Data Tables of Semiconductor, High-k Dielectrics, and Metal Constants

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Samares Kar
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Appendices

Appendix I: Fundamental Constants

We have included those fundamental constants which are frequently used when dealing with MOSFETs, IC technology, and dielectric materials.

The values of fundamental constants quoted are accurate.

Constant	Symbol	Value	Unit	Remarks
Avogadro constant	N_A	$6.022\ 141\ 79 \times 10^{23}$	mol^{-1}	
Boltzmann constant	k	$1.380\ 6504 \times 10^{-23}$	JK^{-1}	
Electron mass	m	$9.109\ 382\ 15 \times 10^{-31}$	kg	
Elementary charge	e, q	$1.602\ 176\ 487 \times 10^{-19}$	C	
Permeability of vacuum (magnetic constant)	μ_0	$12.566\ 370\ 614 \times 10^{-7}$	NA^{-2}	Exact
Permittivity of vacuum (electric constant)	ε_0	$8.854\ 187\ 817 \times 10^{-12}$	Fm^{-1}	Exact
Planck constant	h	$6.626\ 068\ 96 \times 10^{-34}$	Js	
		$4.135\ 667\ 33 \times 10^{-15}$	eVs	
	$h/2\pi$	$1.054\ 571\ 628 \times 10^{-34}$	Js	
		$6.582\ 118\ 99 \times 10^{-16}$	eVs	
Speed of light in vacuum	c	299 792 458	ms^{-1}	Exact

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Appendix II: Periodic Table of the Elements

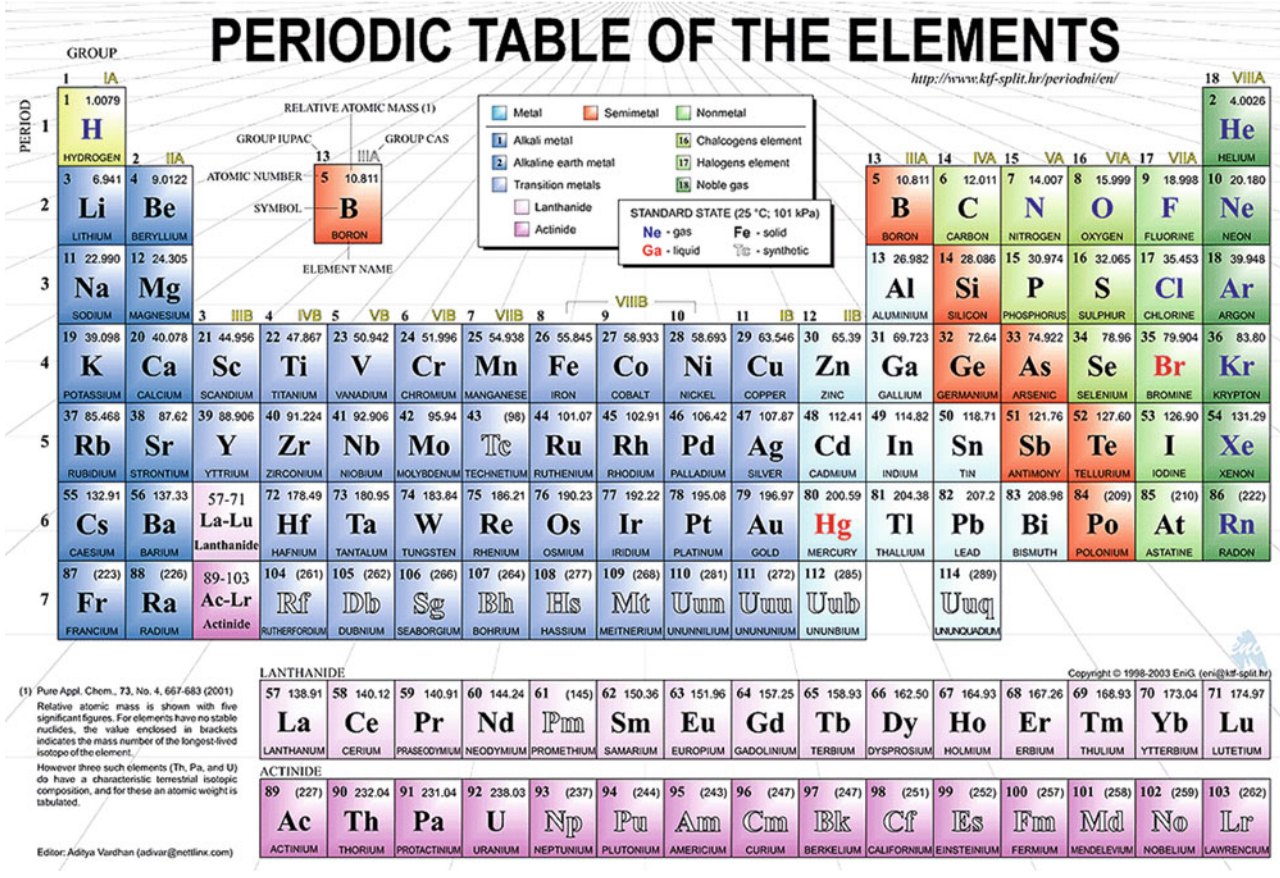
A visual display of the periodic table can greatly help in the study of and search for the high permittivity materials for the gate dielectrics, high mobility semiconductors for the MOSFET channel, and high and low work function metals for the gate electrode. A thorough understanding of and familiarity with the numerous salient features of the periodic table could inspire the appropriate ideas for research.

