

# Investigating the Role of Trace Additions to Al-Cu-X Alloys; A Kinetic Monte Carlo Study

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## Introduction

The influence of early-stage clustering on the competitive precipitation in age-hardenable aluminium alloys has been a long-standing focus of metallurgical research. Unfortunately, the precise mechanisms responsible for the development of beneficial or deleterious clusters are not well understood and until recently have been limited to laboratory observations. We have used kinetic Monte-Carlo simulations to reproduce the formation of these clusters. In an attempt to better understand the competition regarding cluster chemistry and number density Al-Cu binary through complex Al-Cu-Mg-Ag-Si alloys were investigated.

## Methodology & Model

The atoms are positioned on a fixed FCC aluminium lattice and we consider only first nearest neighbours interaction. The diffusion process occurs via a vacancy-assisted mechanism. For each iteration, every vacancy exchange rate is calculated, and the performed exchanges are chosen by a Monte-Carlo procedure. The exchange rate between a configuration 1 and a configuration 2 is given by (cf. Fig. 1) :

$$W_{1 \rightarrow 2} = \nu \exp(-E_a/kT)$$

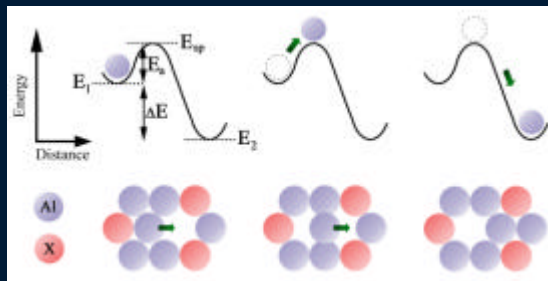


Figure 1 – Determination of the vacancy exchange rate

## Derivation of Input Parameters

To derive the input parameters, former clustering KMC studies have used either *ab initio* simulations [1] or experimental values such as solubility limits [2-3]. Some authors have not tried to reproduce a particular physical system, but have tried to be very general [4]. We have fitted our system to semi-empirical thermodynamics descriptions from ThermoCalc databases, which intrinsically capture some effects due to strain, for example, though limited to the nearest neighbour distance (cf. Fig. 2).

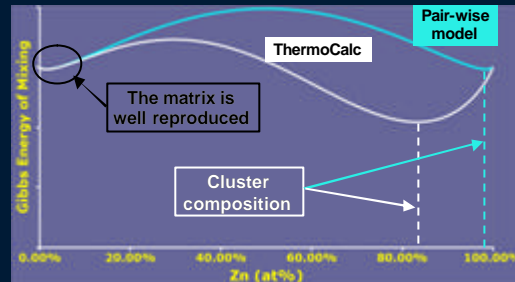


Figure 2 – Fitting the energy curve with a pair-wise model

For a satisfactory fit in both matrix and cluster we had to include multi-body interactions. This means that the system can not only be described as the sum of pair-wise interactions (cf. Fig. 3).

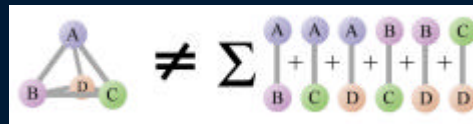


Figure 3 – Four-body model vs pair-wise model

## Clustering Tendencies

The clustering tendency (or binding energy) is given by the energy difference between the clustered atoms and the isolated atoms.

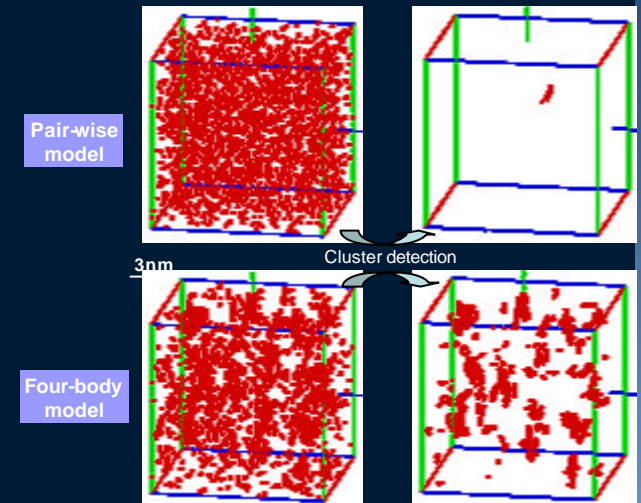
$$\text{Pair-wise: } E_{X-Y}^{\text{bin}} = e_{AIX} + e_{AIY} - e_{AIAI} - e_{XY}$$

Four-body:

$$E_{AI-AI-X-Y}^{\text{bin}} = 2 ( e_{AIAIAIX} + e_{AIAIAIY} - e_{AIAIAIAI} - e_{AIAIXY} )$$

Atomic Pair	Hirosawa [3]	Current Study (pair-wise)	Current Study (Al-Al-X-Y tetrahedron)
Mg-Ag	0.7 kJ/mol	5.2 kJ/mol	0.8 kJ/mol
Cu-Mg	2.9 kJ/mol	1.3 kJ/mol	4.9 kJ/mol
Mg-Mg	2.3 kJ/mol	1.1 kJ/mol	2.1 kJ/mol
Cu-Cu	4.4 kJ/mol	-2.3 kJ/mol	11.4 kJ/mol
Ag-Ag	2.6 kJ/mol	-5.3 kJ/mol	-14.3 kJ/mol
Cu-Ag	1.1 kJ/mol	-8.0 kJ/mol	-6.0 kJ/mol

## Visualisation of the Simulation Results



## Conclusions

This preliminary study has shown that a realistic KMC simulation study of the clustering in multi-component aluminium alloys is possible provided that a many-body interaction model is used. Pair-wise interactions have been shown to insufficiently reproduce the behaviour of the solute elements. The derivation of the energetic parameters from thermodynamic databases has been shown to be successful. Further work is being done on the confrontation between simulation and experiments.

## References

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