Chemical order transitions within interfacial segregation zones in NbMoTaW

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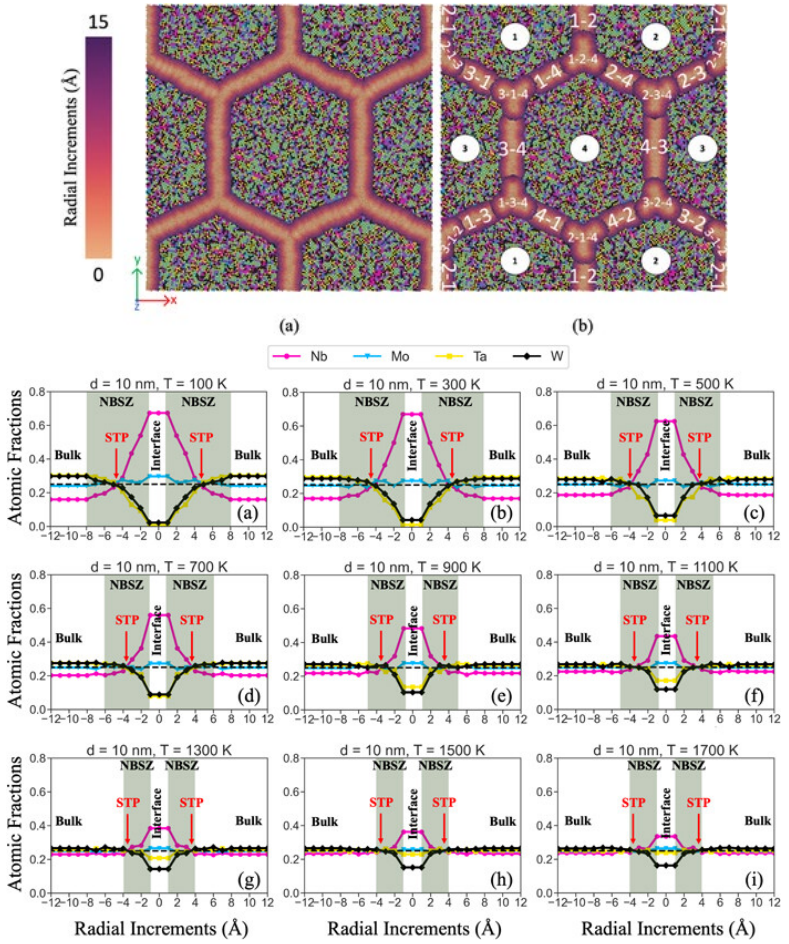
- The effect of chemical ordering with grain boundaries was investigated in a NbMoTaW refractory complex concentrated alloy (RCCA).
- Atomistic simulations were performed at 100 - 2000 K on hexagonal grain models of sizes of 5-20 nm. Interface regions were sliced and partitioned for investigation of near-boundary segregation and structural transitions with the boundaries.
- At the interface regions, heavy Nb enrichment and W and Ta depletion were observed. The near-boundary segregation zone and structural transitioning point width are dependent on grain size and temperature. The widths decrease as temperature increases up to the order-disorder transition temperature.
- The two most frequent cluster types, Nb-Nb and Mo-Ta exhibit opposite chemical short-range ordering (CSRO) behavior by displaying ordered-to-disordered and disordered-to-ordered transitions from interfaces to bulk, respectively.
- The findings demonstrate how different parameters such as grain size, temperature, and crystallographic orientation modify segregation both at and near the interfacial regions in refractory complex concentrated alloys with strong CSRO.



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