

Atomistic Modeling of Grain Boundary Segregation Strengthening in Nanocrystalline Aluminum Alloys

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Background & Motivation

Advancements in fabrication methods have enabled the development of nanocrystalline materials with superior properties – high strength, diffusivity and electrical resistivity- that are directly from the grain boundary content[1].

- Thermodynamic instabilities of the nanocrystalline state is often produce rapid grain growth at low homologous temperatures [2-5].
- Solute segregation to grain boundaries can reduce the driving force for grain growth and in turn, stabilize the nanostructures against thermally driven coarsening. [6,7].

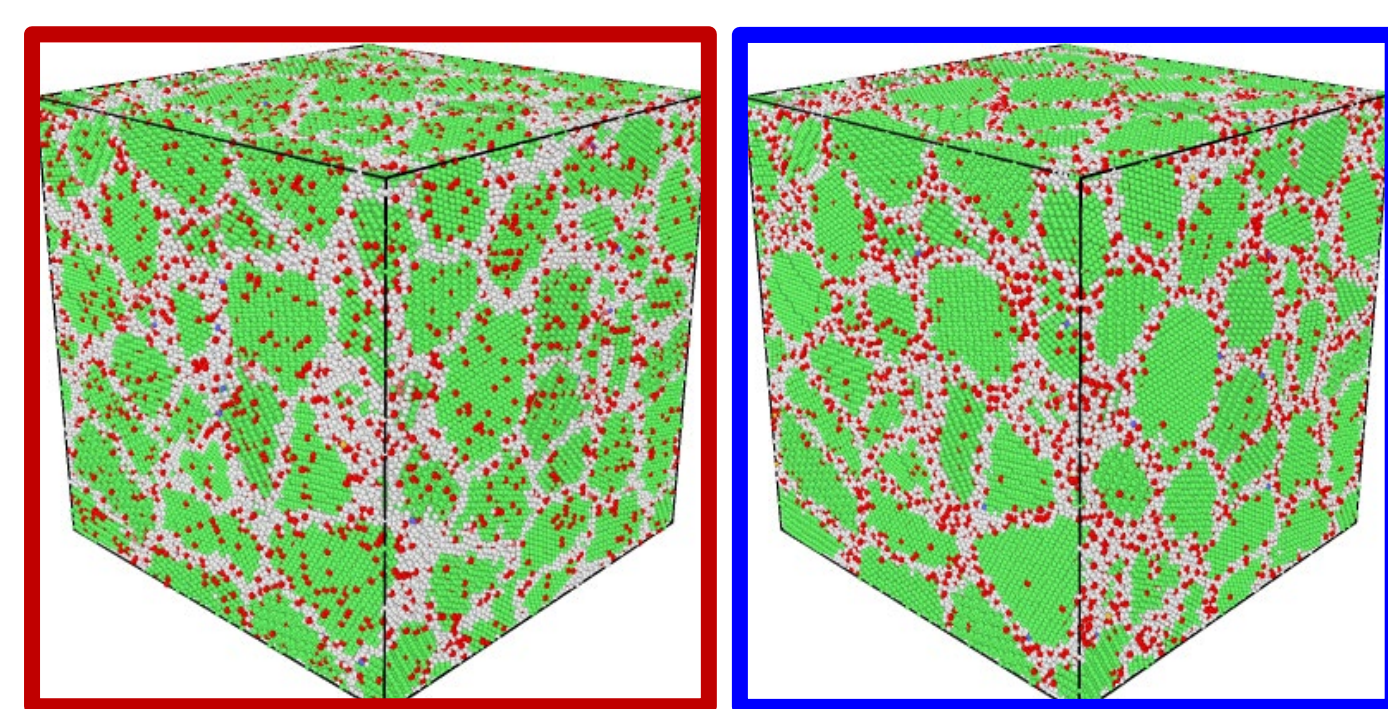
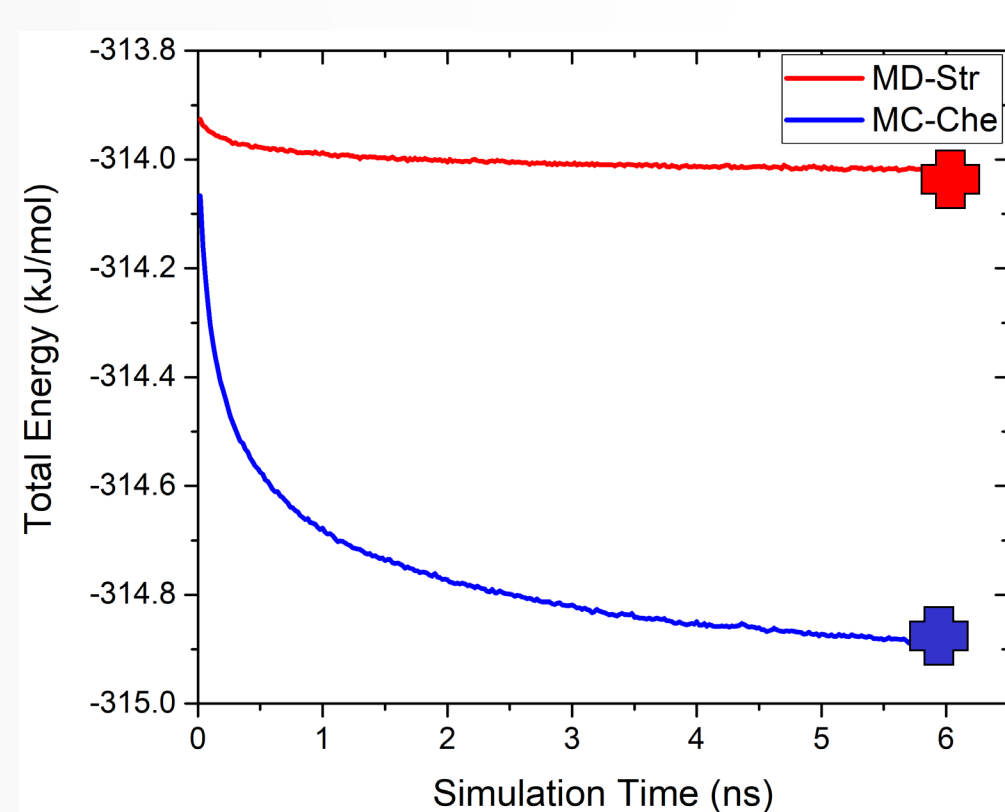
The focus of this study is to examine the effects of grain boundary segregation on the strength of nanocrystalline Al-Mg alloys by Molecular Dynamics (MD) simulations.

