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# Molecular dynamics simulations of deformation behaviour of Cu-Al alloys: solute-planar fault interactions

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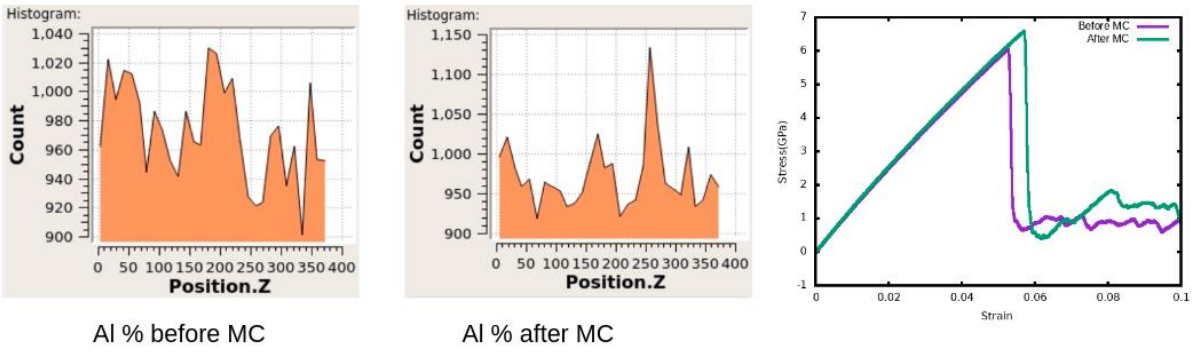
We have carried out molecular dynamics (MD) simulations of tensile deformation on pure copper and Cu-Al alloys that contain planar faults such as stacking faults and twin boundaries. The simulations are carried out using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) [1] and the system is modelled using EAM potentials. In the case of Cu-Al alloys, we carry out Monte Carlo (MC) moves to allow for the structure to relax through solute-planar fault interactions. We show that the Al atoms do indeed prefer to segregate to the planar fault. By carrying out tensile simulations on the same systems before and after MC moves and comparing the stress-strain curves as well as the defect structure and microstructure evolution, we show the effect of solute-planar fault interaction on the mechanical behaviour. In the presentation, finally, we will also indicate how thermodynamic integration can be used to evaluate the changes in stacking fault energies due to segregation which can then be used to rationalise the simulations results.




Al % before MC  Al % after MC

Fig. Al segregation at the fault after MC and the stress-strain curves before and after segregation

*Keywords: Cu-Al, Suzuki effect, MD, MC, Stacking fault*

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**References:**

[1] LAMMPS - A flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, A. P. Thompson et a.l, Comp Phys Comm, 271 (2022) 10817.