Lecture Note #1

Introduction

1. Introduction to lecture (syllabus)
2. Electrochemical energy engineering
3. Surface chemistry
4. Surface chemistry & electrochemistry

Electrochemical energy engineering

- Materials, device, process, analysis/measurement/evaluation, and other technologies for fuel cell, battery, supercapacitor, solar cell, and others below

- **Examples of Electrochemical devices/technologies**

Battery or Fuel cell: chemical state changes(electrochemistry) → electric power
Supercapacitor: double layer phenomena → electric power
Photoelectrochemical cell (Solar cell): light + electrochemistry → electric power
Photocatalysis: light → hydrogen or chemical reaction
Electrochromic display: chemical state changes by electric signal → coloration
Sensors: chemical state changes by mass → electric signal
Electrolysis: electric power → chemical species by chemical state changes
Electrodeposition: electric power → chemical change: thin film, Cu metallization
Electrochemical synthesis: electric power → chemical change
Corrosion: potential difference → chemical change
Etching

Electrical quantities & their SI units

Quantity	Unit
Current (I)	Ampere (A)
Current density (i)	Ampere per square meter (A/m^2)
Charge (q)	Coulomb (C = As)
Charge density (ρ)	Coulomb per cubic meter (C/m^3)
Potential (ϕ)	Volt (V = J/C)
Field strength (X)	Volt per meter (V/m)
Conductivity (κ)	Siemens per meter (S/m)
Resistance (R)	Ohm (Ω =1/S = V/A)
Conductance (G)	Siemens (S = A/V)
Permittivity (ε)	Farad per meter (F/m = C/Vm)
Energy of work (w)	Joule (J = VC)
Power	Watt (W = J/s = AV)
Capacitance (C)	Farad (F = s/Ω = Ss), F = C/V

Electrochemical cell potential (V, volts)

1 V = 1 J/C, energy to drive charge between electrodes
<u>Electrochemical cell notation</u>:

$Zn/Zn^{2+}, Cl^-/AgCl/Ag$ $Pt/H_2/H^+, Cl^-/AgCl/Ag$

slash(/): phase boundary,
comma(,): two components in the same phase

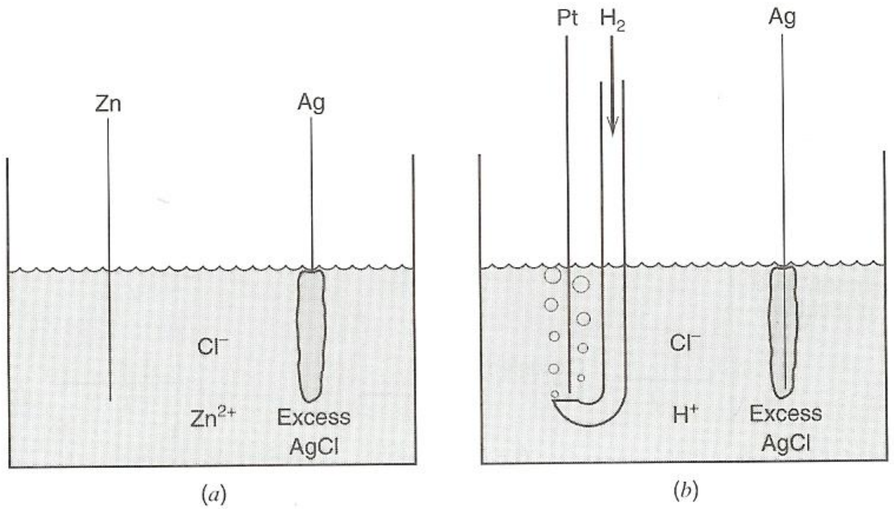


Figure 1.1.1 Typical electrochemical cells. (*a*) Zn metal and Ag wire covered with AgCl immersed in a $ZnCl_2$ solution. (*b*) Pt wire in a stream of H_2 and Ag wire covered with AgCl in HCl solution.

Figure) A.J. Bard, L. R. Faulkner, Electrochemical Methods, Wiley, 2001.