- Mg is selected as the alloying element (or dopant) of interest due to its large positive heat of segregation, which will promote Mg enrichment of the grain boundaries.
- The implications of stabilizing GBs through doping on the governing deformation mechanisms is studied by MD simulation.

Molecular Dynamics Simulations

Nanocrystalline Al-Mg models constructed with different grain sizes and solute contents using two energy minimization procedures.

- In this research, the equiaxed polycrystalline structures were first be built by a Voronoi tessellation procedure. The structures were then relaxed and deformed using LAMMPS and an Al-Mg EAM potential to describe the interatomic forces.
- Solute atoms are introduced into the pure Al systems through a random replacement of Al atoms with Mg. The structure is then subjected to two minimization procedures: (1) a structural relaxation through MD (MD-Str) and (2) a hybrid MD-Monte Carlo scheme [8] to further allow for chemical relaxation (MC-che).

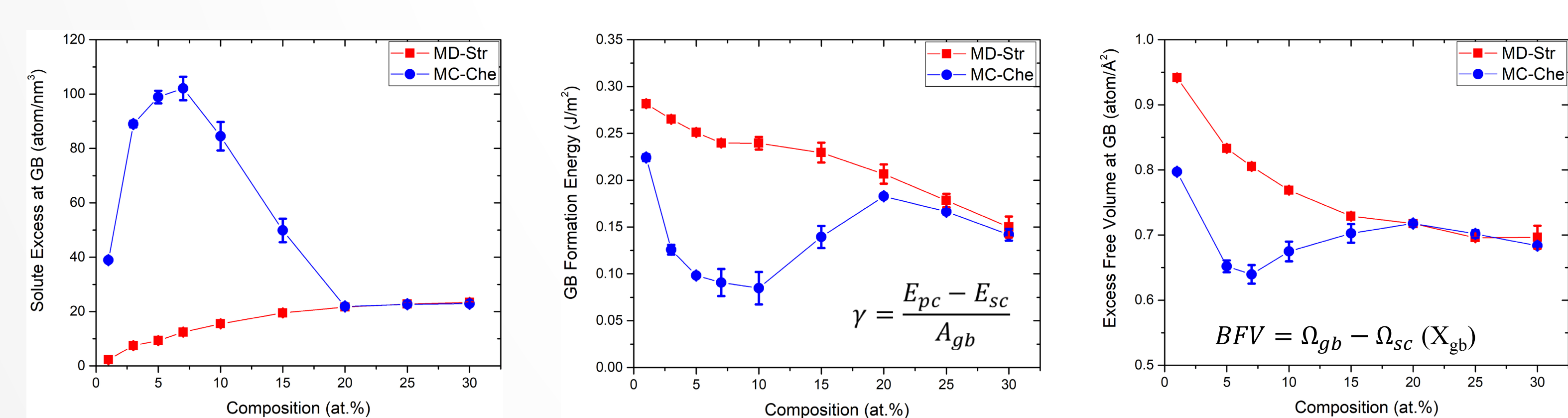


Energy Minimization

- Conjugate gradient (CG) relaxation to a final energy convergence of 10^{-12}
- MD relaxation at 50K for 0.2 ns
- Average grain size of 10 nm

- Al-Mg alloys are deformed in uniaxial tension at a strain rate is 10^9 s^{-1} . The deformation behavior is quantified using analysis methods for atomistic simulations including a CNA (Common Neighbor Analysis) scheme, slip vector quantification, microrotation metric.

