# 論文 / 著書情報
# Article / Book Information

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| Title(English) | Experimental and Molecular Dynamics Study on Metallic Impurity Diffusion in Liquid Lead Alloys |
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Doctoral Program

# 論 文 要 旨

THESIS SUMMARY

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| 専攻：<br>Department of | 原子核工学 専攻 | 申請学位（専攻分野）：<br>Academic Degree Requested | 博士 （原子核工学）<br>Doctor of |
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要旨（英文 800 語程度）
Thesis Summary（approx.800 English Words ）


Fe and Ni diffusion in liquid Lead-bismuth eutectic (LBE) and Pb-17Li (17mol% Li) are studied experimentally and computationally. A conventional long capillary method is improved to perform the diffusion experiment and a new measurement method by using ion exchange ion chromatography with ICP-MS is developed to measure the diffused Fe and Ni concentrations. On the other hand, the classical molecular dynamics simulation where the potential energy of the atoms are presented by using embedding atom method is developed and applied to simulation the Fe and Ni diffusion in liquid LBE and Pb-17Li. The quantitative and qualitative study of Fe and Ni diffusion in both liquid LBE and Pb-17Li are estimated by those experimental and computational methods. The temperature dependence of Fe and Ni diffusion coefficients are obtained experimentally. It is found that the diffusion coefficients increase with temperature and they are independent on the time. The diffusion coefficient of Fe is lightly bigger than that of Ni in liquid LBE since the radius of Fe is bigger than Ni. The diffusion of Fe and Ni in liquid Pb-17Li at temperature of 723K show roughly the same value. It is assumed that the diffusion coefficient of Fe is smaller than that of Ni at temperature lower than 723K and the diffusion coefficient of Ni is smaller than that of Fe at temperature higher than 723K through the experimental results.

On the other hand, the simulation results show that Fe and Ni atom aggregation happen during the diffusion when temperature is not sufficiently high. The atomic diffusion of Fe and Ni are in good agreement with the theoretical results from Stokes Einstein, however, they are 1 order in magnitude bigger than the experimental results. It is considered that the aggregation of Fe and Ni atoms happened just after the dissolution in the experiment. Since Fe and Ni are saturated, the atoms aggregate fast, then the formed clusters diffusing into the LBE. According to results comparison, it is also assumed that the aggregation will not happen when the temperature is higher than 2000K and the diffusion would be atomic diffusion. Furthermore, it is found that the diffusion activation energy of Fe is twice bigger than that of Ni. It is because the radius of Fe is bigger than that of Ni, Fe needs more energy to jump into a vacancy in the liquid LBE. Besides, Fe and Ni atoms show stronger affinity for Bi atom during the diffusion. In case of Fe and Ni diffusion in Pb-17Li, there is no Fe and Ni atom aggregation during the diffusion. Fe atom show stronger affinity for Li atom but Ni atom has stronger affinity for Pb atom during the diffusion. The diffusion activation energy of Fe is lightly smaller than Ni, which shows reverse tendency compared to the diffusion in liquid LBE. This result assume that the diffusion activation energy may also influenced by the affinity. Since Ni has stronger affinity for Pb atom of which radius is significantly larger than Li atom, Ni needs more energy to jump to the vacancy site. Besides, the diffusion coefficient of Fe increases with

decreasing the lithium concentration in solvent. By contrast, the diffusion coefficient of Ni decreases with the lithium concentration. The reasons are considered as the different affinities of Fe and Ni during the diffusion.

Overall, since the liquid LBE and Pb-17Li show similar physical properties to each other, Fe and Ni diffusion coefficient in both alloys show comparable values. However, the diffusion mechanism of them are largely different. It is implied that the corrosion phenomenon of Fe and Ni in liquid LBE may differ from that in liquid Pb-17Li.