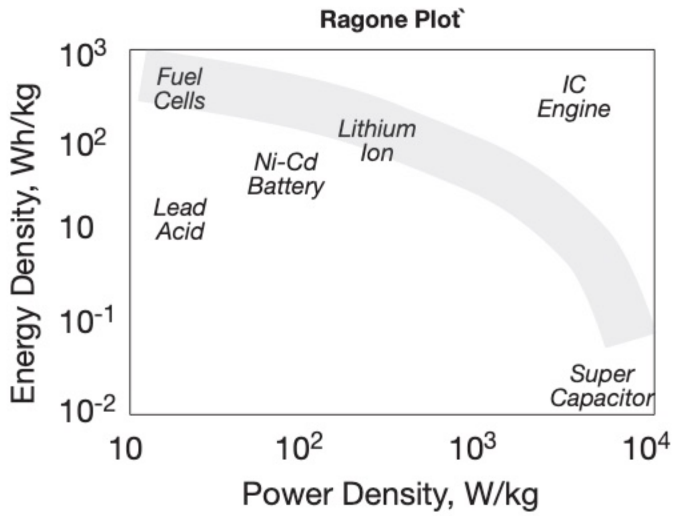
4B_Li+ battery: Energy Density



- The Ragone plot, shown above, shows the give and take between the power density (W/kg) and the energy density (Wh/kg). Note that the plot uses logarithmic scale.
- Let us compare Li+ battery with the Internal Combustion Engine: while both have comparable energy density, the IC engine can deliver a higher power density. The power delivered by a Li+ battery is limited by its internal resistance.
- The fundamental units for energy density are kJ/kg.
- The fundamental units for power density are kJ s^{-1}/kg, or kW/kg since a Watt is doing work at the rate of one J per sec.

They are converted into engineering units in the following way.

	Engineering	Basic units	Conversion into different units	
Energy Density	kWh/kg	kJ/kg	convert kWh/kg to kJ/kg	multiply by 3600
Power Density	kW/kg	kW/kg	n/a	n/a
Energy Density in one gallon of gas	1 gallon of gas (1 gallon of gas weighs 2.7 kg and has energy of 121, 000 kJ) i.e. 44815 kJ/kg	J/g	convert into energy density of a battery (in kWh/kg) which at a weight of 2.7 kg will have the same energy as one gallon of gas.	Energy in one gallon = (12.5 *2.7 kWh) where one gallon weighs 2.7 kg

Capacity

While the voltage of the battery depends on the activity of Li in the anode and the cathode, the energy density (J per kg of battery weight) depends on how much lithium can be held the anode for it to be saturated, that is how much lithium would cause the activity of lithium in the anode to be equal to unity.

Units of mAh/g for capacity

The amount of lithium is specified in units of how many lithium atoms per gram of the anode (or the cathode). It is called the capacity of the anode and the cathode.

It is written in terms of mAh/g, or

mAs*3600/g, since one As is one Coulomb we have

mC*3600/g, i.e. 3.6C/g where C is the Coulombs held in the electrodes.

One lithium atom can provide a charge of one electron. Therefore the charge C is equal to the number of Li that can be supplied at the electrodes multiplied by the charge on one electron.

Example Capacity of Carbon, the current material for the anodes

The theoretical capacity of carbon is 352 mAh/g. Let us calculate the ratio of Li/C atoms in the lithiated carbon.

Method: Convert mAh/g to moles of Li atoms per g of carbon, let us call it m_{Li} . Then calculate the moles of carbon (approximately) in on mole of carbon, calling it m_C.

$$m_{Li} = (\frac{mAh}{g})*\frac{3600}{1000}*\frac{1}{1.6*10^{-19}}\frac{1}{N_A}$$

Multiplying by 3600 converts *h* into *s*; dividing by 1000 converts *mA* into *A*; dividing by the charge on an electron converts C into number of lithium atoms (remember one Li atom can produce a charge of one electron); and finally dividing by the Avogadro's number converts (*mAh/g*) into mole of Li per gram. Note that N_A=6.03*10^{23}.

Substituting a capacity of 352 mAh/g, gives

$$m_{Li} = 0.013 \text{ mol/g}$$

The atomic weight of carbon is 12 g/mol, which means

m_C = 0.083 mol/g

Therefore at a capacity of 352 mAh/g, there would be on Li for every 6 atoms of carbon. However, a practical values of the capacity is ~150 mAh/g.

What are the numbers?

Current anode material is graphite. It has a theoretical capacity of 320 mAh/g. More realistically it is only about 150 mAh/g

The battery is not just the anode.. it is also the cathode, the electrolyte and the current collectors.

The anode is nominally equal to one third of the total weight of the battery.

Energy Density of a Li+ Battery

Energy density is the work equivalent that is stored per unit weight of the battery. Units in common use are:

kWh/kg

Fundamentally, the energy is the product of voltage (in V)*charge (in C) = Joules. Therefore the charge held in the battery per kg weight multiplied by the battery voltage (2.5 V) will give the energy density.

Caveat: so far we have considered the capacity of the anode (in mAh/g); but the battery contains other components: the cathode, the electrolyte and the current collectors. As a rule of thumb we assume that the battery weight is three times the weight of the anode. But let us leave that open for now, and insert this correction as a factor say, H.

Let us now see how the capacity of the anode translates into the energy density of the battery in kWh/kg:

$$E^{*}(kWh/kg) = \frac{1}{H}\left(\frac{mAh}{g}\right)\frac{1}{1000}2.5 \text{ kWh/kg} \qquad (1)$$

Note that dividing by 1000 converts mA into A, and multilying by the battery voltage (2.5 V) converts the product of Amps and Volts into Watts. No other factor is needed since kW/kg is the same is W/g. Note that the factor H is in the denominator since the weight of other components reduces the overall energy density of the battery. Substituting H=3, and mAh/g = 200 for the anode, gives the energy density equal to

$$E^{*} = 0.17 \text{ kWh/kg} \qquad (2)$$

Let us estimate the weight of this battery that will have the same energy as one gallon of gasoline. From the table as the very start of this section one gallon of gasoline is equivalent to 33.75 kWh of energy. Therefore:

(33.75/0.17) = 200 kg of battery would be needed for the battery to have the same energy as one gallon of gasoline. However the batteries can be three to five times more efficient than the internal combustion engine. Therefore the effective energy equivalent is possible wit 40 kg of Li+ battery. Therefore, for the same driving range as say 15 gallons of gasoline would require a battery weighing 600 kg.

Note however, that new materials, and a battery with a higher Nernst potential can bring dramatic improvements in the energy density. For example consider new materials for the anode as explained in the box below:

You can now appreciate the incentive to find anode materials with higher capacity than carbon. For example pure lithium metal can be used as the source of lithium atoms at the anode. Lithium metal has a capacity of about 3800 mAh/g. Silicon is even greater about 4000 mAh/g.

But changing a material has a cascading influence on battery design and materials selection. Lithium metal reacts with the liquid electrolyte current used in batteries (this is the cause of batteries catching fire). Therefore an inert electrolyte, a ceramic, is being considered. However, the bonding between lithium metal and the ceramic is difficult - blank spots are left where the current concentrates causing early failure. Thus fabrication and manufacturing of Li-ceramic interface is a large question.

While silicon has a high capacity, it expands 400% percent when lithiated. The volume expansion and contraction when the battery is charged and discharged causes the silicon to fracture and battery to fade (lose voltage). In this course we shall consider nanoscale design of the anode which may pre-empt fracture in silicon. The idea will be similar to the concept that was invoked in the first topic in this course on fracture at small length scales.