Notes and Comments

1. There are labels and notes on the periodic table explaining the features and the arrangement of the periodic table.
2. There are two nomenclatures in use for the designation of the groups: the classical Chemical Abstracts Service (CAS) group number and the more recent International Union of Pure and Applied Chemistry (IUPAC) group number.
3. A guide in the search of elements for the semiconductor is the four electrons per average atom criterion. This criterion leads to the elements of group IVA (elemental semiconductors), groups IVA and IVA (IV-IV compound semiconductors), groups IIIA and VA (III-V compound semiconductors), groups IIB and VIA (II-VI compound semiconductors), groups IB, IIIA, and VIA (I-III-VI_2 compound semiconductors), and groups IIB, IVA, and VA (II-IV-V_2 compound semiconductors), cf. Appendix III. There are exceptions to this criterion, e.g. the IV-VI compound semiconductors, cf. Appendix III.
4. Among group IVA natural elements, C, Si, and Ge are semiconductors, Sn is a semi-metal, whereas Pb is a metal.
5. The genesis of the criterion of an average valency of four is the fact that semiconductors are covalent or largely covalent material; a valency of four can be linked to covalent bonds, unless the electro-negativity difference is too high. The I-VII compounds are not semiconductors because these are ionic or largely ionic materials on account of the large difference between the anion and the cation electro-negativity.
6. In contrast to the search for the semiconductor behavior, we need to look for ionic oxides/insulators when searching for the high-k gate dielectrics. The genesis behind the search for high ionicity is the following. At the MOSFET operating frequency of a few GHz, only electronic and ionic polarizations count; as the former is not large enough even for the heavy elements, one has mainly to depend upon the ionic polarization to contribute to a high value of the dielectric constant k. Generally, large electro-negativity difference may lead to large ionic polarization, although the latter also depends upon the molecular volume and the phonon frequency. In a high-k material, the anion is generally oxygen, which has a Pauling electro-negativity of 3.44 (one of the highest values of electro-negativity), cf. Appendix VI. This means that to enhance the electro-negativity difference, we have to look for a cation (metals) with a small

value of the electro-negativity; in other words an element from the left side of the periodic table—from groups IIIB, IVB, and VB, including the lanthanides, cf. Appendix VI.

7. A guide in the search for the gate electrode metal is the value of the vacuum work function of the metal; however, the vacuum work function is less relevant on the high-k gate stack than on the SiO_2 gate dielectric, because of the very high trap density at the high-k/metal interface and the resultant Fermi level pinning. Still the vacuum work function of about 4.0 eV for the n-channel metal and of about 5.0 eV for the p-channel metal can be a starting point. There appears to be some correlation between the vacuum work function of the metal and the position of the metal on the periodic table. The vacuum work function tends to increase going from the left to the right columns of metals in the periodic table cf. Appendix VII.



Source for the periodic table of the elements: http://www.periodni.com

Appendix III: Physical Constants of Semiconductors

Notes

1. The values in the table are mostly those which obtain at 300 K and in the intrinsic semiconductor.
2. The values have been taken from multiple sources; a list of some important sources is given under the references.
3. Where two values of the electron effective mass occur, the first represents the longitudinal and the second the transverse electron effective mass. Where two values of the hole effective mass occur, the first represents the light and the second the heavy hole effective mass.
4. Where two values of the lattice constant occur, the first represents lattice constant a and the second the lattice constant c.
5. Many semiconductors may crystallize in more than one atomic arrangement. For example, many III-V compound semiconductors may solidify with either the zinc blende or the wurtzite crystal structure. We have presented values for the crystal structure with the more reliable and complete values.

