JASMAC Conference of the Japan Society of Microgravity Application

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分子動力学法を用いた液体 Al-Ni 合金中における原子の拡散挙動評価

Diffusion behavior of individual atoms in liquid Al-Ni alloy calculated using molecular dynamic simulation

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1. Introduction

Diffusion in liquid metal is an important physical phenomenon for solidification simulation in casting. In self-diffusion, the squared displacements of individual atoms increased suddenly due to the jump diffusion in molecular dynamic (MD) simulation of Sn and Pb[1)]. However, in impurity diffusion, it has not been clear how the impurity atoms move individually. The objective of this study is to clarify the characteristics of trajectories with individual Ni atoms in liquid Al-Ni alloy.

2. Computational analysis procedures

The MD simultion of liquid Al-5 at.%Ni alloy was performed. This calculation was carried out with PreFerred Potential[2)] version 4.0.0 on Matlantis[3)]. 4000 Al atoms were arranged in a cubic simulation box which had an fcc structure. 200 atoms were replaced with Ni atoms. Each atom was given a serial number (ID). The number density was 0.0272 $Å^{-3}$. The equilibration process was carried out for the time of 1 fs × 2000 steps under the canonical ensemble at 973 K. After the equilibration process, the targeted simulation was performed with the time of 1 fs × 3000 steps.

3. Results

The squared displacements of Ni calculated between the positions at 0 and 2999 fs were distributed over a range of 0 to 21 $Å^2$. The average of this distribution was 4.56 $Å^2$. One of the smallest and largest squared displacements were 0.679 $Å^2$ of ID 1071 and 18.7 $Å^2$ of ID 3954, respectively. From fitting the mean square displacement of Ni using least-square analysis, the calculated impurity diffusion coefficient of Ni was 2.57×10^{-9} m^2s^{-1}. This value was approximately 30 % smaller than reliable experimental data measured by using shear cell technique under the microgravity condition[4)] and on the ground[5)].

4. Discussion

Figure 1 shows the time evolution of the squared displacements after equilibration and the trajectories for the atoms of ID1071 and ID3954. The trajectories were visualized by OVITO[6)]. ID1071 oscillated around almost the same location and its squared displacement remained. On the other hand, ID3954 oscillated in-situ up to 1000 fs, and its squared displacement increased markedly from 1000 fs to 2000 fs like jump diffusion. From 2000 fs to 2999 fs, the atom oscillated again.

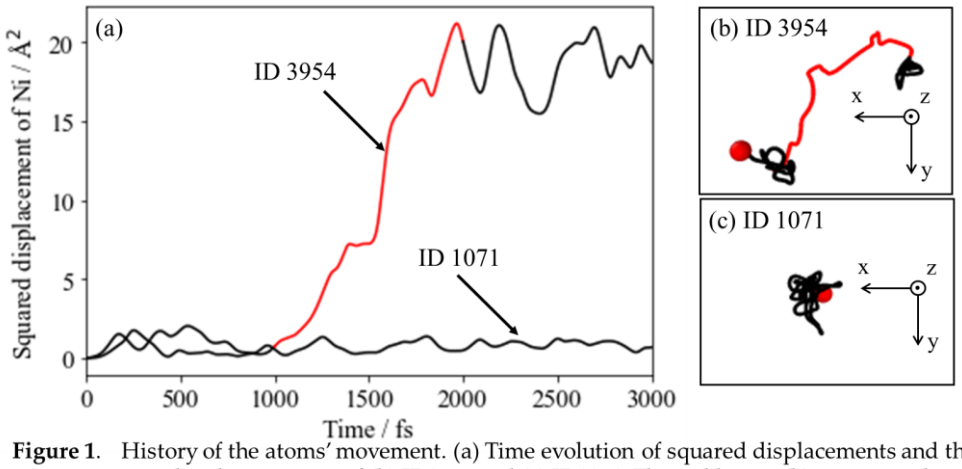

Figure 1. History of the atoms' movement. (a) Time evolution of squared displacements and the visualized trajectories of (b) ID3954 and (c) ID1071. The red line in (b) corresponds to the range of red squared displacement of ID3954 from 1000 fs to 2000 fs. The red spheres in (b) and (c) express the atomic locations at 0 fs.

5. Conclusion

In liquid Al-Ni, the Ni atom with large squared displacement has the characteristic of the transition from staying at the position to moving suddenly.

Acknowledgement

This study was supported by Grant-in-Aid for Scientific Research (C) Grant Number JP23K04364, Grant-in-Aid for Research Activity Start-up Grant Number JP24K23035, Grant-in-Aid for JST SPRING Grant Number JPMJSP2128, the "FY2023 Waseda University-ENEOS FS Research Grant"., Waseda Research Institute for Science and Engineering Grand-in-Aid for Young Scientists (Early Bird) (Yoshihiro Kobayashi) and Kimura Foundry Co., Ltd. for financial support.

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