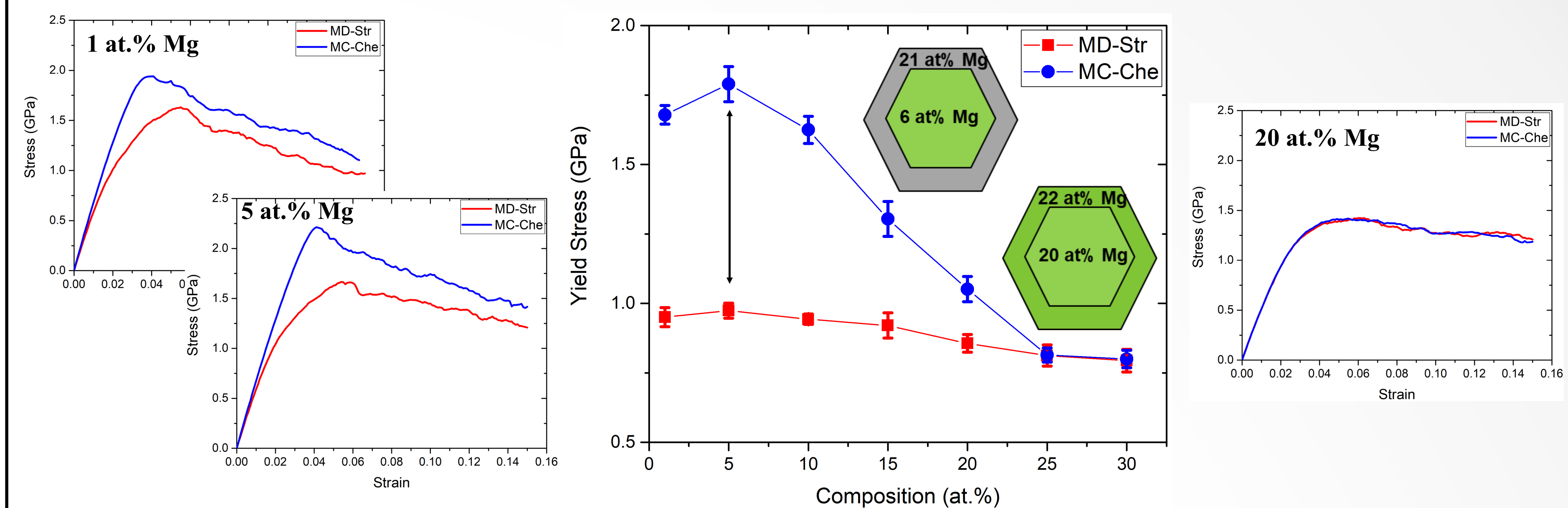
Quantifying Grain Boundary Segregation



- Allowing for solute redistribution during the hybrid MD/MC energy minimization produces a grain boundary segregated nanocrystalline structure with a maximum segregation state at a global (average) alloy composition of Al-7.5 at.% Mg.
- Grain boundary segregation drives down the grain boundary energy and excess free volume relative to the chemically homogeneous state produced from the MD-Str process.