Observations

1. The most common crystal structure among the semiconductors is the tetrahedral crystal structure with four nearest neighbors. This promotes covalent chemical bonding. The tetrahedral crystal structure is equivalent to two face-centered-cubic (fcc) structures displaced from each other by one–fourth of its body diagonal.
2. The covalent bond is strongly directional in nature; this does not promote close packing; hence most of the semiconductors have low packing density and expand on solidification.
3. The average valency of most of the semiconductors is four. This is true for the group IV elemental, group III-V compound, group II-VI compound, group I-III-V_2 compound, and group II-IV-VI_2 compound semiconductors.
4. Compound semiconductors are not completely covalent, but are partly ionic. The ionicity in general increases going from group IV elemental to group IV-IV compound to III-V compound to II-VI compound semiconductors.
5. The defect density increases going from group IV elemental to group IV-IV compound to group III-V compound to group II-VI compound to group II-IV-V_2 compound to group I-III-VI_2 compound semiconductors; the doping efficacy decreases in this order because of a variety of reasons including the self-compensation effect. Silicon is one of the easiest semiconductors to dope. In contrast, many of the II-VI compound semiconductors can be doped either p- or n-type but not both.

Semiconductor	Band gap (eV)	Gap transition	Mobility (cm^2 V^{-1} s^{-1})		Effective mass		Electron affinity (eV)	Dielectric constant	Crystal structure	Lattice constant (Å)	Melting point (°C)
			μ_e	μ_h	m_e^*/m	m_h^*/m					
Group IV elements											
C (Diamond)	5.46–5.60	Indirect	1,800–2,200	1,600–1,800	1.40/0.36	0.70/2.12		5.5–5.7	Diamond	3.56–3.57	3,800
Si	1.11–1.12	Indirect	1,350–1,500	450-600	0.97–0.98/ 0.19	0.16/0.49–0.50	4.01–4.24	11.7–12.0	Diamond	5.43	1,410–1,420
Ge	0.66–0.67	Indirect	3,600–3,900	1,800–1,900	1.60-1.64/ 0.08	0.04/0.30–0.33	4.00–4.13	16.0–16.3	Diamond	5.64-5.66	937–958
Group IV-IV compounds											
4H-SiC	2.99–3.23	Indirect	400-900	50–120	0.29/0.42			10.0–10.2	Wurtzite	3.07/10.05	2,830
3C-SiC	2.36	Indirect	800	320	0.68/0.25	1.00–1.20		9.66–9.72	Zinc Blende	4.36	2,830
Group III-V compounds											
BN	6.10–6.40	Indirect	200	500	0.35/0.24	0.15/0.38	4.50	7.1	Zinc Blende	3.62	2,973
AlN	6.02	Direct	300	14	0.40	0.24/3.53	0.60	8.5–9.1	Wurtzite	3.11/4.98	3,000
AlP	2.45–3.00	Indirect	80					9.8–11.6	Zinc Blende	5.46	1,500–2,000
AlAs	2.11–2.16	Indirect	180–280				3.50	8.5–12.0	Zinc Blende	5.66	1,600
AlSb	1.52–1.65	Indirect	200-900	400–420	0.30–0.39	0.40	3.65	10.1–14.4	Zinc Blende	6.13-6.14	1,050
GaN	3.25–3.50	Direct	1,000	200	0.19–0.20	0.30/1.40	4.10	8.9–12.2	Wurtzite	3.16–3.18/ 5.16–5.18	1,500
GaP	2.24–2.26	Indirect	110–300	75–150	0.12–0.35	0.14/0.79	3.80–4.30	8.5–11.1	Zinc Blende	5.45	1,465
GaAs	1.42–1.43	Direct	8,500–8,600	250–420	0.06–0.07	0.08–0.12/ 0.51–0.68	4.07	10.9–13.1	Zinc Blende	5.63–5.65	1,238
GaSb	0.67–0.78	Direct	3,000–5,000	850–1,400	0.04–0.05	0.05–0.06/ 0.30–0.50	4.06	14.0–15.7	Zinc Blende	6.09–6.10	712
InN	2.05–2.40	Direct	3200		0.11	0.27/1.63	4.38	15.3–19.3	Wurtzite	3.53/5.69	1,100
InP	1.27–1.35	Direct	4,500–4,600	100–150	0.07–0.08	0.08/0.40–0.60	4.38–4.40	9.6–12.4	Zinc Blende	5.67–5.87	1,070
InAs	0.33–0.36	Direct	30,000–40,000	450–500	0.03	0.03/0.41	4.90–4.96	12.3–15.1	Zinc Blende	6.05–6.06	943
InSb	0.16–0.18	Direct	77,000–80,000	450–1,250	0.01	0.02/0.39–0.43	4.59	15.9–17.9	Zinc Blende	6.47–6.48	536

