Application of Quasi-Lattice Models for Predicting the Temperature Dependence of Thermodynamic Properties in Liquid Binary Alloys

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ABSTRACT

This study applies the quasi-lattice model (QLM) incorporating temperature- and composition-dependent parameters to predict the thermodynamic properties of liquid binary alloys. By focusing on key alloys such as Cu-Pb and In-Tl, the model effectively captures temperature-induced variations in free energy, entropy, heat of mixing, and concentration fluctuations. Validation against experimental data demonstrates the model's capability to describe non-ideal mixing and phase stability, offering valuable insights for alloy design and processing optimization.

Keywords: quasi-lattice model, thermodynamic properties, alloy

INTRODUCTION

Liquid binary alloys are essential in metallurgical and materials engineering applications, where their thermodynamic behavior governs phase stability and microstructural evolution. Properties like free energy of mixing, entropy, heat of mixing, and concentration fluctuations are strongly temperature-dependent and influence processes such as melting, solidification, and heat treatment.

Traditional models, including regular and sub-regular solutions, often inadequately represent these complex dependencies, especially near critical points. The quasi-lattice model (QLM) which models atomic bonding within a temperature- and composition-dependent coordination environment—has emerged as a robust framework to fill this gap. This paper aims to apply the QLM to understand and predict temperature-dependent thermodynamic properties of liquid binary alloys, validating outcomes with experimental observations for industrially relevant systems.

LITERATURE REVIEW

The QLM advances beyond classical solution theories by statistically modeling atomic pair interactions and short-range order fluctuations through a coordination number □ and interaction energy □, both dependent on temperature □ and composition □. Prior works demonstrate QLM's success in describing asymmetric and non-ideal mixing behaviors across various systems including Al-Sn, In-Tl, and Cu-Pb. Refined parameterizations with temperature-dependent coordination numbers have notably enhanced the agreement between theory and experiment. Studies by Shrestha et al. (2017) and Singh et al. (2018) exemplify the model's application and validation across temperature ranges.

Theoretical Framework and Mathematical Formulation

In QLM, atoms in the liquid phase form quasi-lattice environments characterized by coordination numbers $Z(T, x)$. Key thermodynamic quantities are expressed as:

- Interaction energy parameter:

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$$W(T) = W_0 + W_1T + W_2T^2 + \cdots$$

- Free energy of mixing:

$$\Delta G_M = RT[x\ln x + (1-x)\ln(1-x)] + x(1-x)W(T)$$

- Heat of mixing:

$$\Delta H_M = x(1-x)\left[W(T) - T\frac{dW}{dT}\right]$$

- Entropy of mixing:

$$\Delta S_M = -R[x\ln x + (1-x)\ln(1-x)] - x(1-x)\frac{dW}{dT}$$

- Concentration fluctuations:

$$S_{cc}(0) = \frac{k_BT}{\left(\frac{\partial^2 G}{\partial x^2}\right)_{T,P}}$$

- Redlich-Kister expansion to model excess properties:

$$W(x,T) = x(1-x)\sum_{k=0}^{n} L_k(1-2x)^k$$

where L_k are temperature-dependent coefficients.

METHODOLOGY

1. Binary liquid alloys Cu-Pb, In-Tl, Al-Sn, and Sn-Zn were selected based on data availability.
2. Thermodynamic data including free energy, heat, entropy of mixing, and concentration fluctuations were gathered from literature.
3. Temperature-dependent coordination numbers and interaction energies were optimized via least squares to fit experimental values.
4. Using these optimized parameters, the model computed continuous thermodynamic property profiles over temperature-composition space.
5. Model predictions were validated through comparison with independent experimental datasets.

RESULTS AND DISCUSSION

The QLM reproduces key temperature-dependent thermodynamic trends observed experimentally:

1. The free energy of mixing (Δ□□) decreases with increasing temperature, indicating enhanced alloy mixing and lowered segregation, as confirmed in Cu-Pb alloys (Shrestha et al., 2017).
2. Entropy of mixing (Δ□□) rises, reflecting greater configurational disorder, matching findings in In-Tl alloys (Singh et al., 2018).
3. Heat of mixing (Δ□□) diminishes, showing reduced enthalpic segregation influence consistent with metallurgical observations.

4. Concentration fluctuations $□_{□□}(0)$ substantially decrease, indicating a shift toward ideal solution behavior and improved microstructural stability (Pathak et al., 2019).

Compared to traditional models with constant coordination, adopting temperature-dependent $□(□, □)$ significantly improves prediction accuracy (Jain et al., 2021). Residual discrepancies, primarily at extreme compositions, suggest directions for future refinement, including vibrational and electronic contributions.

These results confirm the QLM's value in elucidating high-temperature alloy behavior, facilitating alloy design and processing decisions by predicting phase stability and mixing characteristics at elevated temperatures.

Case Studies

- In Cu-Pb alloys, QLM predicted reductions in $Δ□_{□}$ and $Δ□_{□}$ over 1300–1500 K consistent with measured data, alongside diminishing concentration fluctuations indicative of homogenization.
- For In-Tl alloys, characterized by asymmetric mixing, the model successfully captured temperature-driven entropy and heat variations between 400–900 K.
- Al-Sn and Sn-Zn alloys displayed monotonic decreases in mixing energy and fluctuations with temperature, conforming to QLM predictions.

CONCLUSION

The quasi-lattice model with temperature- and composition-dependent parameters accurately predicts thermodynamic property variations in liquid binary alloys. This approach offers enhanced insights for alloy thermodynamics and supports industrial metallurgical applications. Future research should extend the framework to multicomponent systems and integrate additional physical phenomena to further refine predictive capabilities.

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