The Implications of Grain Boundary State for Mechanical Properties

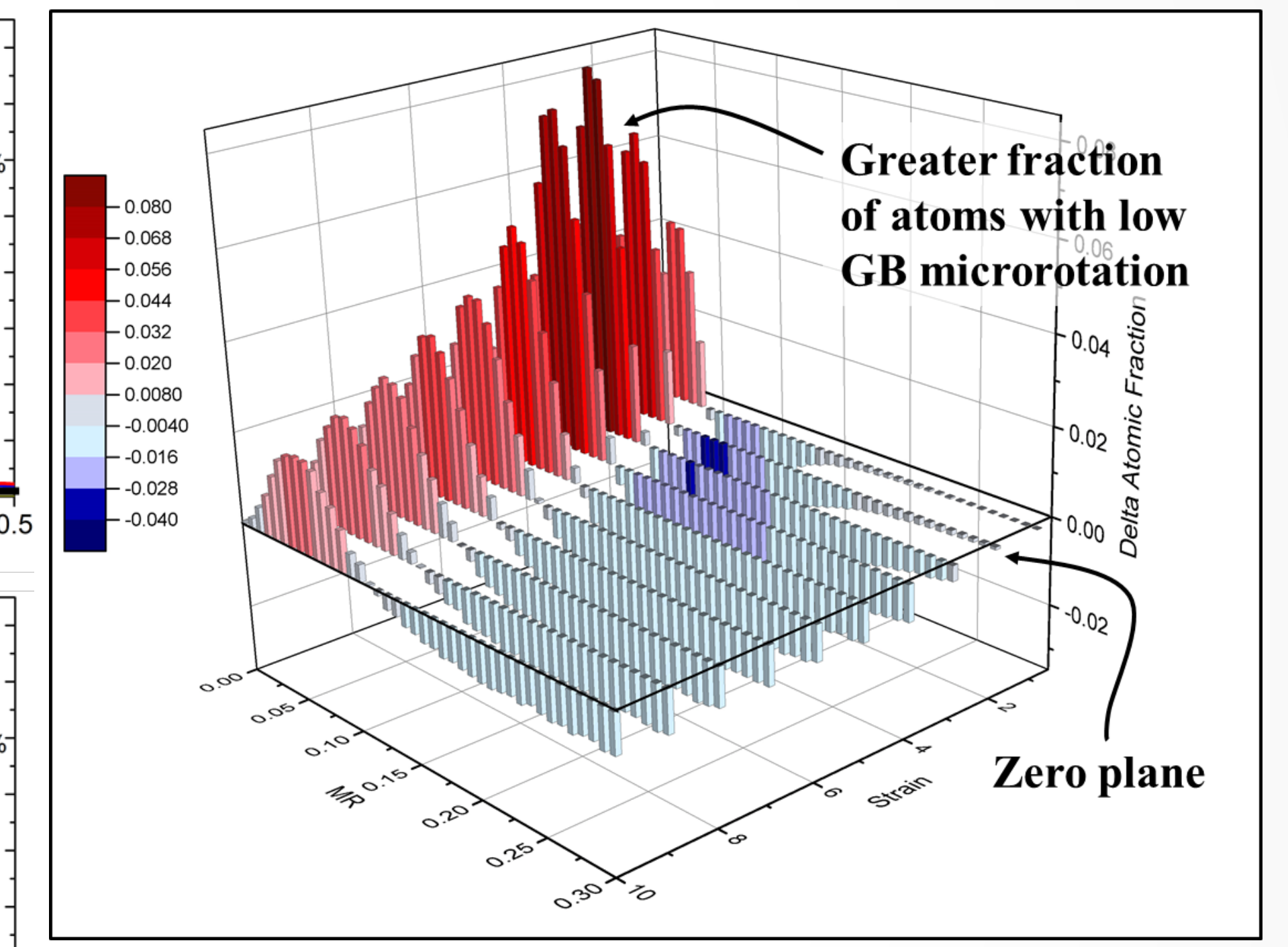
