Supplementary information for machine learning enhanced empirical potentials for metals and alloys

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TABLE I. Model parameters of the $\rho(r)$, $\phi(r)$ and $F(\rho)$ functions of elementary Ni and Mo. 'Zjw04' denotes the original parameters published by Zhou et al.

Parameter	Ni		Mo		
	Zjw04	ML-EAM	Zjw04	ML-EAM	ML-ADP
r_e	2.488746	2.184066	2.728100	2.7281	2.7281
f_e	2.007018	2.534902	2.723710	3.4736385	3.5863051
ρ_e	27.562015	27.242392	29.354065	36.638607	37.623623
ρ_s	27.930410	28.503098	29.354065	23.207705	22.683228
α	8.383453	8.808985	8.393531	7.3310647	7.6616936
β	4.471175	2.875468	4.476550	4.783378	5.5784864
A	0.429046	0.693091	0.708787	0.9908045	0.9215712
B	0.633531	0.624794	1.120373	1.8643652	1.7317773
κ	0.443599	0.591682	0.137640	0.16669716	0.1413604
λ	0.820658	1.102230	0.275280	0.22740759	0.24908023
F_{n0}	-2.693513	-3.785397	-3.692913	-6.025855	-6.270608
F_{n1}	-0.076445	-0.123840	-0.178812	2.4391363	2.2659059
F_{n2}	0.241442	-2.315715	0.380450	-0.20683534	-0.18881902
F_{n3}	-2.375626	-9.106957	-3.133650	-3.3985534	-3.2595265
F_0	-2.70	-3.727002	-3.71	-5.551877	-5.8015256
F_1	0	0.316349	0	3.2580216	3.2561238
F_2	0.265390	0.740672	0.875874	0.82902724	1.1035414
F_3	-0.1528856	0.936249	0.776222	-0.003057075	-0.95508283
η	0.469000	0.950386	0.790879	0.81461126	0.7645085
F_e	-2.699486	-3.638958	-3.712093	-6.0208893	-6.360732

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TABLE II. Model parameters of the $\mu(r)$ and $\omega(r)$ functions of the elementary Mo ML-ADP.

Parameter	ML-ADP
d_1	-0.10194129
d_2	-2.098797
d_3	6.1936436
q_1	0.08105006
q_2	-1.6661074
q_3	-9.597149
r_c	4.4990587
h	6.757866

APPENDIX

A. Elementary Ni and Mo

Table I summarizes the model parameters of $\rho(r)$, $\phi(r)$ and $F(\rho)$ functions of the original Zjw04 EAM, ML-EAM and ML-ADP of elementary Ni and Mo.

Table II summarizes the model parameters of $\mu(r)$ and $\omega(r)$ for the elementary Mo ML-ADP.

B. Binary Mo-Ni

Table III summarizes the model parameters of $\rho(r)$, $\phi(r)$ and $F(\rho)$ functions of ML-EAM and ML-ADP. One should note that the pairwise interaction of Mo-Ni in our tests are also described by the following function:

$$\phi(r)^{\text{MoNi}} = \frac{A \exp\left[-\alpha\left(r/r_e - 1\right)\right]}{1 + \left(r/r_e - \kappa\right)^{20}} - \frac{B \exp\left[-\beta\left(r/r_e - 1\right)\right]}{1 + \left(r/r_e - \lambda\right)^{20}} \tag{1}$$

Table IV summarizes the model parameters of $\mu(r)$ and $\omega(r)$ functions of ML-ADP. h and r_c of each type (Ni-Ni, Mo-Mo, Mo-Ni) are shared by the corresponding $\mu(r)$ and $\omega(r)$.

TABLE III. Model parameters of the $\rho(r)$, $\phi(r)$ and $F(\rho)$ functions of the binary Mo-Ni.

Parameter	Ni-Ni		Mo-Mo		Mo-Ni	
	ML-EAM	ML-ADP	ML-EAM	ML-ADP	ML-EAM	ML-ADP
r_e	2.488746	2.488746	2.728100	2.728100	2.248422	2.236042
f_e	1.573611	1.493597	3.293607	3.100258		
ρ_e	26.041567	22.907389	32.334946	32.181946		
ρ_s	27.513889	23.965549	21.431379	26.999769		
α	8.357251	7.890068	7.578850	7.282433	9.165461	8.311396
β	3.262010	3.530539	5.271230	6.306448	3.448286	3.984799
A	0.341653	0.376238	1.082262	1.217825	0.920266	1.378780
B	0.590183	0.551236	1.795642	1.890288	1.353243	1.595449
κ	0.419685	0.389896	0.146541	0.139798	0.477891	0.682473
λ	0.861396	0.856361	0.211250	0.451321	0.426472	0.840181
F_{n0}	-3.276638	-3.882192	-6.873109	-6.547637		
F_{n1}	0.065121	-0.385112	1.600031	1.067100		
F_{n2}	-2.030634	-1.666104	0.328615	-0.091667		
F_{n3}	-7.037966	-7.832167	-2.389441	-2.622464		
F_0	-3.208834	-3.890994	-6.542728	-6.249061		
F_1	0.418720	-0.068532	2.241790	2.177628		
F_2	0.562025	0.839004	0.663757	1.889595		
F_3	-2.041830	0.106350	-4.500637	-3.193933		
η	1.260760	0.844734	0.667079	1.021184		
F_e	-3.110896	-3.896700	-6.763651	-6.256578		

TABLE IV. Model parameters of the $\mu(r)$ and $\omega(r)$ functions of the binary Mo-Ni ML-ADP.

Parameter	Ni-Ni	Mo-Mo	Mo-Ni
d_1	-23.871168	11.369281	0.212463
d_2	1.598995	0.526101	-1.505769
d_3	0.698707	-2.479640	-4.198265
q_1	8.238647	6.791066	6.186455
q_2	0.482742	0.465529	-6.073431
q_3	-2.888822	-1.810418	-4.659296
r_c	5.436740	5.301004	2.200823
h	5.642247	3.834129	5.152708