Table S1. Properties of Al reproduced by different interatomic potentials: lattice constant a_0 and c_0, cohesive energy E_c, bulk modulus B_0, elastic constants C_{ij} and melting point T_m The symbol of *ab* indicates that the data is calculated by first principle calculations in this work.

		Exp	Y22	P15 [65]	W09 [66]	Z09 [67]	M08 [68]	L04 [69]	Z04 [70]	L03 [71]	Z03 [72]	S00 [73]
			eam/fs	meam	eam/alloy	eam/alloy	eam/fs	eam/alloy	eam/alloy	meam	eam/alloy	eam/fs
fcc-Al	a_0 (Å)	4.0496 [33]	4.0497	4.0500	4.0248	4.0320	4.0453	4.0320	4.0502	4.0447	4.0500	4.0500
	E_c (eV)	3.3900 [34]	3.3896	3.3600	2.6460	3.3607	3.4107	3.3600	3.5800	3.3600	3.3600	3.3900
	B_0 (GPa)	72.2 [34]	72.2	78.9	79.1	81.6	74.7	81.6	76.0	79.4	79.0	77.0
	C_{11} (GPa)	106.8 [33]	83.1	96.9	113.8	105.1	105.1	118.9	107.0	114.3	116.8	94.6
	C_{12} (GPa)	60.4 [33]	66.7	69.9	61.7	69.8	59.5	62.9	60.5	61.9	60.1	68.2
	C_{44} (GPa)	28.3 [33]	29.1	31.3	31.2	44.1	30.7	33.0	28.3	31.6	31.7	42.5
	T_m (K)	933.5 [75]	740±1	794±1	823±1	930±1	908±1	845±1	566±1	913±1	849±1	908±1
bcc-Al	a_0 (Å)	3.2347[ab]	3.2151	3.3193	3.2238	3.1957	3.2384	3.1305	3.3100	3.2269	3.2355	3.2081
	E_c (eV)	3.2929[ab]	3.3748	3.2778	2.5165	3.3256	3.3088	3.2758	3.5463	3.2417	3.2674	3.3558
	B_0 (GPa)	68.4[ab]	70.7	47.6	39.2	76.4	39.3	94.6	72.3	75.4	52.9	67.5
	C_{11} (GPa)	41.3[ab]	70.6	-10.5	-8.2	70.9	12.9	120.7	71.4	26.0	20.9	54.4
	C_{12} (GPa)	81.9[ab]	70.8	76.7	62.9	79.2	52.5	81.6	72.8	100.2	68.9	74.0

		ref										
	C_{44} (GPa)	41.3[ab]	33.2	13.7	27.6	53.2	18.8	67.1	30.0	31.2	38.0	47.3
hcp-Al	a_0 (Å)	2.8514[ab]	2.8495	2.8348	2.8252	2.8490	2.8451	2.8220	2.8312	2.8326	2.8357	2.8631
	c_0 (Å)	4.7273[ab]	4.7241	4.8186	4.7479	4.6550	4.7462	4.8931	4.8933	4.7946	4.8983	4.6805
	E_c (eV)	3.3570[ab]	3.3890	3.3291	2.6159	3.3572	3.3831	3.3363	3.5788	3.3305	3.3384	3.3853
	B_0 (GPa)	74.4[ab]	72.0	72.0	64.9	79.6	69.3	85.4	82.9	77.9	72.3	72.2
	C_{11} (GPa)	106.1[ab]	97.6	117.4	98.7	125.5	117.2	146.2	131.4	128.8	116.9	114.4
	C_{12} (GPa)	67.8[ab]	66.2	49.3	48.0	68.0	60.4	72.0	71.4	60.0	60.9	66.5
	C_{44} (GPa)	6.5[ab]	15.0	21.1	17.3	24.2	12.8	19.3	16.2	26.8	13.4	18.2

Table S2. Properties of Ni reproduced by different interatomic potentials.

