6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

# ANALYSIS OF INTRINSIC DIFFUSION IN FCC METALS THROUGH MOLECULAR DYNAMICS SIMULATION

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**Key Words:** *Intrinsic Diffusion, Molecular Dynamics, Dislocation, Diffusion.*

Although, enhanced diffusivity in the core of lattice dislocations have been reported for a number of crystalline materials [1, 2], the mechanisms remains debated. Recently, Pun and Mishin [3] revealed existence of enhanced diffusion along the dislocation core in Al even in the absence of pre-existing point defects: "the intrinsic mechanism." It is shown that the contribution of vacancies and self-interstitials to diffusion is negligible compared to the intrinsic diffusion. In our previous work [4] using molecular dynamics (MD) occurrence of intrinsic diffusion in aluminum, nickel, copper, and silver is studied. High diffusivity along the dislocation core was observed and quantified in Al, Ni and Cu. Moreover, high frequency of constriction of partials at elevated temperatures were observed in these three FCC metals. The observation of these two phenomena at core regions suggested that there might be a correlation between the two. In the present work, using MD techniques, this hypothesis is tested through i) analyzing the generation of point defects and their migration paths in core regions, and ii) investigating the role of constricted partial dislocations on enhanced diffusivity by computing the vacancy formation energy on different atomic sites (i.e. on partial dislocations, in stacking fault ribbon, and on the constricted node of partial dislocations). It is observed that the formation energy of point defects is much lower at the constriction nodes compared to the bulk. This shows that these nodes can perform as desired positions for nucleation of point defects. It is revealed that, even in materials with low stacking fault energy, when constriction is enforced, intrinsic diffusion may occur. These results imply that the reversion and constriction of partial dislocations is the essential requirement for generation of point defects, which lead to the high diffusivity in the core region.

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