

Table A.1: Mechanical properties of 12 MPEAs from MS calculations. Lattice distortion coefficient: δ ; Lattice parameter (\AA): a_0 ; Elastic constants (GPa): C_{11} , C_{12} , C_{44} ; Zener ratio: A_c ; Cohesive energy (eV): E_{coh} ; Unstable stacking fault energy (mJ/m^2): $\gamma_{\text{usf}}^{110}$, $\gamma_{\text{usf}}^{112}$, $\gamma_{\text{usf}}^{123}$. Ideal shear strength (GPa): τ_{ISS}^{110} , τ_{ISS}^{112} , τ_{ISS}^{123} .

Composition	Values													
	δ	a_0	C_{11}	C_{12}	C_{44}	A_c	E_{coh}	$\gamma_{\text{usf}}^{110}$	$\gamma_{\text{usf}}^{112}$	$\gamma_{\text{usf}}^{123}$	τ_{ISS}^{110}	τ_{ISS}^{112}	τ_{ISS}^{123}	
NbTaTi	0.0126	3.295	196.24	124.39	66.37	1.85	-6.76	559.34	645.25	635.36	6.99	8.13	7.99	
MoNbTi	0.0282	3.233	241.38	133.00	76.32	1.41	-6.43	742.35	857.21	845.89	7.44	8.38	8.32	
HfNbTa	0.0371	3.383	201.27	132.08	68.54	1.98	-7.39	647.42	758.90	745.44	7.51	8.86	8.72	
NbTiZr	0.0429	3.391	143.32	110.55	56.85	3.47	-6.31	459.61	537.78	529.89	5.17	6.03	5.95	
HfNbTi	0.0400	3.386	146.02	115.97	65.41	4.35	-6.29	474.26	566.09	556.67	5.35	6.35	6.25	
HfTaTi	0.0356	3.381	154.69	119.64	82.03	4.68	-6.45	511.04	610.78	599.62	5.81	7.03	6.93	
TaTiZr	0.0387	3.385	153.52	116.17	71.84	3.85	-6.46	494.45	579.18	569.42	5.57	6.60	6.53	
MoTaTi	0.0254	3.240	234.35	140.46	92.70	1.97	-6.59	786.30	910.26	897.48	8.45	9.87	9.76	
MoNbTa	0.0260	3.243	308.55	158.28	76.84	1.02	-7.57	877.23	1016.40	1000.05	9.31	10.63	10.48	
HfNbTaTi	0.0354	3.361	175.31	123.25	70.57	2.71	-6.73	553.96	653.34	641.87	6.46	7.62	7.53	
HfMoNbTaTi	0.0374	3.310	205.97	141.21	82.20	2.54	-6.82	666.67	782.60	769.12	7.38	8.67	8.55	
HfNbTaTiZr	0.0420	3.405	157.62	118.17	67.61	3.43	-6.69	522.79	615.94	605.31	5.82	6.88	6.80	

Table A.2: The LSR values (MPa) of edge and screw dislocations on the {110}, {112}, and {123} planes for 12 MPEAs from MS calculations.

Composition	Values											
	σ_e^{110}	σ_s^{110}	σ_e^{112}	σ_s^{112}	σ_e^{123}	σ_s^{123}	$\frac{\sigma_e^{110}}{\sigma_e^{123}}$	$\frac{\sigma_s^{110}}{\sigma_s^{123}}$	$\frac{\sigma_e^{112}}{\sigma_e^{123}}$	$\frac{\sigma_s^{112}}{\sigma_s^{123}}$	$\frac{\sigma_e^{110}}{\sigma_e^{112}}$	$\frac{\sigma_s^{110}}{\sigma_s^{112}}$
NbTaTi	443.03	1731.11	514.18	1616.89	340.94	1737.92	3.91	3.14	5.10	0.86	1.07	1.30
MoNbTi	797.49	2016.97	1085.82	1634.26	795.84	1776.54	2.53	1.51	2.23	0.73	1.23	1.00
HfNbTa	777.59	1394.83	708.49	1104.07	592.07	1032.13	1.79	1.56	1.74	1.10	1.26	1.31
NbTiZr	956.74	1226.94	556.23	877.68	344.02	811.20	1.28	1.58	2.36	1.72	1.40	2.78
HfNbTi	617.74	1021.31	590.82	994.67	413.33	674.14	1.65	1.68	1.63	1.05	1.03	1.49
HfTaTi	857.43	1013.25	758.30	1012.44	549.66	740.18	1.18	1.34	1.35	1.13	1.00	1.56
TaTiZr	1138.82	1414.79	732.28	1098.29	474.18	842.95	1.24	1.50	1.78	1.56	1.29	2.40
MoTaTi	922.53	1975.66	1185.92	1686.38	736.58	1742.48	2.14	1.42	2.37	0.78	1.17	1.25
MoNbTa	949.41	2320.54	1303.57	1645.52	798.93	1977.64	2.44	1.26	2.48	0.73	1.41	1.19
HfNbTaTi	884.90	1155.84	637.74	1062.53	624.89	1220.25	1.31	1.67	1.95	1.39	1.09	1.42
HfMoNbTaTi	1543.22	2017.60	878.73	1772.92	772.36	1395.88	1.31	2.02	1.81	1.76	1.14	2.00
HfNbTaTiZr	923.91	1084.82	659.58	1021.67	458.90	782.21	1.17	1.55	1.70	1.40	1.06	2.01