Energy

Heat: a form of energy

Quantity of heat (Q)

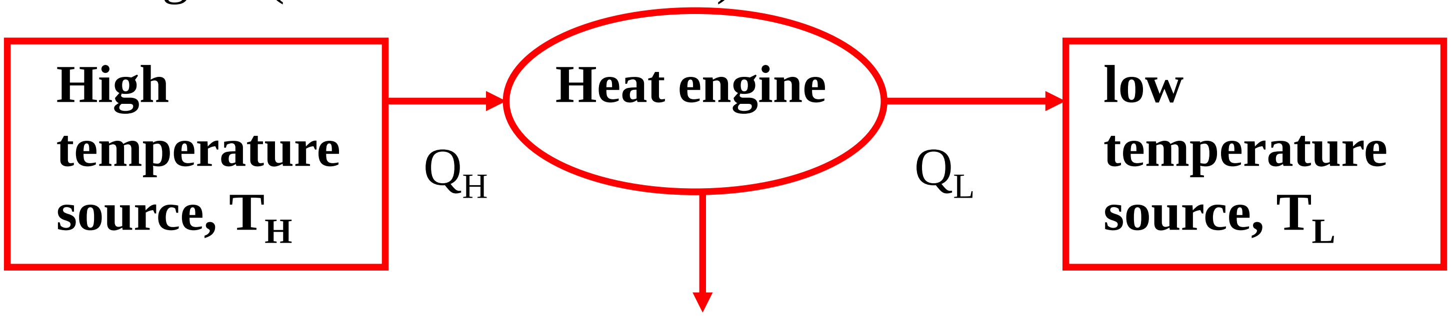
1 calorie: heat to raise 1 g of water through 1℃

1 BTU (British thermal unit): 1 pound (lb) of water through 1℉

Mechanical equivalent of heat

1 cal = 4.186 J   1 BTU = 7718 ft lb = 252 cal = 1054.7 J ~ 0.293 kWh

Ideal heat engine (heat-work converter)



External work

$W = Q_H - Q_L$

$Q_H - Q_L = W$ (1st law of thermodynamics)

Efficiency η = work output / work input = $W/Q_H = 1 - Q_L/Q_H$

Power

Power: the time rate of doing work or of expending energy

Power = energy/time = work/time

Instantaneous power $P = dW/dt$

Average power $P = W/t$

Unit: watt (W) = J/s

1 horsepower (HP) = 746 W

Power ratings of various devices & animals

10^{18} W solar power input to earth

10^{12} W electricity capacity in USA (2000)

10^{9} W large electric power plant

10^{7} W train

10^{5} W automobile

1000 W horse

100 W man/woman resting

0.1~1 W Si solar cell

0.01 W human heart

e.g., 5933000 BTU = 6259 MJ = 6259 MWs = 6259/3600 MWh (1.739 MWh)

1 kWh = 1000 x 60 x 60 = 3.6 x 10^6 J ~ 3411 BTU ~ 859.6 Kcal

cf. 1 barrel = 42 US gallons ~ 0.136 tonnes ~ 159 L

Fuel equivalence: 1 tonnes oil ~ 1.5 tonnes hard coal ~ 3 tonnes lignite ~ 12000 kWh

Million tonnes of oil equivalent (1 Mtoe = 41.9 PJ)

MW(mega-), GW,(giga-) TW(tera-), PW(peta-), EW(exa-):

10^6, 10^9, 10^{12}, 10^{15}, 10^{18} W

Faraday's law

charge(Q, C(1 C = 6.24 x 10^{18} e^-) vs. extent of chemical reaction

"the passage of 96485.4 C causes 1 equivalent of reaction (e.g., consumption of 1 mole of reactant or production of 1 mole of product in a one-electron rxn)"

$$F = N_A Q_e = (6.02 \times 10^{23}\ \text{mol}^{-1})(1.6022 \times 10^{-19}\ \text{C}) = 96485\ \text{Cmol}^{-1}$$

- <u>Current</u> (i): rate of flow of coulombs (or electrons) (1 A = 1 C/s)

Surface chemistry

- Catalysis, electrochemistry, photography, tribology, surface instrumentation, thermodynamics, colloids, adsorption science, electron emission, surface charge, electron transport, monolayer science, microporous solids, thin film technologies, semiconductor technologies, nanotechnology

- Materials: crystals, clusters, thin films, small particles, microporous solids (internal surface)

- Surface: interface between immiscible bodies

- Surfaces on earth are exposed to another solid or gas or liquid → interface: *s/s, s/l, s/g, l/g*

