Supplementary Information for "Probing multi-dimensional composition spaces in search of strong metallic alloys"

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Supplementary Table 1: Plastic strength and specific plastic strength of component metals and alloys from the Fe-Ta-W ternary family predicted in MD simulations with the EAM potentials: σ in the 2nd column is the simulated strength of an elemental metal or a RCCA random solution alloy, σ_{A} in the 3d column is the simulated strength of the A-atom model of the same composition and σ_{V} in the 4th column is the V-baseline expectation for strength of the same alloy computed from strength values of its component metals. For pure metals $\sigma = \sigma_A = \sigma_V$ by definition. All strength values in columns 2-4 are given in GPa. Columns 5-7 contain specific strength (= simulated strength divided by mass density) of the same alloy compositions : γ in the 5th column is simulated specific strength of an elemental metal or a RCCA random solution alloy, γ_{A} in the 6th column is simulated strength predicted of the A-atom model of the same composition and γ_{V} in the 7th column is the V-baseline expectation for specific strength of the same alloy computed from specific strength values simulated for its component metals. For pure metals $\gamma = \gamma_A = \gamma_V$ by definition. All values of specific strength in columns 5-7 are given in GPa·cm^3/g.

Composition	σ	σ_{A}	σ_{V}	γ	γ_{A}	γ_{V}
Fe	1.59	-	-	0.22	-	-
Ta	1.83	-	-	0.11	-	-
W	4.19	-	-	0.22	-	-
FeTaW	4.42	1.89	2.54	0.29	0.12	0.18
$Fe_{25}Ta_{25}W_{50}$	4.69	2.33	2.95	0.29	0.14	0.19
$Fe_{27}Ta_{10}W_{63}$	5.21	2.77	3.25	0.32	0.17	0.21
$Fe_{35}W_{65}$	5.51	2.85	3.25	0.36	0.18	0.22
$Fe_{38}W_{62}$	**5.55**	2.77	3.20	0.35	0.18	0.22
$Fe_{52}W_{48}$	5.22	2.36	2.84	**0.38**	0.17	0.22

[1]Maximum values of simulated strength and simulated specific strength are shown in bold.

[2]Strength values listed above the upper dividing line are from five MD simulations performed prior to GPR-guided search. Strength values below the same line are from three MD simulations with compositions selected in a GPR-guided search for highest strength. Strength value below the lower dividing line is from an MD simulation with alloy composition selected in a GPR-guided search for highest specific strength. Two iterative GPR-guided searches - one for maximum strength and another for maximum specific strength - were conducted simultaneously and strength values computed in MD simulations were shared among two iteratively updated GPR models.

Supplementary Table 2: Plastic strength and specific plastic strength of component metals and alloys from the Nb-Mo-Ta-W quaternary family predicted in MD simulations with the EAM potentials. Columns and units are as described in caption for Table 1.

Composition	σ	σ_A	σ_V	γ	γ_A	γ_V
Nb	1.08	-	-	0.13	-	-
Ta	1.83	-	-	0.11	-	-
Mo	3.01	-	-	**0.30**	-	-
W	**4.19**	-	-	0.22	-	-
NbTa	1.54	1.11	1.46	0.12	0.09	0.12
NbMo	2.07	1.49	2.05	0.22	0.16	0.22
NbW	2.71	2.71	2.63	0.20	0.20	0.19
TaMo	2.35	1.93	2.42	0.17	0.14	0.18
TaW	2.95	2.40	3.01	0.17	0.13	0.17
MoW	3.60	3.53	3.60	0.25	0.24	0.25
NbTaMo	1.96	1.61	1.98	0.17	0.14	0.17
NbTaW	2.32	1.79	2.37	0.16	0.12	0.16
NbMoW	2.78	2.15	2.76	0.22	0.17	0.22
TaMoW	2.93	2.48	3.01	0.19	0.16	0.20
NbTaMoW	2.49	1.89	2.53	0.18	0.14	0.19

[1]Maximum values of simulated strength and simulated specific strength are shown in bold.

