Supplementary Materials for

Construction and experimental validation of embedded potential functions for Ta-Re alloys

Figure S1

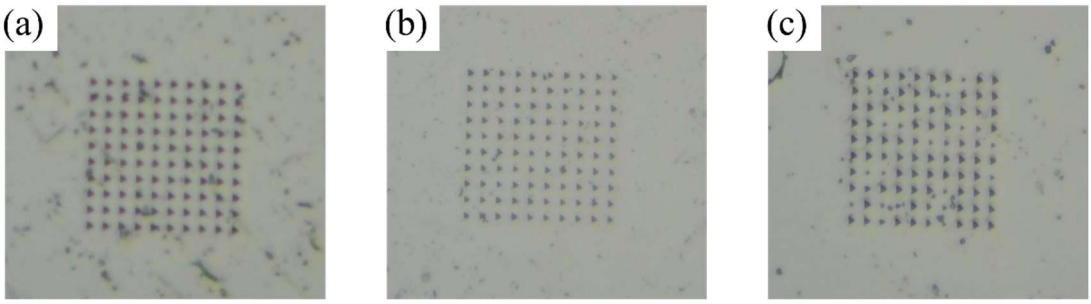

Figure S1. Dot plots for different Ta and Re content mass ratios (a)7.77:1; (b)1.21:1; (c)0.12:1

Below are the dot matrix data for different Ta and Re content mass ratios (a) 7.77:1; (b) 1.21:1; (c) 0.12:1

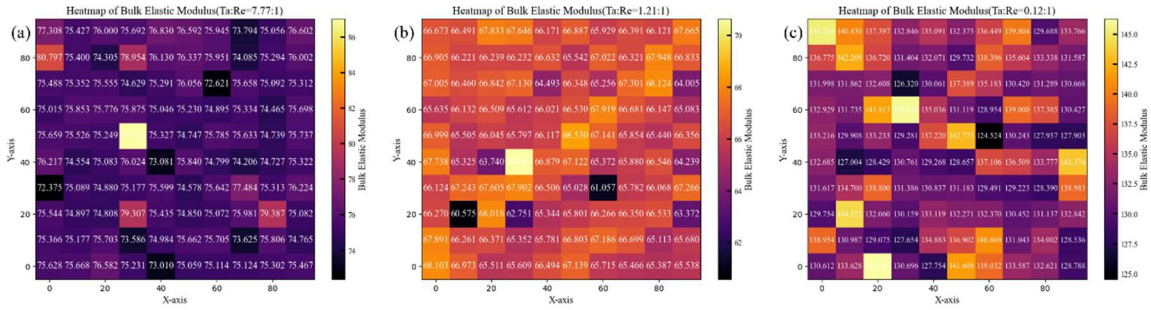

Figure S2

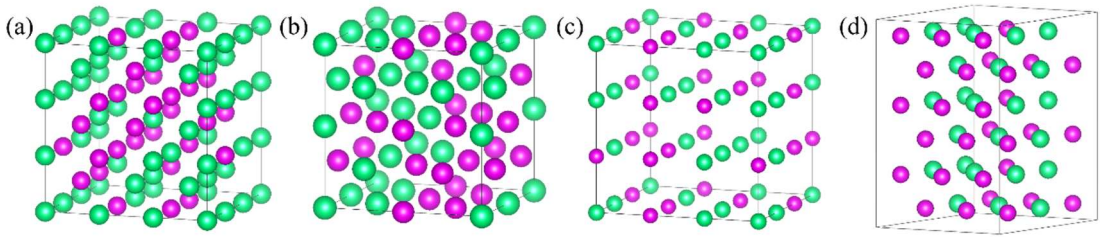

Figure S2. Perturbation structure: (a) bcc, (b) fcc, (c) sc, (d) hcp. Among them, green spheres represent Ta atoms, while purple spheres denote Re atoms.

