Self-Diffusion in solid solutions of α-Cu-Zn alloys using Molecular Dynamics simulations

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Abstract

The investigation of self-diffusion behavior in solid solutions of α-Cu-Zn alloys has been a subject of great interest. They play a critical role in comprehending material properties and developing advanced materials with tailored diffusion properties in industrial applications. In this work, Molecular Dynamics (MD) simulations were employed to investigate the self-diffusion of Zn in α-Cu-Zn (brass) alloys, specifically focusing on the 37 at. % Zn composition, at elevated temperatures ranging from 900 K to 1220 K. The calculated diffusion coefficients exhibit fair agreement with the experimental values from earlier literature, determined by the residual activity method, particularly after applying a necessary correlation factor correction for face-centered cubic lattices. Our results support an Arrhenius-type relationship where the self-diffusion coefficient increases with temperature, signifying that diffusion is thermally activated. Single vacancy simulations yielded results closely aligned with experimental data, in contrast to the simulations with higher vacancy concentrations. This work highlights the potential of MD simulations for determining diffusion coefficients as an alternative to expensive and time-consuming extensive experimental methods.

Motivation

- Compound casting offers a method to tailor a component's mechanical properties by directly integrating dissimilar metals in a single casting process. This technique creates a strong interface with unique properties, as seen when liquid Al bonds with a solid Cu-Zn substrate.
- The limited availability of diffusion data for higher compositions, specifically with 37 at.% Zn, hampers the comprehensive understanding of the Al-Cu-Zn system.
- Investigating diffusion coefficients in the α-Cu-Zn system provides initial insights into the ternary Al-Cu-Zn system.
- Molecular dynamics simulations offer a comprehensive approach to studying diffusion kinetics.

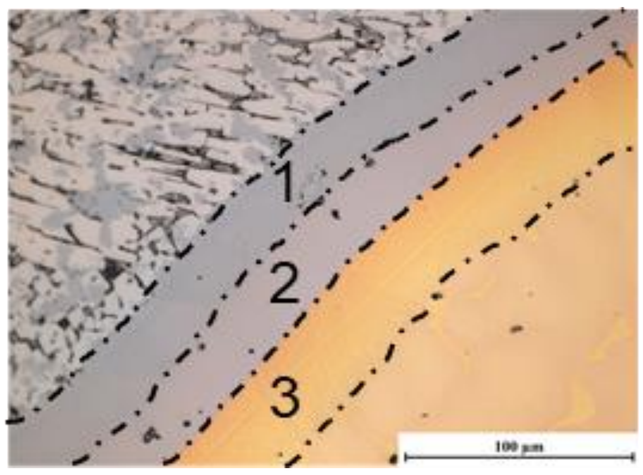

Fig. 1: Microstructure at the diffusion-reaction interface between AA6060 – CuZn37 solid-liquid diffusion couple annealed at 660°C for 90s, where 3 distinct intermetallic layers are observed