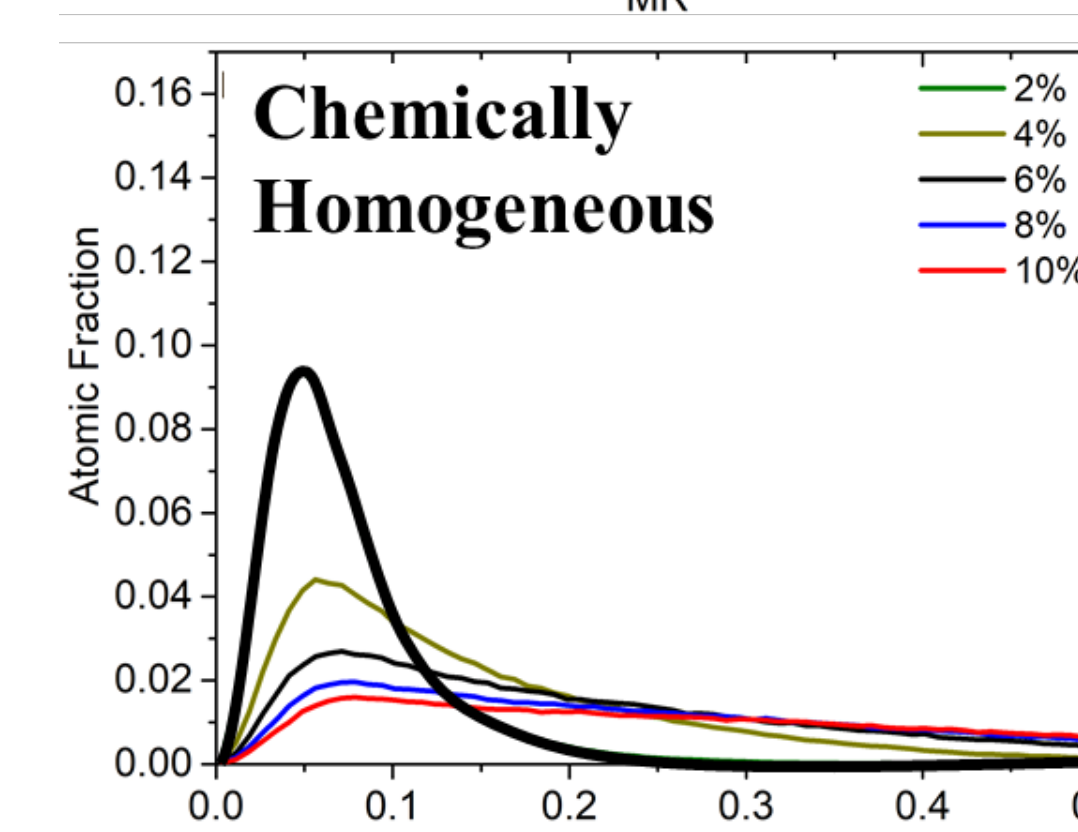
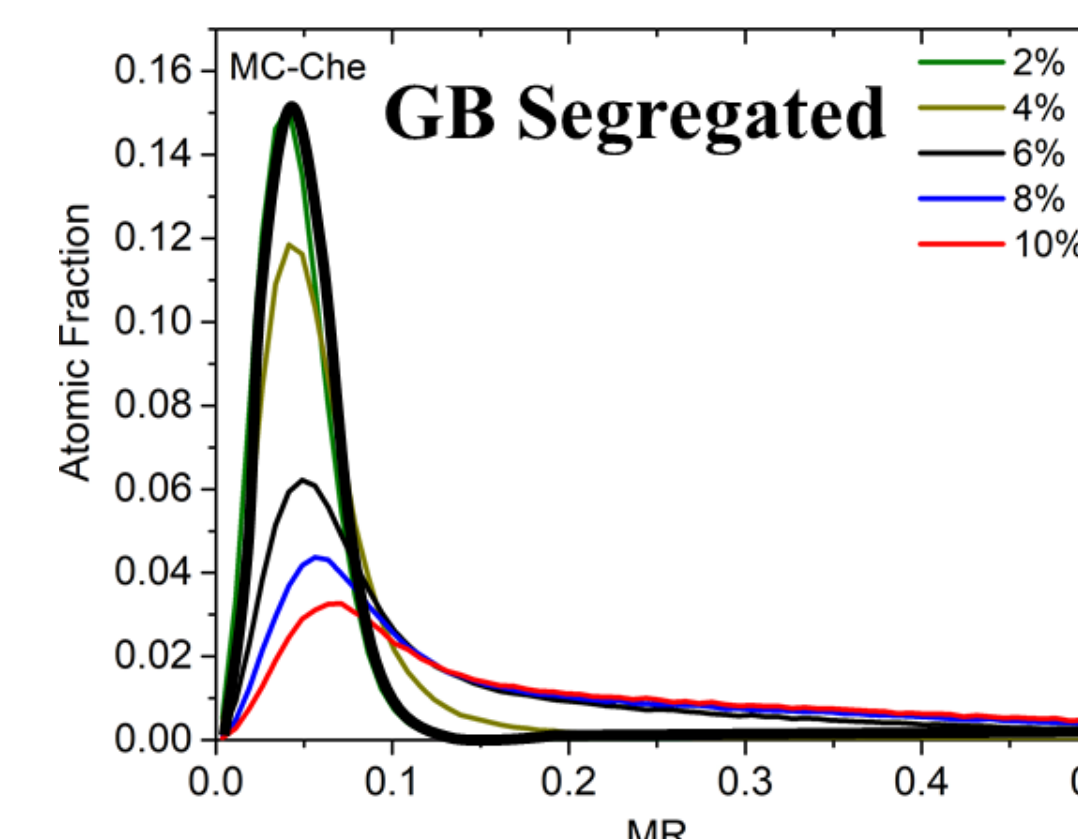
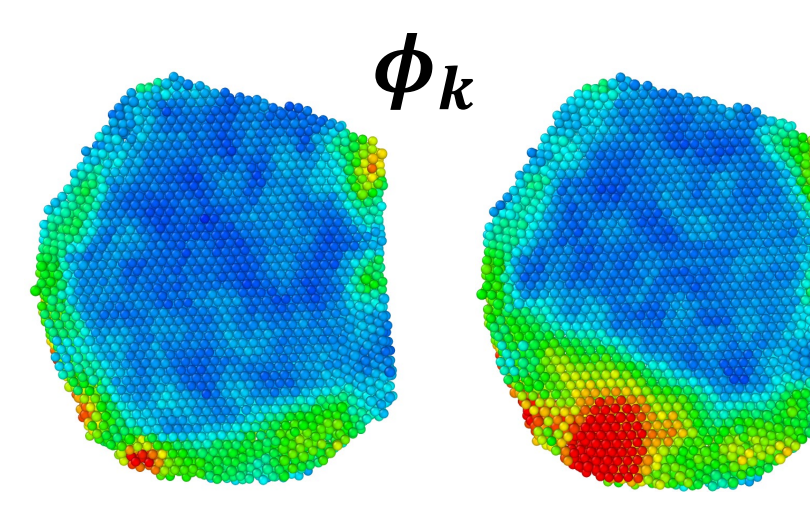