(continued)

(continued)

Semiconductor	Band gap (eV)	Gap transition	Mobility ($cm^2\ V^{-1}\ s^{-1}$)		Effective mass		Electron affinity (eV)	Dielectric constant	Crystal structure	Lattice constant (Å)	Melting point (°C)
			μ_e	μ_h	m_e^*/m	m_h^*/m					
Group II-VI Compounds											
ZnS	3.58–3.68	Direct	120-165	5	0.25	0.50–1.00	3.90	8.0–8.3	Zinc Blende	5.41–5.42	1,830
CdS	2.42	Direct	340–400	9–50	0.10–0.17	0.40–0.80	4.50	8.3–9.0	Zinc Blende	5.82–5.83	1,750
HgS	2.00	Direct	250					30.7	Zinc Blende	5.85	1,450
ZnSe	2.60–2.67	Direct	530	16	0.15–0.17	0.60	4.09	8.1–9.1	Zinc Blende	5.67	1,515
CdSe	1.70–1.80	Direct	600–800	9–10	0.13	0.45	4.95	10.0–10.7	Zinc Blende	6.05	1,258
CdSe	1.70–1.74	Direct							Wurtzite	4.30/7.01	1,350
HgSe	0.60	Direct	20,000		0.04–0.05	0.02–0.08		25.6–25.8	Zinc Blende	6.08	800
ZnTe	2.26	Direct	530	130–900	0.20	0.10–0.30	3.50–4.80	10.1	Zinc Blende	6.10	1,295
CdTe	1.44–1.56	Direct	300–1,050	65–100	0.14	0.37	4.28–4.30	9.6–11.0	Zinc Blende	6.48	1,098
HgTe	0.15	Direct	22,900		0.02	0.003		48.0	Zinc Blende	6.46–6.52	670
Group IV-VI Compounds											
PbS	0.41	Indirect	600	700	0.66	0.50		205/17	NaCl	5.93–5.94	1,077
PbSe	0.27	Direct	900	700	0.33	0.34		280	NaCl	6.15	1,062
PbTe	0.29–0.32	Indirect	2,500–6,000	1,000–4,000	0.22	0.29		400/30	NaCl	6.46	904
Group I-III-VI_2 Compounds											
$CuInSe_2$	1.00–1.04	Direct	320	10			4.15		Chalcopyrite	5.77/11.54	990
$CuInTe_2$	0.95	Direct	200	12					Chalcopyrite	6.16/12.32	780
Group II-IV-V_2 Compounds											
$CdSnP_2$	1.17	Direct	2,000		0.04				Chalcopyrite	5.90/11.51	570
$CdSnAs_2$	0.26		11,000						Chalcopyrite	6.08/11.91	593–595

6. Doping ease correlates well with covalency.
7. For the semiconductors with the same class of crystal structure, the band-gap in an approximate manner is inversely proportional to the lattice constant. Hence, on an average, smaller lattice constant correlates with higher band-gap, stronger bond, and higher melting point.
8. Mixed semiconductors can be formed easily, particularly in the case of the III-V compound semiconductors as the rules of solid solutions are well satisfied for many combinations.
9. Nearly equal values of electron and hole mobility is rare in semiconductors. Only diamond and PbTe are among the exceptions with reasonable values of both electron and hole mobility. This rare property makes these two semiconductors potentially ideal channel materials for CMOSFETs.
10. Most semiconductors have disappointingly low values of the hole mobility. Diamond, Ge, GaSb, and PbTe are among the rare semiconductors with reasonable values of hole mobility.
11. Some III-V compound semiconductors and a few other compound semiconductors (InSb, InAs, HgTe, HgSe, $CdSnAs_2$, GaAs) have enormous values of electron mobility. Equally striking are their disproportionately low values of hole mobility. While InSb has the highest value of electron mobility, GaAs—a leading candidate for high mobility MOSFET channel—has much lower electron mobility than the other semiconductors with the highest electron mobility.
12. For most semiconductors, the value of hole mobility is lower than its value of electron mobility. There are some exceptions to this rule; among the exceptions are ZnTe and PbS in which the electron mobility is lower than the hole mobility.
13. PbTe is a rare semiconductor with high values of both electron and hole mobilities—6,000 and 4,000 $cm^2\ V^{-1}\ s^{-1}$ respectively.
14. No clear correlation can be observed between electron mobility and crystalline perfection including its chemical purity and absence of mechanical imperfections. IC grade silicon is the most perfect crystal available today, yet values of its electron and hole mobility are among the lower values.
15. Silicon has been and still is by far the leading CMOSFET channel material, but values of its electron and hole mobility remain perhaps its most potent weakness for this application.
16. Carrier mobility is proportional to the mean free time and inversely proportional to the effective mass. Many semiconductors with high electron mobility exhibit low effective mass for electrons; but the same semiconductors also exhibit low effective mass for holes as well; yet values of hole mobility are abysmally low.

