Optimization of Refractory High Entropy Alloy (RHEA) MoNbTaW via Molecular Dynamics Simulation

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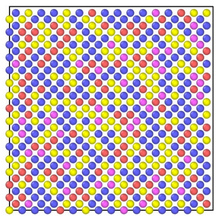
Motivation

High entropy alloys (HEA) are proposed to be the alloys of the future, being chemically complex with a high concentration spread of 4+ atoms that give them unique properties when compared to conventional alloy compositions. MoNbTaW is one of these HEAs comprised of refractory metals that can maintain adequate mechanical properties at extreme temperatures exceeding 1200°C. Application for this alloy would be in aircraft jet engines by taking advantage of its extreme temperature resistance, where those engines could be operated at much higher temperatures to improve efficiency. This then poses the question: what is the most optimized elemental concentration of MoNbTaW that has the greatest mechanical strength at extreme temperatures using molecular dynamics simulations? HEAs have a massive compositional space which culminate in many degrees of freedom, like controlling Nb for more lightness or increasing W for greater temperature resistance and strength. The main parameters that are being looked at are lattice distortion, diffuse anti-phase boundary energy (DAPBE), and stress. Lattice distortion is correlated to ductility which needs to be maximized due to the HEA being too brittle at room temperature. DAPBE is being calculated as it is an energy barrier to dislocation motion which will increase strength. Finally, stress will be analyzed to provide an initial look at the strength of the alloy as a perfect crystal.

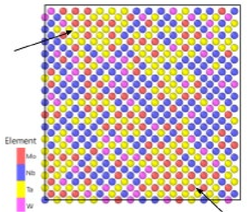
Research Method

To gain insight into possible compositions that fulfill the criteria, LAMMPS, a molecular dynamics program designed for modeling materials, was used to run simulations at the atomic scale to get quantitative answers. Over the course of the project, three main simulations were run: lattice relaxation for calculating lattice distortion, DAPBE as an estimation of an energy barrier, and simulated tensile testing for an approximation of strength. Chemical ordering tuning was also used to magnify its influence on lattice distortion and DAPBE. 84 different compositions were analyzed with 10% being the minimum composition percent for all elements.

Composition Labeling: Mo:Nb:Ta:W

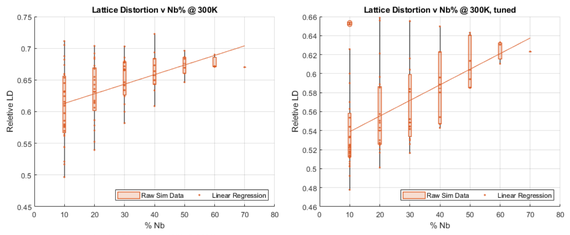


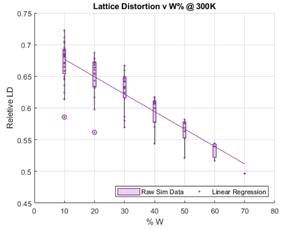
Left: A random structure tuned to optimized chemical order.
Right: Arrows point towards clusters of Mo and Ta in a presumed B2 structure.

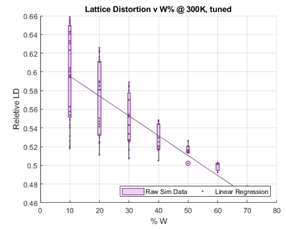


Current Results & Discussion

Lattice Distortion



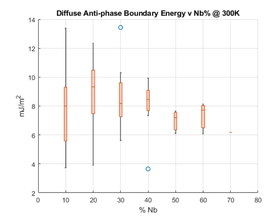


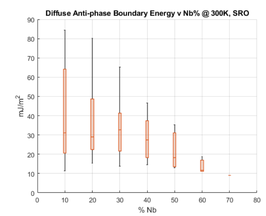


Lattice Distortion					
Random			Tuned for SRO		
Rank	Comp	Rele. LD	Rank	Comp	Rele. LD
1	20:40:30:10	0.7226	1	10:20:60:10	0.6587
2	20:10:60:10	0.7113	2	20:20:50:10	0.6559
3	30:10:50:10	0.7051	3	20:30:40:10	0.6553
4	20:20:50:10	0.7036	4	10:30:50:10	0.6551
...	...	...	...	...	...
81	10:20:10:60	0.5394	81	30:10:10:50	0.5021
82	30:10:10:50	0.5211	82	10:20:10:60	0.5012
83	20:10:10:60	0.5167	83	20:10:10:60	0.4923
84	10:10:10:70	0.4966	84	10:10:10:70	0.4777

The composition that showed the highest lattice distortion with a random structure is 20:40:30:10. When tuned, the 3rd highest composition of 20:30:40:10 is quite like the random structure. A high lattice distortion correlates to a more imperfect crystal, potentially enabling more elongation. Both compositions are most promising to have plasticity at room temperature.