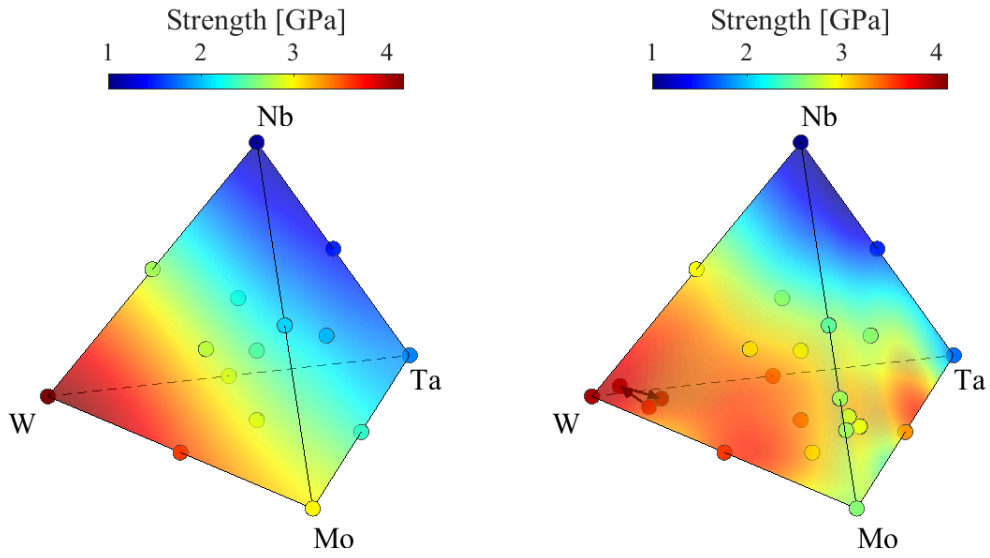
[2]Two GPR-guided searches - one for maximum strength and another for maximum specific strength - both converged in one iteration to pure W and pure Mo, respectively.

Supplementary Table 3: Plastic strength and specific plastic strength of component metals and alloys from the Nb-Mo-Ta-W quaternary family predicted in MD simulations with the SNAP potentials. A-models are not available for the SNAP potentials, otherwise columns and units are as described in caption for Table 1.

Composition	σ	σ_V	γ	γ_V
Nb	1.04	-	0.13	-
Ta	1.72	-	0.11	-
Mo	2.59	-	0.26	-
W	3.99	-	0.21	-
NbTa	1.51	1.38	0.13	0.12
NbMo	2.47	1.81	0.26	0.19
NbW	2.94	2.51	0.22	0.17
TaMo	3.26	2.15	0.25	0.19
TaW	3.55	2.85	0.20	0.16
MoW	3.54	3.29	0.25	0.24
NbTaMo	2.61	1.78	0.23	0.17
NbTaW	2.73	2.25	0.19	0.15
NbMoW	3.06	2.54	0.25	0.20
TaMoW	3.48	2.77	0.23	0.19
NbTaMoW	3.07	2.33	0.23	0.18
$Ta_7Mo_{12}W_{81}$	3.87	3.66	0.22	0.21
$Nb_3Ta_6W_{91}$	4.04	3.76	0.22	0.21
$Ta_{14}Mo_7W_{79}$	**4.07**	3.57	0.23	0.20
$Nb_8Ta_5Mo_{70}W_{17}$	3.10	2.66	0.27	0.24
$Nb_{17}Ta_{13}Mo_{70}$	2.88	2.21	0.28	0.22
$Nb_{23}Ta_5Mo_{72}$	2.83	2.19	0.29	0.22
$Nb_{30}Mo_{70}$	2.67	2.12	0.29	0.22
$Nb_{21}Mo_{79}$	2.68	2.25	**0.31**	0.23

[1]Maximum values of simulated strength and simulated specific strength are shown in bold.

