# Self- and Inter-Diffusions in Liquid Binary Alloys

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The self- and inter-diffusion processes in liquid Al-Cu and Ni-Cu alloys are studied by using molecular dynamics simulations. The self-diffusivity is calculated via the Green-Kubo method. The results show exponential growth with the increase of Al and Cu compositions for both species in Al-Cu and Ni-Cu alloys. Although the self-diffusivities of Al, Cu and Ni in pure liquid metals exhibit obvious differences, those in Al-Cu and Ni-Cu alloys are almost identical. The Maxwell-Stefan (M-S) interdiffusivities of Al-Cu and Ni-Cu alloys are calculated over the whole composition range with the Green-Kubo method and the Darken relation respectively. For Al-Cu alloy, the results from the two method show good agreements in low concentration region (<10% Al), whereas the M-S diffusivities from the Darken relation are markedly larger than those by the Green-Kubo method for medium concentration systems. This departure reaches the maximum at 70% Al, suggesting the failure of the Darken relation for predicting the M-S diffusivity of Al-Cu alloy effectively, especially in the medium concentration range. In contrast, the M-S diffusivities of Ni-Cu alloy are nearly the same over the whole compositions. The validation of the Darken relation depends on the alloy type and the concentration. Based on the M-S diffusivity and the activity analysis, the Fick diffusivities are calculated and the results show strong dependences on composition. In particular, the Fick diffusivities of $Al_{60}Cu_{40}$ and $Ni_{50}Cu_{50}$ melts as a function of undercooling are provided, which could be helpful in improving the quantitative predictions of solidification.