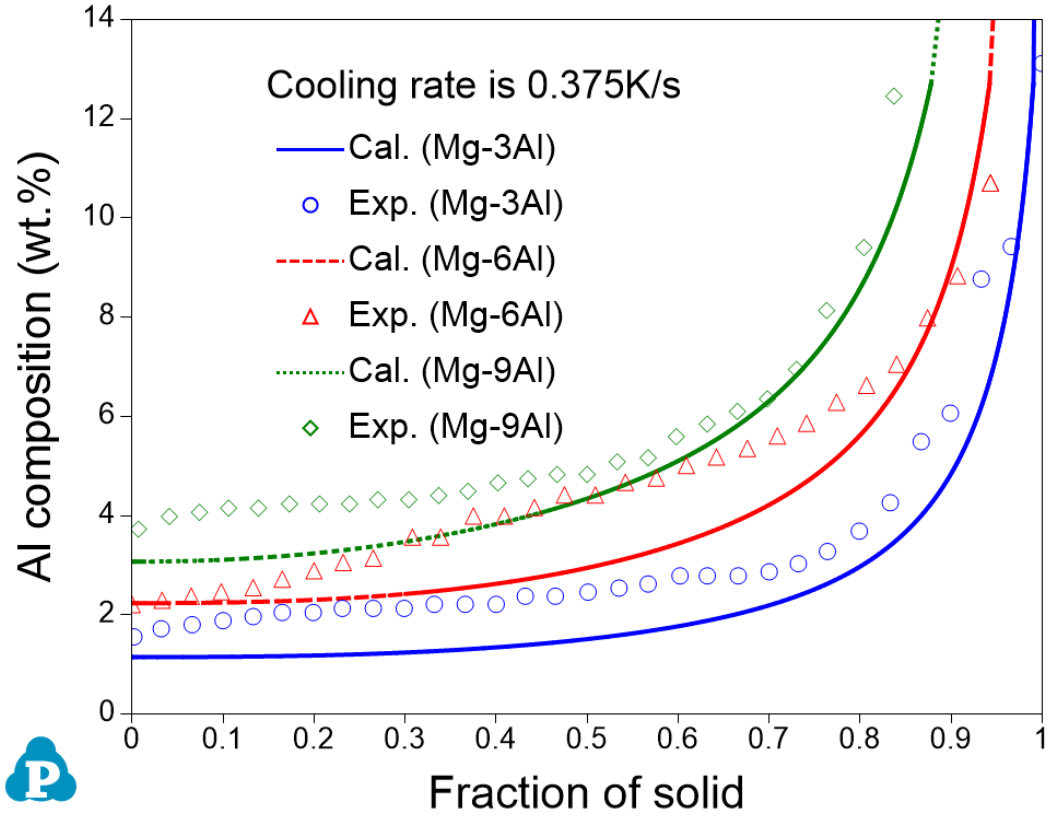

Figure 1.5: Comparison between the simulated and measured [7] Al composition profiles in the hcp_α(Mg) phase vs. f_s for Mg-xAl (x=3, 6 ,9) alloys

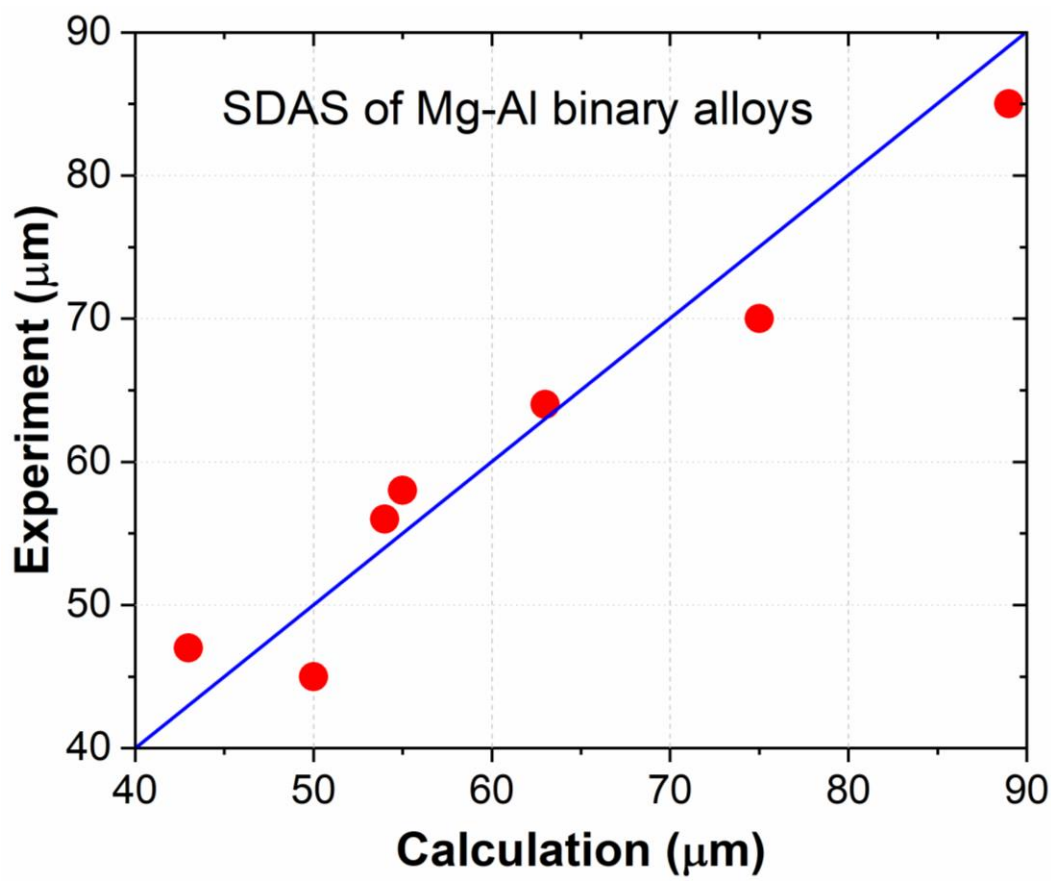

Figure 1.6: Comparison between the simulated and measured SDAS [8] for Mg-Al binary alloys.

1.7 References

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