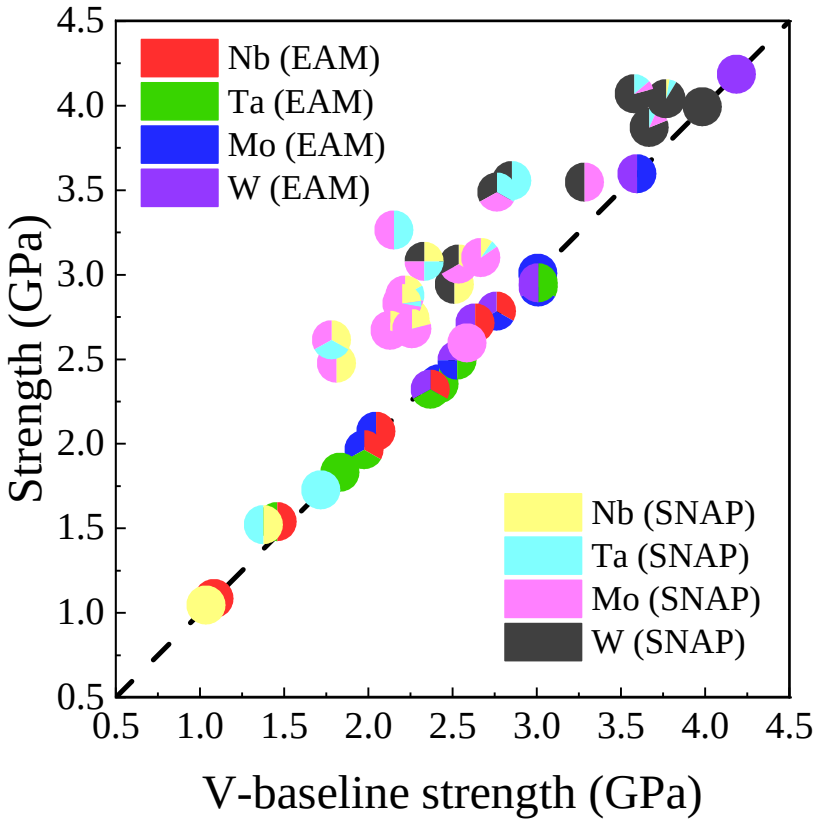
[2]Strength values listed above the upper dividing line are from fifteen MD simulations performed prior to GPR-guided search. Strength values below the same line are from three MD simulations with compositions selected in a GPR-guided search for highest strength. Strength values below the lower dividing line are from five MD simulations with alloy compositions selected in a GPR-guided search for highest specific strength. Two iterative GPR-guided searches - one for maximum strength and another for maximum specific strength - were conducted simultaneously and strength values computed in MD simulations were shared among two iteratively updated GPR models.



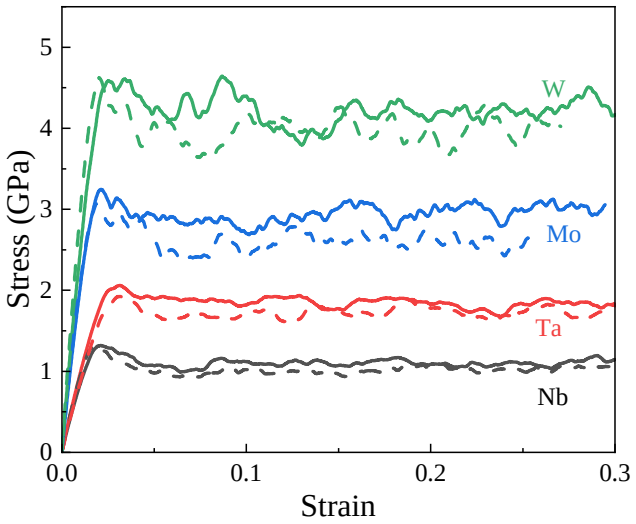
(a) Nb-Mo-Ta-W (EAM)

(b) Nb-Mo-Ta-W (SNAP)

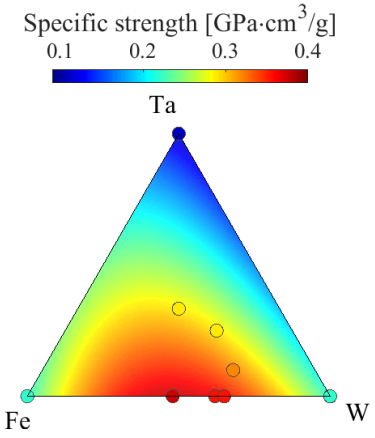
Supplementary Figure 1: Strength as a function of alloy composition predicted for Nb-Mo-Ta-W quaternary alloys. Dots mark compositions for which MD simulations where actually performed, whereas colors elsewhere on the tetrahedron faces show variations of strength predicted using a GPR surrogate model fitted to all simulated alloy compositions. (a) Strength variations predicted with the EAM potentials. (b) Strength variations predicted with the SNAP potentials. Arrows connect three alloy compositions selected for sampling during an iterative GPR-guided search.



