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Ab initio simulations to investigate the correlation between the local melt structure and segregation behavior of Fe, V, Ti, and Si in liquid Al

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ABSTRACT

In this study, the elements Fe, Si, V, and Ti, which exhibit typical segregation behavior in Al, were chosen as the solute atoms to be analyzed. The structure of the molten Al, the local structure around the atoms, and the diffusion of the solute atoms were investigated with *ab initio* molecular dynamics simulations. The results showed that the minimum addition of a solute (1 atom) does not significantly influence the overall structure of the liquid Al. However, the local structure around the solute atoms varied dramatically depending on the solute added. The local structure around the Fe atom was the most compact and stable of the four solutes tested, and thus, this local structure had the lowest diffusion coefficient. Conversely, the local structure around the Si atom was the most relaxed structure. For the transition metal elements (Fe, V, and Ti), there was a correlation between the equilibrium partition coefficients and local structures around these solutes in the molten Al. This simple relationship between the solute atmosphere, chemistry, and temperature requires further study. In summary, the close packing and stable local structure around the solute atoms can affect both their diffusion and segregation behavior in the melt. In addition, we suggest that more transition metal elements should be investigated to corroborate the results of this study.

KEYWORDS: *ab initio*, melt structure, segregation, diffusion coefficient