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Electron Work Function: A Novel Probe for Toughness

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Table I Calculated lattice constants, elastic constants, bulk modulus (B), shear modulus (G), Young modulus (E)

	Lattice Constants(**Error!**)		Elastic Constants and Modulus (GPa)							
	a	c	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	B	G	E
Be	2.257	3.563	320.6	22.5	14.8	378.6	163.7	124.6	159.5	335.3
	2.286[a]	3.585[a]	292.3[a]	26.7[a]	14.0[a]	336.4[a]	162.5[a]	100[b]		303[c]
Mg	3.195	5.2	68.1	21.3	19.9	61.9	12.6	35.5	18.1	46.4
	3.209[a]	5.211[a]	59.50[a]	26.12[a]	21.80[a]	61.55[a]	16.35[a]	35.4[b]		44[c]
Sc	3.309	5.253	102.7	27.8	26.3	100.9	31.1	51.9	34.8	85.4
	3.309[a]	5.268[a]	99.3[a]	39.7[a]	29.4[a]	107[a]	27.7[a]	56.6[c]	29.1[c]	74.4[c]
V	3.0		265.5	139			28.4	181.1	39.4	110.2
	3.024[a]		228.7[a]	119[a]			43.2[a]	161.9[b]	46.4[c]	124[c]
Fe	2.829		286.9	163.9			110	204.9	87.2	229
	2.866[a]		226[a]	140[a]			116[a]	168.3[b]	80.6[c]	208.2[c]
Co	2.5	3.941	404.75	149.5	138.9	428.1	99.6	232.5	118.1	303.1
	2.507[a]	4.069[a]	307.1[a]	165[a]	102.7[a]	358.1[a]	75.5[a]	191.4[b]		211[c]
Ni	3.525		248.8	140.8			117.7	176.8	86.1	222.1
	3.524		248.1[a]	154.9[a]			124.2[a]	186[b]	76[c]	207[c]
Cu	3.595		170.2	120.3			57.9	136.9	41.3	112.5
	3.615[a]		168.3[a]	122.1[a]			75.7[a]	137[b]	46.8[c]	128[c]
Y	3.644	5.78	76.5	19	20.5	77.8	25.2	39	27.2	66.2
	3.648[a]	5.732[a]	77.90[a]	28.50[a]	21.00[a]	76.90[a]	24.31[a]	36.6[b]	25.6[c]	63.5[c]
Nb	3.309		240	132.3			12.7	168.2	23.7	68
	3.3[a]		246.5[a]	134.5[a]			28.73[a]	170[b]	37.5[c]	103[c]
Mo	3.161		454	167.2			103.7	262.8	118	308
	3.147[a]		463.7[a]	157.8[a]			109.2[a]	272.5[b]		329[c]
Rh	3.836		337.2	145.4			148.3	209.3	124.5	311.8
	3.803[a]		413[a]	194[a]			184[a]	270.4[b]		293[c]
W	3.185		493.8	204			136.8	300.6	140	363.5
	3.165[a]		522.4[a]	204.4[a]			160.83[a]	323.2[b]		375[c]
Ir	3.873		583.9	241.9			249.59	355.9	214.5	535.85
	3.839[a]		580[a]	242[a]			256[a]	355[b]		517[c]
Cr	2.8778		451.2	145.03			106.3	247.1	123.1	316.7

	2.8848[a]		339.8[a]	58.6[a]			99[a]	190.1[b]		248[c]
Ti	2.9348 2.9506[a]	4.6585 4.6835[a]	160.7 162.4[a]	84.9 92[a]	80.5 69[a]	164.7 180.7[a]	13.5 46[a]	108.7 105.1[b]	25.6	71.4
Zn	2.6695 2.665[a]	4.9553 4.947[a]	146.3 163.6[a]	47.3 36.4[a]	50.3 53[a]	75 63.47[a]	23.3 38.79[a]	70.1 59.8[b]	31.4	81.9
Zr	3.2315 3.2316[a]	5.1473 5.1475[a]	134.4 143.4[a]	67.4 72.8[a]	70.9 65.3[a]	156.9 164.8[a]	13.4 32[a]	93.5 83.3[b]	23.9	66.1 99.2[c]
Ru	2.721 2.7058[a]	4.3057 4.2816[a]	536.5 562.6[a]	212.5 187.8[a]	201.1 168.2[a]	570.9 624.2[a]	165.7 180.6[a]	319.2 320.8[b]	167.1	426.9