		Exp or cal	Y22	E18 [76]	S16 [77]	A15 [78]	M12 [79]	Z04 [80]	L03 [81]
			eam/fs	meam	eam/alloy	meam	eam/fs	eam/alloy	meam
fcc-Ni	a_0 (Å)	3.5240 [34]	3.5229	3.5214	3.5200	3.5214	3.5181	3.5197	3.5214
	E_c (eV)	4.4400 [74]	4.4385	4.4500	4.4500	4.4500	4.3855	4.4500	4.4500
	B_0 (GPa)	186.0 [74]	189.6	187.6	180.6	187.6	180.5	180.6	187.6
	C_{11} (GPa)	248.1 [34]	242.5	270.8	240.9	261.7	247.0	247.0	261.2
	C_{12} (GPa)	154.9 [34]	163.1	146.0	150.5	150.5	147.3	147.3	150.8
	C_{44} (GPa)	124.2 [34]	123.4	132.5	127.1	131.7	122.8	124.9	131.7
	T_m (K)	1728.3 [75]	1753±1	2064±1	1636±1	1984±1	1709±1	1480±1	2164±1
bcc-Ni	a_0 (Å)	2.7893[ab]	2.8052	2.80676	2.7687	2.7868	2.7570	2.8061	2.7945
	E_c (eV)	4.3873[ab]	4.3912	4.37218	4.3827	4.2786	4.2945	4.3671	4.2893
	B_0 (GPa)	200.9[ab]	177.4	245.1	148.9	184.3	93.5	89.1	181.0
	C_{11} (GPa)	178.5[ab]	162.7	282.8	141.9	89.0	100.3	40.6	89.0
	C_{12} (GPa)	212.0[ab]	184.8	226.2	152.5	231.9	90.0	113.4	227.0
	C_{44} (GPa)	147.6[ab]	121.0	229.1	127.3	156.4	83.1	91.8	158.5
hcp-Ni	a_0 (Å)	2.4713[ab]	2.4835	2.48607	2.4819	2.4844	2.4859	2.4829	2.4844
	c_0 (Å)	4.0915[ab]	4.0928	4.08227	4.1048	4.0914	4.1204	4.1168	4.0914
	E_c (eV)	4.4141[ab]	4.4379	4.43858	4.4279	4.4293	4.3534	4.4339	4.4293
	B_0 (GPa)	203.2[ab]	189.6	187.0	159.4	186.5	136.8	159.8	186.4
	C_{11} (GPa)	300.5[ab]	303.1	329.1	298.5	332.0	267.0	302.6	332.7
	C_{12} (GPa)	180.1[ab]	158.4	140.1	145.2	138.4	134.2	138.1	139.0
	C_{44} (GPa)	48.9[ab]	67.6	76.6	48.6	75.7	39.0	55.6	75.0

Table S3. Properties of Ti reproduced by different interatomic potentials.

		Exp or cal	Y22	M16_1 [82]	M16_2 [83]	M16_3 [83]	H08 [84]	K06 [85]	Z04 [70]
			eam/fs	eam/fs	eam/fs	eam/fs	meam/spline	meam	eam/alloy
hcp-Ti	a_0 (Å)	2.9506 [34]	2.9494	2.9465	2.9487	2.9507	2.9305	2.9453	2.9405
	c_0 (Å)	4.6835 [34]	4.6816	4.7043	4.6983	4.6879	4.6783	4.6874	4.7721
	E_c (eV)	4.8500 [74]	4.8456	5.3455	5.2465	5.4017	4.8312	4.8727	4.8700
	B_0 (GPa)	105.1 [74]	106.4	110.5	100.4	111.2	112.8	109.7	105.9
	C_{11} (GPa)	162.4 [74]	131.2	160.8	160.2	164.8	174.2	170.0	148.5
	C_{12} (GPa)	92.0 [34]	94.0	80.3	69.6	87.8	94.7	80.4	88.4
	C_{44} (GPa)	46.7 [34]	61.9	52.6	54.3	57.7	57.7	42.1	36.8
	T_m (K)	1941.0 [75]	1552±1	1750±1	1233±1	1200±10	1803±1	1638±1	1480±1
bcc-Ti	a_0 (Å)	3.2455[ab]	3.2822	3.2513	3.2563	3.2422	3.2716	3.2661	3.2919
	E_c (eV)	4.7379[ab]	4.8150	5.3162	5.1726	5.3130	4.7201	4.8489	4.8502
	B_0 (GPa)	109.6[ab]	102.1	307.6	414.7	255.2	105.6	113.9	112.9
	C_{11} (GPa)	98.6[ab]	81.8	308.8	394.2	236.6	94.9	129.7	120.4
	C_{12} (GPa)	115.0[ab]	112.2	306.9	425.0	264.5	111.0	105.9	109.2
	C_{44} (GPa)	45.4[ab]	97.8	28.6	21.9	33.9	52.9	78.1	77.3
fcc-Ti	a_0 (Å)	4.0972[ab]	4.1313	4.1820	4.2133	4.1313	4.1467	4.1330	4.1491
	E_c (eV)	4.7919[ab]	4.8484	5.2867	5.1947	5.3488	4.7925	4.8245	4.8637
	B_0 (GPa)	111.5[ab]	106.2	6.5	78.7	95.4	97.6	108.6	-1444.7
	C_{11} (GPa)	140.0[ab]	169.8	106.8	121.4	91.4	125.8	148.4	-6846.5
	C_{12} (GPa)	97.2[ab]	74.5	-43.7	57.3	97.4	83.5	88.7	-161.0
	C_{44} (GPa)	59.2[ab]	33.8	43.6	62.5	60.1	58.7	62.6	57.3

Table S4. Properties of Al-Ni reproduced by different interatomic potentials.