Method

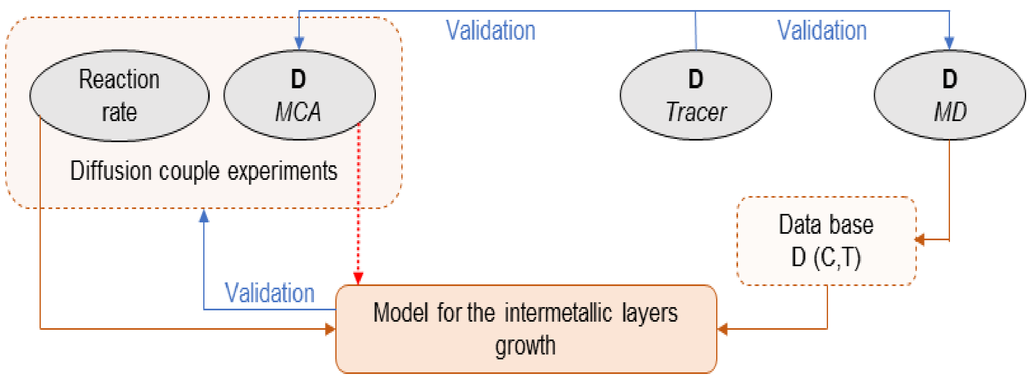

Fig. 2: Interaction between experiments and numerical simulations

- Atomistic simulations have been performed with the open-source code LAMMPS.
- Embedded-Atom-Method potential has been employed to define the interaction between Cu-Zn [1]
- Periodic boundary conditions are employed, and the time step in all the simulations is 6 ns.
- The samples are relaxed using NPT ensemble.
- All visualizations are done by the software tool OVITO PRO.

Future Work

- Developing an interatomic potential for Al-Cu-Zn using traditional empirical methods presents a significant challenge due to the combined complexities of the Cu-Zn system (disparate bonding types and ordered phases) and the additional considerations for Al.
- The vast range of potential intermetallic compounds formed further adds complexity, requiring careful modeling and analysis.
- Our future work aims to develop a high-dimensional neural network potential for the ternary Al-Cu-Zn system, based on the algorithms proposed by Jörg Behler et al.,[3] to accurately model diverse bonding types, ordered phases, and intermetallic compounds.

Results

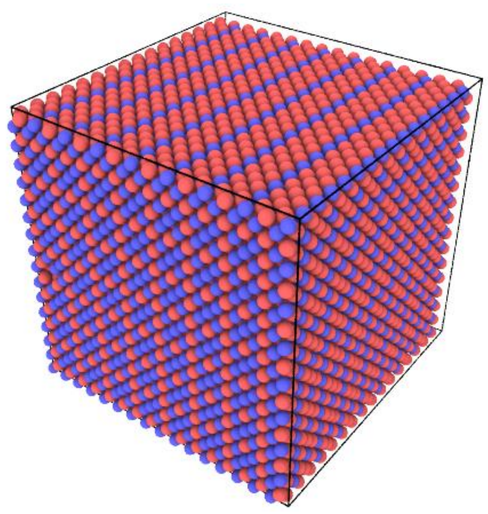

Fig. 3: Initial atomic Arrangement (red= Cu, Blue = Zn)

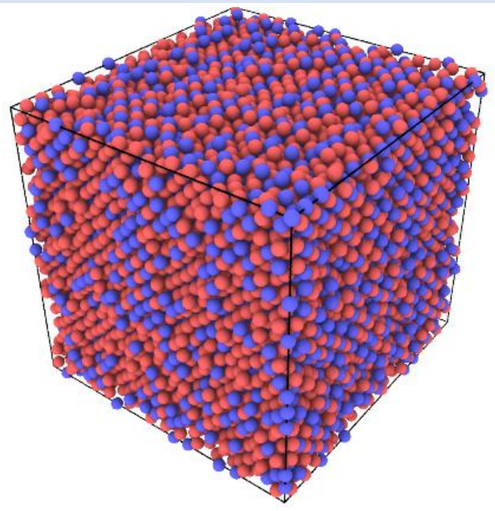

Fig. 4: After Diffusion

- The mobility of the Zn atoms is described by their mean square displacement (MSD)

$$MSD = \langle |\mathbf{r}(t) - \mathbf{r}(0)|^2 \rangle$$

- According to the Einstein's relation Diffusion coefficient is related to MSD as:

$$D' = \frac{1}{6t}\frac{\mathrm{d}(MSD)}{\mathrm{d}t}$$

- Enhancing accuracy in molecular dynamics simulations, a correlation factor correction is employed to address correlated motion effects, facilitating precise comparisons between simulated and experimental diffusion coefficients

$$D = f_c \frac{1}{6t}\frac{\mathrm{d}(MSD)}{\mathrm{d}t} \quad , f_c = 0.7815 \text{ for FCC lattice}$$