Note: the data with superscript (a) are cited from ref. [1]., (b) are cited from ref.[2], (c) are cited from ref.[3]

Table II Surface energy (γ_s), electron work function (φ), elongation (El(%)), the ideal tensile strength (ITS), the ideal shear strength(ISS), the tensile strain energy density ($W_{tensile}$), the shear strain energy density (W_{shear}), the reciprocal of brittleness (β^{-1}) and the fracture toughness (K_{IC})

	γ_s (J/m^2)	φ (eV)	El(%)	ITS (GPa)	ISS (GPa)	$W_{tensile}$ (GPa)	W_{shear} (GPa)	β^{-1}	K_{IC} (MPam$^{0.5}$)
Be	1.71 1.68[a]	5.09 4.98[c]	2[d]	23.3	15.9	3.4	1.4	2.45	6.2 10.9[g]
Mg	0.58 0.76[b]	3.69 3.66[c]	5[d]	5.9	1.4	1.5	0.13	11.51 13.04[f]	18.3 15~40[h]
Sc	1.450 1.28[b]	3.47 3.5[c]	5e	13	2.8	3.8	0.24	15.75	42.1
V	2.399 2.55[b]	4.12 4.3[c]	39[d]	34	6.3	10.4	0.86	12.02	90.8 124[i]
Fe	2.16 2.48[b]	4.61 4.5[c]	45[d]	32.4	7.8	10.1	0.92	10.97 12.89[f]	87.9 50~90 [j]
Co	2.43 2.55[b]	4.77 5.0[c]	14[d]	34.2	6.9	7.6	0.67	11.42	104.8
Ni	2.6 2.45[b]	4.9 5.15[c]	30[e]	33.1	5.9	7.4	0.73	10.21 22.59[f]	68.1 100~`50[f]
Cu	1.460 1.83[b]	4.26 4.65[c]	48[d]	24.5	2.8	5.4	0.36	14.9 33.86[f]	90.4 100~107[f]
Y	1.11 1.13[b]	2.87 3.1[c]	25[d]	9.7	2.2	2.8	0.19	14.9	30.7
Nb	2.8 2.7[b]	4.27 4.3[c]	30[e]	27.6	7.0	8.7	1.04	8.4	53.6 37[k]
Mo	2.824 3.0[b]	4.62 4.6[c]	20[d]	41.2	15.5	10.3	2.27	4.53 8.94[f]	34.5 21[k]
Rh	2.32 2.7[b]	5.1 4.98[c]		37.6	12.9	6.8	1.59	4.27	24.8

W	3.266 3.68[b]	4.38 4.55[c]	30[e]	49.4	17.5	12.9	2.62	4.94 9.95[f]	44.7 9~39[k]
Ir	2.67 3.0[b]	5.37 5.27[c]	13[e]	46	18.6	6.0	2.29	2.63	21.5
Cr	3.0 2.3[b]	4.81 4.5[c]	3[e]	45.64	16.64	13.83	2.99	4.63	31.9
Ti	2.7 2.1[b]	4.46 4.33[c]	54[e]	23.97	2.87	8.55	0.44	19.26 53[f]	110.12
Zn	0.71 0.99[b]	4.29 4.33[c]		4.47	2.16	1.84	0.23	7.96 13.733[f]	20.15 28.3[l]
Zr	1.91 2.0[b]	4.32 4.05[c]	32[e]	19.34	1.57	4.87	0.26	18.7	95.38 30~120[m]
Ru	2.58 3.05[b]	4.77 4.71[c]		43.55	16.47	10.06	2.0	5.02	47.27

Note: the data with superscript (a) cited from ref. [4], (b) cited from ref. [5], (c) cited from ref.[6], (d) cited from ref. [7], (e) cited from ref.[3], (f) cited from ref.[8], (g) cited from ref. [9], (h) cited from ref. [10], (i) cited from ref. [11], (j) cited from ref.[12], (k) cited from ref.[13], (l) cited from ref[14]., (m) cited from ref.[15].

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