DAPBE

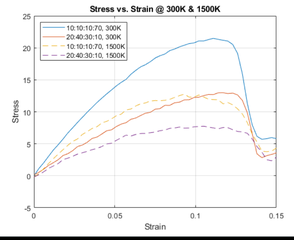




Diffuse Anti-Phase Boundary Energy					
Random			Tuned for SRO		
Rank	Comp	mJ/m^2	Rank	Comp	mJ/m^2
1	40:30:20:10	13.4355	1	40:10:40:10	84.4518
2	40:10:30:20	13.3984	2	40:10:30:10	82.6901
3	20:10:60:10	13.3330	3	30:10:40:20	80.1165
4	30:20:40:10	12.3383	4	30:10:40:20	79.3339
...	...	...	...	...	...
80	30:10:10:50	3.8997	75	10:60:10:20	11.7447
81	10:20:20:50	3.8912	76	10:10:10:70	11.3029
82	10:10:10:70	3.7434	77	10:60:20:10	11.0286
83	20:40:10:30	3.6529	78	10:70:10:10	8.9233

Tuning for short range order massively increased the energy barrier. This is most obviously seen in the composition 40:10:40:10 with mostly Mo and Ta, suggesting strong bonding between the elements.

Tensile Test

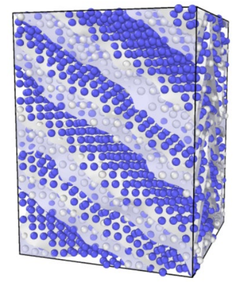


Ultimate Strength			
Comp	300K	1500K	% Retained
10:10:10:70	21.4805	12.7547	59.378041
20:30:40:10	13.1628	7.8548	59.674233
20:40:30:10	12.9873	7.7456	59.639802
20:50:20:10	12.9587	7.7738	59.989042

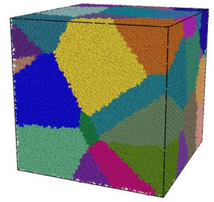
The low lattice distortion, high percent W shows the greater strength in comparison to the first ranking 20:40:30:10 composition. This suggests that with the system used for the simulation, the element with the strongest structure and bonds will also be the most resilient. Failure of the system appears to also occur at the same amount of strain for both temperatures.

Conclusions & What's Next

Lattice distortion and DAPBE both show compositions that are promising for further testing. In both cases, but more strongly for DAPOBE, there is a correlation between Mo and Ta and having a similar composition percent. This suggests the pair of elements have some mechanism that warrants them to bond together and the potential strength that may arise from that. The tensile test simulations also show that ~60% of room temperature strength is maintained at ~1200°C which proves the high temperature durability of the alloy. Molecular dynamics is not necessarily indicative of what is possible in the real world. A direct result of this are the tensile test results as perfect crystals were used; in reality, no metal alloy is a perfect crystal as many strengthening mechanisms are related to defects and polycrystallinity. Additionally, the time scale of molecular dynamics is immeasurably small in real life, which is an advantage in some situations, but for the tensile test simulations, it is a downside due to the system being elongated too quickly which does not allow certain defects from forming and acting a barrier to the strain. This is the main factor for why the 70% W composition shows a much higher stress value than 20:40:30:10. One final issue is the time needed for simulations to complete, for very large systems this can take days to weeks depending on the number of particles and the complexity of the simulation.



Above: Strained crystal showing twinning at slip system
Below: Generated polycrystalline system, ~400,000 atoms



Going forwards, more sophisticated simulations like screw/edge dislocation mobility and nano-indentation will be run on select compositions from the high-ranking lattice distortion and DAPBE lists to further understand dislocation behavior and insight into directly manipulating ductility.

Acknowledgements

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