Surface vs. bulk

D = number of surface atoms / total number of atoms

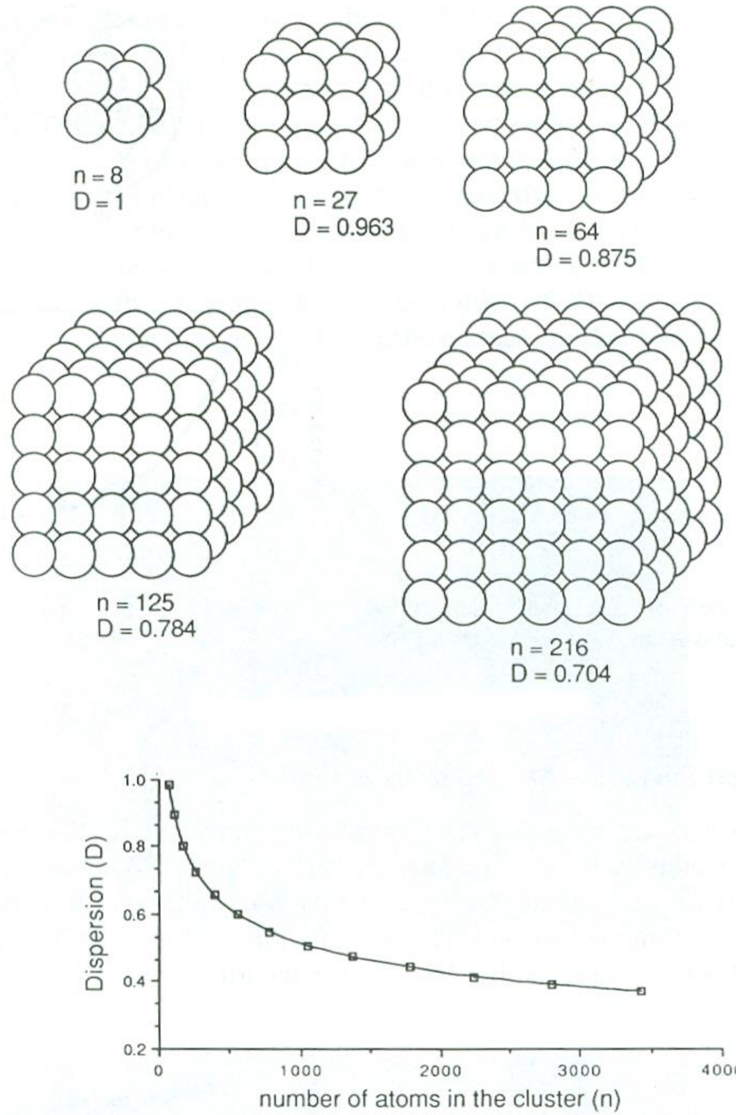


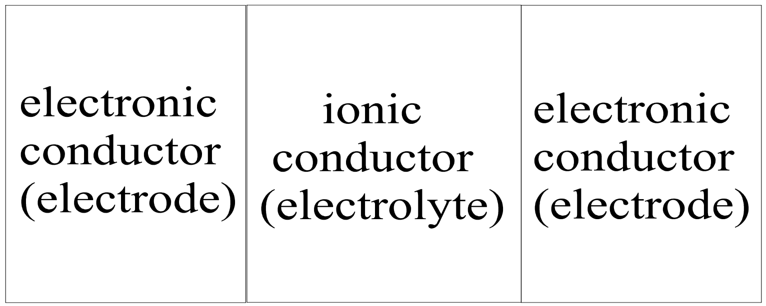
Figure 1.7. Clusters of atoms with single cubic packing having 8, 27, 64, 125, and 216 atoms. In an eight-atom cluster, all of the atoms are on the surface. However, the dispersion, 𝔇, defined as the number of surface atoms divided by the total number of atoms in the cluster, declines rapidly with increasing cluster size. this is shown in the lower part of the figure.

Somorjai, p.9

Surface chemistry & electrochemistry

<u>Electrode & electrochemical cell</u>

The interface between electronic conductor and ionic conductor that the chemistry of electrochemistry occurs



<u>Surface electrochemistry</u>: well-defined electrode (single crystal..), surface kinetics, *in situ* analysis (IR, XPS, STM…), photoelectrochemistry

<u>Electrochemical surface area(ESA)</u>: ‘real area’, microelectrode, nanoelectrochemistry

<u>Interfacial structure</u>: double layer, potential of zero charge, intercalation in battery electrodes