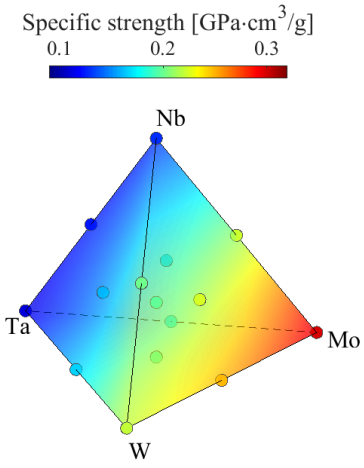
Supplementary Figure 2: Strength of elemental metals and alloys of the Nb-Ta-Mo-W quaternary family computed in MD simulations with EAM and SNAP potentials. The legends show colors assigned to elemental metals in the pies. Pie symbols above the dashed line correspond to model alloys exhibiting cocktail strengthening with respect to V-baseline.



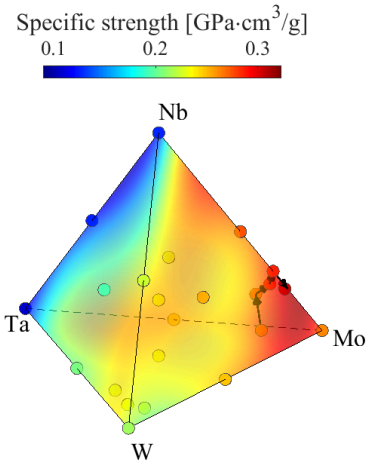
Supplementary Figure 3: Stress-strain curves extracted from MD simulations of component metals of the Nb-Ta-Mo-W quaternary family of alloys. Solid lines are from MD simulations with the EAM potentials and dashed lines are from MD simulations with the SNAP potentials. Element symbols are placed next to the corresponding stress-strain curves in matching colors.



(a) Fe-Ta-W (EAM)

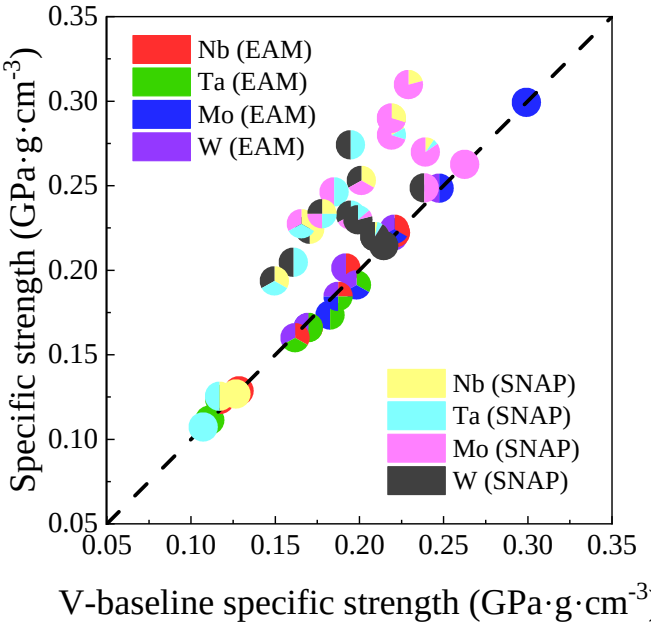


(b) Nb-Mo-Ta-W (EAM)



(c) Nb-Mo-Ta-W (SNAP)

Supplementary Figure 4: Specific plastic strength as a function of alloy composition predicted in MD simulations of elemental metals and alloys. Dots mark compositions for which MD simulations where actually performed, whereas colors elsewhere within the triangle and on the tetrahedron faces show variations of strength predicted using a GPR surrogate model fitted to all simulated alloy compositions. Colors are as shown in the color maps at the top. (a) Variations of specific strength predicted for the Fe-Ta-W ternary alloys simulated using the EAM potentials. (b) Variations of specific strength predicted for the Nb-Ta-Mo-W quaternary alloys simulated using the EAM potentials. (c) Variations of specific strength predicted for the Nb-Ta-Mo-W quaternary alloys simulated using the SNAP potentials. Arrows connect five alloy compositions selected for sampling during an iterative GPR-guided search.



Supplementary Figure 5: Specific plastic strength of elemental metals and alloys of the Nb-Ta-Mo-W quaternary family computed in MD simulations with EAM and SNAP potentials. The legends show colors assigned to elemental metals in the pies. Pie symbols above the dashed line correspond to model alloys exhibiting cocktail strengthening with respect to V-baseline.