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Appendix IV: Physical Constants of Si, Ge, GaAs (Values at 300 K)

Physical constant (unit)	Ge	Si	GaAs	Remarks
Acceptors	B, Al, Ga, In	B, Al, Ga, In	Zn, Si, C, Ge, Sn	
Atomic density (cm^{-3})	4.42×10^{22}	5.00×10^{22}	4.42×10^{22}	
Atomic number	32	14	31, 33	
Atomic weight	72.60	28.09	144.63	
Avalanche (breakdown) field ($V\ cm^{-1}$)	2×10^5	3×10^5	3.5×10^5	
Band-gap—direct (eV) E_G	0.81	2.5	1.43	
Band-gap—indirect (eV) E_G	0.66	1.11	—	
Bulk modulus ($N\ cm^{-2}$)	7.5×10^6	9.8×10^6	7.53×10^6	
Cleavage plane	{001}	{111}	{110}	
Crystal structure	Diamond	Diamond	Zinc blende	
Density ($g\ cm^{-3}$)	5.327	2.329	5.317	
Dielectric constant k	16.3	11.7	11.5	
Diffusion coefficient ($cm^2\ s^{-1}$): electrons	93	35	200	
Diffusion coefficient ($cm^2\ s^{-1}$): holes	47	12.5	8	
Donors	P, As, Sb	P, As, Sb	Te, Si, Ge, S, Sn, Se	
Effective density of states in the conduction band (cm^{-3}) N_c	1.04×10^{19}	2.8×10^{19}	4.7×10^{17}	
Effective density of states in the valence band (cm^{-3}) N_v	6.0×10^{18}	1.04×10^{19}	7.0×10^{18}	
Effective mass (m_0): holes m_{hh}*, m_{lh}*	0.33, 0.043	0.49, 0.16	0.51, 0.082	
Effective mass (m_0): electrons m_l*, m_t*	1.6, 0.08	0.98, 0.19	0.07	
Electron affinity (eV) χ_s	4.13	4.05	4.07	
Hardness (Mohs scale)	6	7	4-5	
Intrinsic carrier density (cm^{-3}) n_i	2.4×10^{13}	1.45×10^{10}	9×10^6	
Intrinsic resistivity (Ω cm)	50	2.5×10^5	3.3×10^8	
Lattice constant (Å) a	5.658	5.431	5.654	

(continued)

(continued)

Physical constant (unit)	Ge	Si	GaAs	Remarks
Melting point (°C)	937	1,412	1,238	
Mobility ($cm^2\ V^{-1}\ s^{-1}$): electrons μ_e	3,900	1,350	8,600	
Mobility ($cm^2\ V^{-1}\ s^{-1}$): holes μ_h	1,900	480	250	
Reflectivity (%)	48	35	30	Normal incidence
Refractive index n	4.0	3.42	3.3	
Specific heat ($J\ g^{-1}\ K^{-1}$)	0.31	0.7	0.35	
Thermal coefficient (K^{-1})	5.75×10^{-6}	2.33×10^{-6}	5.73×10^{-6}	
Thermal conductivity ($W\ cm^{-1}\ K^{-1}$)	0.58	1.5	0.55	
Thermal velocity ($cm\ s^{-1}$): electrons	3.1×10^7	2.3×10^7	4.4×10^7	
Thermal velocity ($cm\ s^{-1}$): holes	1.9×10^7	1.65×10^7	1.8×10^7	
Vapor pressure (Pa)	1 (1,330 °C)	5×10^{-3} (1,300 °C)	1 (900 °C)	

Appendix V: Physical Constants of High Permittivity Dielectrics

Please see Sect. 1.4 for observations on the data presented below.