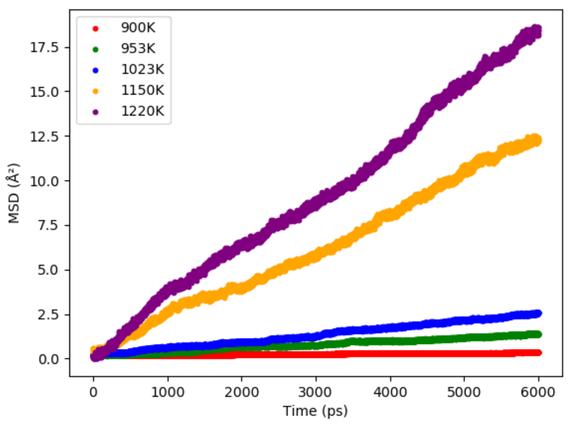

Fig. 5: Mean-square displacement of Zn at various temperatures

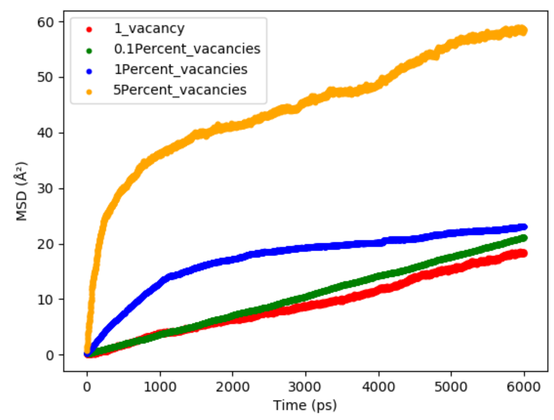

Fig. 6: Mean-square displacement of Zn at 1220 k at various vacancy concentrations

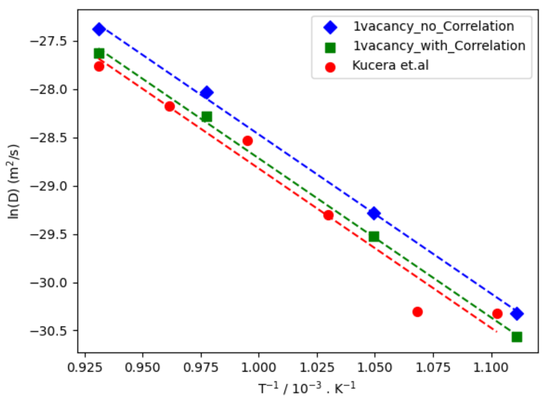

Fig. 7: Experimental results[2] Vs Molecular Dynamics simulations at various vacancies ranging from 1 vacancy to 5% vacancies

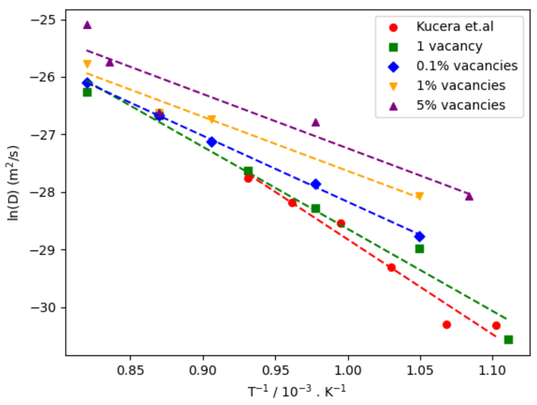

Fig. 8: Experimental results [2] vs Molecular Dynamics simulations with and without correlation factor correction

- The results are in good agreement with experiments[2].
- The results show strong temperature dependencies supporting the Arrhenius-type relationship confirming that diffusion is thermally activated.
- This work emphasizes the potential of MD simulations as a cost-effective and time-consuming alternative to experimental methods.

Acknowledgment

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Literature

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[3] Andreas Singraber, Jörg Behler, and Christoph Dellago Journal of Chemical Theory and Computation 2019 15 (3), 1827-1840 DOI: 10.1021/acs.jctc.8b00770