Figure S3

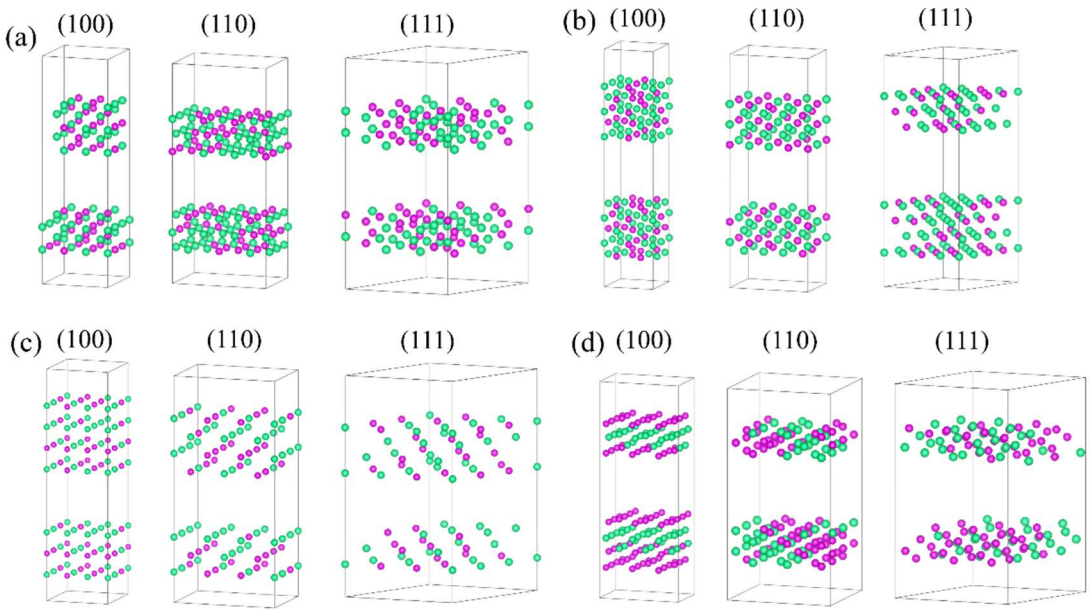

Figure S3. Low index surfaces of structures: (a) bcc, (b) fcc, (c) sc, (d) hcp. Among them, green spheres represent Ta atoms, while purple spheres denote Re atoms.

Figure S4

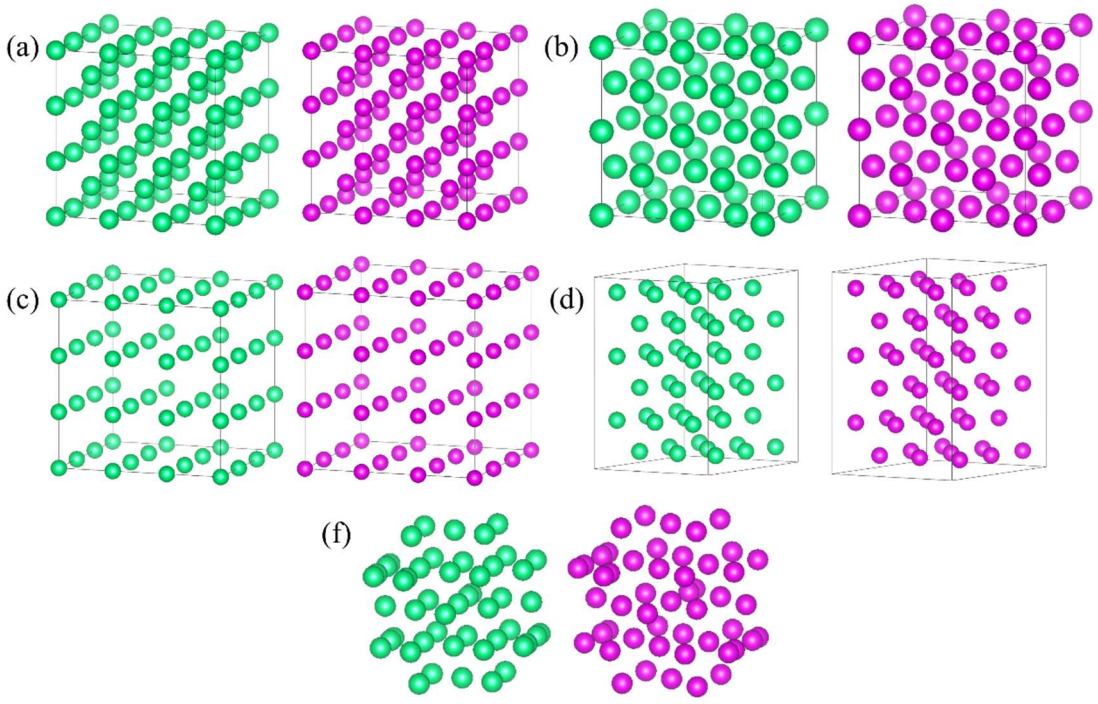

Figure S4. Pure tantalum and rhenium in various configurations: (a) bcc, (b) fcc, (c) sc, (d) hcp, (f) cluster. Among them, green spheres represent Ta atoms, while purple spheres denote Re atoms.