Table A Experimental values of important material constants of various high-k dielectrics

Material	Si	Al_2O_3	SiO_2	TiO_2	Y_2O_3	ZrO_2
Atomic number	14	13–8	14–8	22–8	39–8	40–8
Cation valency		3	4	4	3	4
Crystal structure (Alternate structure)	Diamond	Hexagonal	Cubic (β Cristobalite)	Tetragonal (Rutile: A; B)	Cubic	Monoclinic (T; C)
Ionicity, I (Pauling)	0	0.57	0.45	0.59	0.71	0.67
Coordination number, CN_c:CN_a	4	6:4	4:2	6:3	6:4	7:3 or 4
Cation-anion distance, $d_{c\text{-}a}$ (Å)	2.35(4X)	1.86(3X) 1.97(3X)	1.61(4X)	1.932(4X) 1.979(2X)	2.25(2X), 2.28(2X) 2.34(2X)	2.051, 2.057, 2.151, 2.163, 2.189, 2.220, 2.285
Specific density, ρ (g cm^{-3})	2.33	3.9–4.1	2.2–2.3	3.9–4.3	4.8–5.0	5.7–5.9
Melting point, m.p. (°C)	1,414	2,020–2,072	1,670–1,728	1,830–1,850	2,376–2,464	2,670–2,710
Thermal exp. coeff., α ($\times 10^{-6}$ K^{-1})	2.5	6.5-8.8	0.5–0.6	7.1–9.2	7.9–9.3	7.0–8.0
Bandgap, E_G (eV)	1.12	8.6–8.8	8.9–9.3	3.1–3.5	5.5–6.0	5.4–5.8
Electron affinity, χ_{di} (eV)	4.05	1.2–2.0	0.9–1.1	3.0–3.2	1.8–2.0	2.0–2.5
Effective mass m_h*/m	0.59	—-	3–10	0.3–0.5	—-	4
Effective mass m_e*/m	1.06	0.35-0.50	0.3–0.5	1.3–13.0	—-	0.3
Dielectric constant, k (frequency range, Hz)	11.9 (10^7–10^9)	9.0–10.0 (10^2–10^{11})	3.8–3.9 (10^{-5}–10^{11})	89–173 (10^2–10^8)	14.0–18.0 (10^3–10^7)	14–18 (10^2–10^{11})

(continued)

Table A (continued)

Material	Si	Al_2O_3	SiO_2	TiO_2	Y_2O_3	ZrO_2
Refractive index, n	3.44	1.6-1.7	1.475	2.3–2.7	1.7–1.9	2.1–2.2
n^2	11.83	2.89	2.22	6.40	3.28	4.71
Relaxation frequencies (non-electronic) (Hz)	—-	Nil	Nil	10^2, 10^3, 10^{10}	—-	10, 10^4

In a majority of cases, for the values of each constant, five independent references were used. The frequency range given in the row for the dielectric constant k, indicates the range over which the measurements were made and the values of k were found to be frequency-independent. A ≡ Anatase(T); B ≡ Brookite(O); C ≡ Cubic; H ≡ Hexagonal; M ≡ Monoclinic; O ≡ Orthorhombic; T ≡ Tetragonal

Table B Experimental values of important material constants of various high-k dielectrics

Material	Si	$ZrSiO_4$	$BaZrO_3$	La_2O_3	HfO_2	Ta_2O_5
Atomic number	14	40-14-8	56-40-8	57-8	72-8	73-8
Cation valency		4;4	2;4	3	4	5
Crystal structure (Alternate structure)	Diamond	Tetragonal (b.c.)	Perovskite	Hexagonal (M;C)	Monoclinic (T;C)	Orthorhombic (H)
Ionicity, I (Pauling)	0	0.57	0.74	0.75	0.68	0.61
Coordination number, CN_c:CN_a	4	(8:2); (4:1)	(12:4); (6:2)	7:3 or 4	7:3 or 4	6:2 or 3
Cation-anion distance, $d_{c\text{-}a}$ (Å)	2.35(4X)	Zr-O: 2.10(4X), 2.24(4X), Si-O: 1.61(4X)	Ba-O: 2.957, Zr-O: 2.094	2.38(3X), 2.45(1X) 2.72(3X)	2.031, 2.052, 2.162, 2.170, 2.174, 2.202, 2.254	2.60, 1.98, 2.13, 1.92, 2.14, 1.97
Specific density, ρ (g cm^{-3})	2.33	4.0–4.9	5.3–6.3	6.5–6.6	9.7–10.0	7.5–8.3
Melting point, m.p. (^oC)	1,414	2,340–2,667	2,500–2,700	2,256–2315	2,780–2,810	1,800–1,877
Thermal exp. coeff., α ($\times 10^{-6}$ K^{-1})	2.5	4.0–5.0	6.3–8.7	5.8–6.6	5.8–6.5	2.5–4.0
Bandgap, E_G (eV)	1.12	6.0–7.6	5.3	5.5–5.8	5.6–5.9	4.0–4.5
Electron affinity, χ_{di} (eV)	4.05	2.2–2.6	2.5–3.5	1.8	2.2–2.8	3.2–3.8
Effective Mass m_h*/m	0.59					0.5
m_e*/m	1.06			0.26	0.18-0.20	0.5
Dielectric constant, k (frequency range, Hz)	11.9 (10^7–10^9)	10.7–12.7	28–43	21–27 (10^4–10^6)	21–25 (10^4–10^6)	22–26 (10–10^6)