		Exp or Cal	Y22	M22 [83]	P09 [84]	S07 [85]	M04 [86]	M02 [35]
			eam/fs	meam	eam/alloy	meam	eam/alloy	eam/alloy
D0$_{11}$-Al$_3$Ni	a_0 (Å)	6.598 [87]	6.559	7.089	6.645	6.622	6.665	6.625
	b_0 (Å)	7.352 [87]	7.307	7.898	7.403	7.378	7.426	7.381
	c_0 (Å)	4.801 [87]	4.772	5.158	4.835	4.818	4.850	4.820
	E_f (eV)	-0.421[ab]	-0.428	0.234	-0.239	-0.255	-0.241	-0.265
	B_0 (GPa)	113.1[ab]	92.6	79.534	119.3	101.6	115.8	117.7
B2-AlNi	a_0 (Å)	2.880 [37]	2.842	3.170	2.832	2.877	2.862	2.859
	E_f (eV)	-0.688[ab]	-0.683	0.266	-0.606	-0.626	-0.590	-0.533
	B_0 (GPa)	160.4[ab]	160.2	127.9	158.9	158.0	236.7	159.7
L1$_2$-AlNi$_3$	a_0 (Å)	3.572 [88]	3.510	3.829	3.533	3.570	3.571	3.526
	E_f (eV)	-0.469[ab]	-0.506	0.151	-0.454	-0.437	-0.448	-0.383
	B_0 (GPa)	183.0[ab]	191.7	162.2	190.3	181.9	181.5	247.3

Table S5. Properties of Al-Ti reproduced by different interatomic potentials.

		Exp or Cal	Y22	K16 [38]	Z03 [72]
			eam/fs	meam	eam/alloy
D0$_{22}$-Al$_3$Ti	a_0 (Å)	3.854 [39]	3.855	3.897	3.929
	c_0 (Å)	8.584 [39]	8.586	8.681	8.752
	E_f (eV)	-0.379 [40]	-0.361	-0.284	-0.263
	B_0 (GPa)	103.0 [47]	116.0	126.8	114.7
L1$_0$-AlTi	a_0 (Å)	2.832 [90]	2.821	2.846	2.856
	c_0 (Å)	4.070 [90]	4.054	4.090	4.105
	E_f (eV)	-0.416 [40]	-0.406	-0.386	-0.401
	B_0 (GPa)	112.1 [89]	136.8	142.7	141.7
D0$_{19}$-AlTi$_3$	a_0 (Å)	5.780 [49]	5.765	5.799	5.827
	c_0 (Å)	4.647 [49]	4.635	4.663	4.685
	E_f (eV)	-0.259 [40]	-0.292	-0.281	-0.287
	B_0 (GPa)	111.9 [89]	112.1	135.6	122.1

Table S6. Properties of Ni-Ti reproduced by different interatomic potentials.

		Exp or Cal	Y22	K19 [90]	K17 [49]	K15 [41]
			eam/fs	meam	meam	meam
$hP16$-Ni$_3$Ti	a_0 (Å)	5.096 [45]	5.103	5.177	5.091	5.165
	c_0 (Å)	8.304 [45]	8.315	8.436	8.295	8.416
	E_f (eV)	-0.360 [48]	-0.381	-0.275	-0.329	-0.329
	B_0 (GPa)	163.4 [42]	130.8	157.5	166.9	152.2
B2-NiTi	a_0 (Å)	3.007 [46]	2.962	3.017	2.968	3.011
	E_f (eV)	-0.351 [43]	-0.358	-0.342	-0.351	-0.357
	B_0 (GPa)	142.0 [48]	123.4	137.3	142.0	129.0
$cF96$-NiTi$_2$	a_0 (Å)	11.278 [50]	11.310	11.260	11.204	11.249
	E_f (eV)	-0.278 [48]	-0.312	-0.278	-0.264	-0.300
	B_0 (GPa)	119.8 [41]	83.4	124.4	126.3	116.1

Table S7. Properties of Al-Ni-Ti reproduced by different interatomic potentials.

		Exp or Cal	Y22	K17 [35]
		eam/fs	meam	eam/fs
$cF16$-AlNi$_2$Ti	a_0 (Å)	5.889 [43]	5.821	6.22334
	E_f (eV)	-0.620 [43]	-0.529	0.0492
	B_0 (GPa)	162.0 [43]	148.8	168.684
$cF116$-Al$_{16}$Ni$_7$Ti$_6$	a_0 (Å)	11.802 [44]	12.086	11.4433
	E_f (eV)	-0.560 [44]	-0.497	-0.8633
	B_0 (GPa)	130.0 [44]	78.7	139.379

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