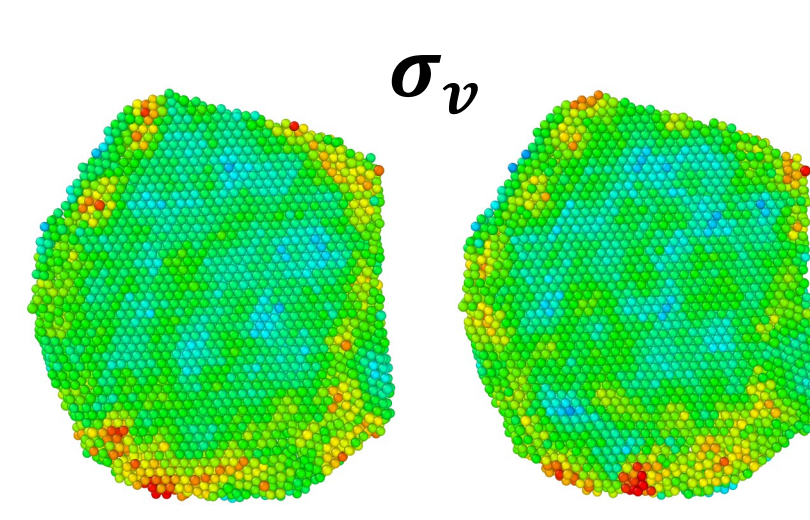
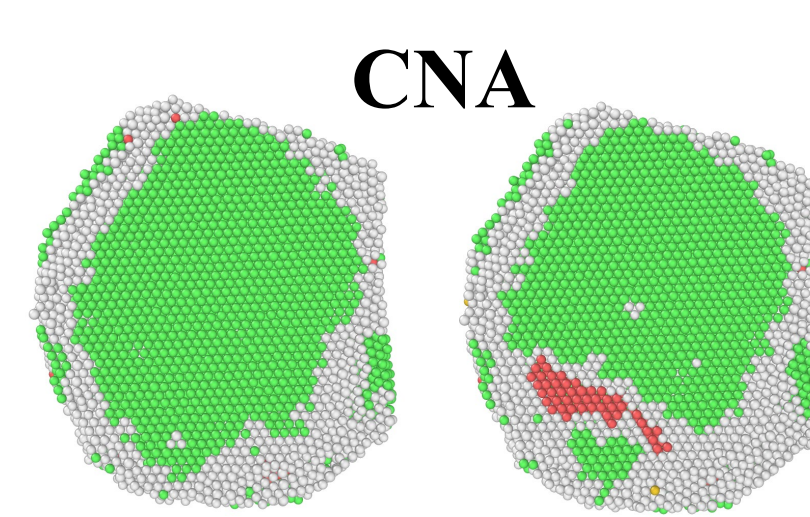
Strength scaling quantified from flow curves:



The peak difference in flow stress between the alloys occurs at the global composition where grain boundary segregation is maximized. This state corresponds to a minimum in the grain boundary energy and excess free volume, which manifests in the mechanical properties as a peak strength.

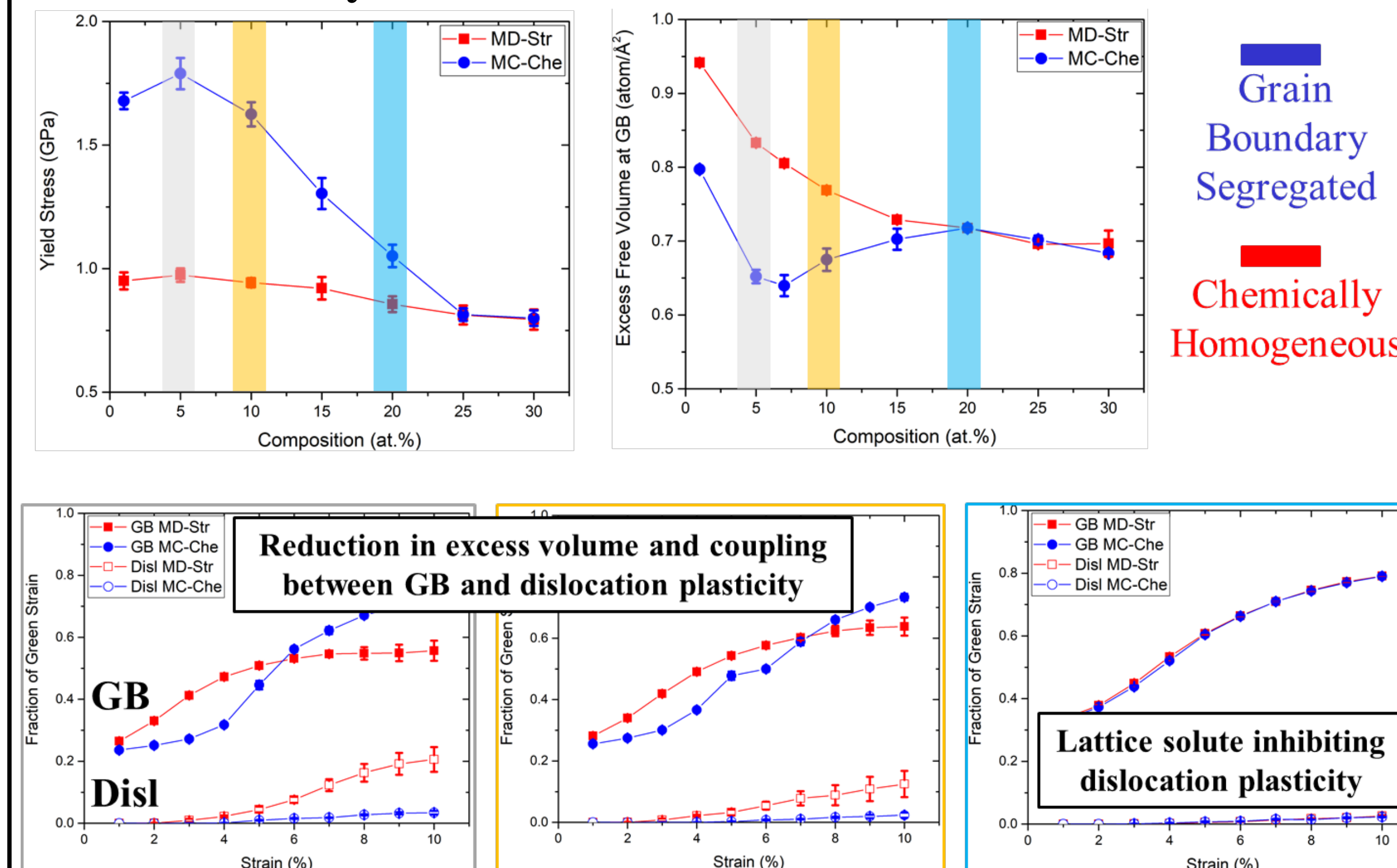
Analysis of dominant deformation mechanisms (coupling between GB and dislocation plasticity):

$\epsilon = 4.20\%$ $\epsilon = 4.26\%$



At low strains, microrotation in the *GB Segregated State* is reduce from the *Chemically Homogenous State*, indicating stabilization of the GBs.

Mechanistically indexed strain accommodation



Comparing trends for the same global composition, strain accommodation by the grain boundaries is suppressed by the segregation of Mg atoms.

A larger stress is required to nucleate dislocations at yielding, thus accounting for the strengthening effect.

At large strains, plastic strain is biased to the grain boundaries in the grain boundary segregated state.

Conclusions

- MD simulations of nanocrystalline Al-Mg alloys with various solute contents and grain sizes were performed to study the effect of grain boundary segregation on the mechanical properties.
- We find that the distribution of dopant atoms in the nanostructure is of significant importance for the strength of the alloys, and this new effect is denoted **grain boundary segregation strengthening**.
- Solute enrichment at grain boundaries reduces their energy and excess free volume, which in turn suppresses grain boundary plasticity via stabilization against local atomic shuffling and rearrangement in the grain boundaries. Stabilization of the grain boundaries delays the onset of dislocation nucleation with an attendant increase in the yield strength of the alloys, thereby providing mechanistic insights into this effect.

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