(continued)

Table B (continued)

Material	Si	$ZrSiO_4$	$BaZrO_3$	La_2O_3	HfO_2	Ta_2O_5
Refractive index, n	3.44	1.9–2.0	2.0	2.0–2.1	2.0–2.2	2.0–2.2
n^2	11.83	3.80	4.00	4.00	4.41	4.41
Relaxation frequencies (non-electronic) (Hz)	—-	—-	—-	—-	—	10^5

In a majority of cases, for the values of each constant, five independent references were used. The frequency range given in the row for the dielectric constant k, indicates the range over which the measurements were made and the values of k were found to be frequency-independent. A ≡ Anatase(T); B ≡ Brookite(O); C ≡ Cubic; H ≡ Hexagonal; M ≡ Monoclinic; O ≡ Orthorhombic; T ≡ Tetragonal

Appendix VI: Electronegativity Table of the Elements

Notes and Comments:

1. Electronegativity represents roughly the strength of an atom to attract electrons to itself.
2. No precise definition or mathematical relation exists for electronegativity. This concept originated from Linus Pauling while he was working on the valence bond theory.
3. Factors influencing electronegativity include the atomic number and the covalent radius.
4. There are several ways of estimating the scale of electronegativity: the classical and the earliest is the Pauling scale, followed by the Allred-Rochow scale, the Mulliken scale, the Sanderson scale, and the Allen scale.
5. In the table below, we have indicated below the symbol of the element, the Pauling electronegativity scale to the left and the Allen electronegativity scale to the right of the solidus.
6. In general, electronegativity increases along the diagonal from the lower left to the upper right of the periodic table.
7. In some cases, there is wide divergence between the Pauling and the Allen electronegativity scale.
8. In the table below, both the IUPAC (to the left of the solidus) and the CAS (to the right of the solidus) group numbers have been indicated.
9. The electronegativity difference ΔEN is often used to classify the type of chemical bond between atoms. The following is an illustration of this kind of an empirical scheme; the range indicated can be considered only an approximate one. Non-polar covalent bond: $\Delta EN < 0.5$; Polar covalent bond: $\Delta EN = 0.5–1.6$; Ionic bond: $\Delta EN > 2.0$.

	Group																	
Period	1 / IA	2 / IIA	3 / IIIB	4 / IVB	5 / VB	6 / VIB	7 / VIIB	8 / VIIIB	9 / VIIIB	10 / VIIIB	11 / IB	12 / IIB	13 / IIIA	14 / IVA	15 / VA	16 / VIA	17 / VIIA	18 / VIIIA
1	H 2.20/2.30																	He 0/4.60
2	Li 0.98/0.91	Be 1.57/1.58											B 2.04/2.05	C 2.55/2.54	N 3.04/3.07	O 3.44/3.61	F 3.98/4.19	Ne 0/4.79
3	Na 0.93/0.87	Mg 1.31/1.29											Al 1.61/1.61	Si 1.90/1.92	P 2.19/2.25	S 2.58/2.59	Cl 3.16/2.87	Ar 0/3.24
4	K 0.82/0.73	Ca 1.00/1.03	Sc 1.36/1.19	Ti 1.54/1.38	V 1.63/1.53	Cr 1.66/1.65	Mn 1.55/1.75	Fe 1.83/1.80	Co 1.88/1.84	Ni 1.91/1.88	Cu 1.90/1.85	Zn 1.65/1.59	Ga 1.81/1.76	Ge 2.01/1.99	As 2.18/2.21	Se 2.55/2.43	Br 2.96/2.69	Kr 3.00/2.97
5	Rb 0.82/0.71	Sr 0.95/0.96	Y 1.22/1.12	Zr 1.33/1.32	Nb 1.60/1.41	Mo 2.16/1.47	Tc 1.90/1.51	Ru 2.20/1.54	Rh 2.28/1.56	Pd 2.20/1.59	Ag 1.93/1.87	Cd 1.69/1.52	In 1.78/1.66	Sn 1.96/1.82	Sb 2.05/1.98	Te 2.10/2.16	I 2.66/2.36	Xe 2.60/2.58
6	Cs 0.79/0.66	Ba 0.89/0.88	La 1.10/	Hf 1.30/1.16	Ta 1.50/1.34	W 2.36/1.47	Re 1.90/1.60	Os 2.20/1.65	Ir 2.20/1.68	Pt 2.28/1.72	Au 2.54/1.92	Hg 2.00/1.76	Tl 2.04/1.79	Pb 2.33/1.85	Bi 2.02/2.01	Po 2.00/2.19	At 2.20/2.39	Rn 2.20/2.60
7	Fr 0.70/0.67	Ra 0.89/0.89	Ac 1.1/	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						
	Lanthanides				Ce 1.12/	Pr 1.13/	Nd 1.14/	Pm 1.13/	Sm 1.17/	Eu 1.20/	Gd 1.20/	Tb 1.10/	Dy 1.22/	Ho 1.23/	Er 1.24/	Tm 1.25/	Yb 1.10/	Lu 1.27/
	Actinides				Th 1.30/	Pa 1.50/	U 1.38/	Np 1.36/	Pu 1.28/	Am 1.13/	Cm 1.28/	Bk 1.30/	Cf 1.30/	Es 1.30/	Fm 1.30/	Md 1.30/	No 1.30/	Lr 1.30/

Color Key:	0-0.66	0.66-1.00	1.00-1.33	1.33-1.66	1.66-2.00	2.00-2.33	2.33-2.66	2.66-

Appendix VII: Work Function Table of the Elements

Notes and Comments:

1. The work function of a metal is the difference in energy between its Fermi level and the vacuum level.
2. The values of work function in the table are in eV.
3. For many metals, there is a wide scatter in the values of the work function reported in the literature.
4. The work function is sensitive to the surface orientation.
5. Group VIIIB elements appear to have the highest work functions, whereas group IA elements seem to have the lowest work functions.

		Group																
Period	1/IA	2/IIA	3/IIIB	4/IVB	5/VB	6/VIB	7/VIIB	8/VIIIB	9/VIIIB	10/VIIIB	11/IB	12/IIB	13/IIIA	14/IVA	15/VA	16/VIA	17/VIIA	18/VIIIA
1	H																	He
2	Li 2.93	Be 4.98											B 4.45	C 5.00	N	O	F	Ne
3	Na 2.36	Mg 3.66											Al 4.06-4.26	Si 4.60-4.85	P	S	Cl	Ar
4	K 2.29	Ca 2.87	Sc 3.50	Ti 4.33	V 4.30	Cr 4.50	Mn 4.10	Fe 4.67-4.81	Co 5.00	Ni 5.04-5.35	Cu 4.53-5.10	Zn 3.63-4.90	Ga 4.32	Ge	As 3.75	Se 5.90	Br	Kr
5	Rb 2.26	Sr 2.59	Y 3.10	Zr 4.05	Nb 3.95-4.87	Mo 4.36-4.95	Tc	Ru 4.71	Rh 4.98	Pd 5.22-5.60	Ag 4.52-4.74	Cd 4.08	In 4.09	Sn 4.42	Sb 4.55-4.70	Te 4.95	I	Xe
6	Cs 2.14	Ba 2.52-2.70	La 3.50	Hf 3.90	Ta 4.00-4.80	W 4.32-5.22	Re 4.72	Os 5.93	Ir 5.00-5.67	Pt 5.12-5.93	Au 5.10-5.47	Hg 4.48	Tl 3.84	Pb 4.25	Bi 4.34	Po	At	Rn
7	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub						

	Lanthanides	Ce 2.90	Pr	Nd 320	Pm	Sm 2.70	Eu 2.50	Gd 2.90	Tb 3.00	Dy	Ho	Er	Tm	Yb 2.60	Lu 3.30
	Actinides	Th 3.40	Pa	U 3.633.90	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

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