What is a model?

There are essentially three kinds of models.

Data Science

Those that are based entirely on data. The recent machine-learning and AI approached have given more "punch" to these models. But they are based upon statistics; they require massive amounts of data. Cloud computing is mainly based on this approach.

Weather prediction (partially), and prediction of the COVID path are good examples.

Analytical

These models are entirely analytical, and derive from fundamental concept in physics, mechanics and materials science; for example, a model that predicts the energy stored in a diving board as a function of its geometry. These models yield closed form predictions. They always depend on fundamental properties of the materials. For example, in the case of the diving board the elastic or the Youngs modulus of the material is needed.

A sterling example of such models lies in mechanics where prediction such as buckling of a cylinder under compression can be made with precision with mathematical models and solid-geometry.

Hybrid

More recently a hybrid approach where machine-learning is combined with analytical models to zero-in quickly, that is with less computation, on the key variables, is being developed.

For example in weather prediction data science is combined with computational fluid mechanics to make the computations more efficient and precise.

THIS COURSE

This course is devoted to the second method, that is, the analytical models approach. Our goal is the link laboratory measurements with the structure, bonding, etc. at the atomic length scale. See the first example of this approach in relating the nature of the bonds among atoms in a crystal to its global elastic modulus. An example of an analytical model is discussed in the beginning of the next chapter on "Elasticity".

Please note that models in materials science, unlike those in mechanics, cannot predict the outcome precisely. This is because of uncertainty in the values of the variables. For example, the grain size is not monotonic but has wide distributions.

However, in the future a combination of analysis and data science will lead to more accurate predictions. This is an emerging field and still in its infancy.

Global Variables (the length scale)

The following are examples of variables that we shall use often as we progress through the course:

(i) Interatomic distance, the area projected by one atom, and the volume occupied by one atom.

We simplify the problem by assuming that each atom occupies a cube which can be stacked to build the crystal. The edge length of this cube is the interatomic distance, the face area is the area per atom, and the volume of the cube is the volume per atom.

We begin with the volume per atom, given the nomenclature Ω (in units of nm^3, 1 nm = 10 Angstroms), since its value can be explicitly derived from handbook parameters, that is

$$\Omega = \frac{\text{molar volume}}{N_A} \text{, where}$$

• N_A is the Avogadro's Number which is the number of atoms (molecules) in one mole = 6.02×10^{23} atoms/mole.

• molar volume = $\dfrac{\text{atomic weight}}{\text{density}}$

• Therefore the length of the bond (equal to the edge of the cube), that is the spacing between atoms, = $\Omega^{1/3}$

• Projected area of the space occupies by one atom = $\Omega^{2/3}$

Note the scaling according to the units. Area has units of $volume^{2/3}$. Length units of $volume^{1/3}$.

Let us apply the above equations to three cases: copper, ice and water. Note that water is not at all a periodic structure but by applying the above model we can quickly get a good estimate of the distance between the H_2O molecules in it.

		Copper	ICE	Water
Atomic wt	gms/mol	2.90E+01	18	18
N_A		6.02E+23	6.02E+23	6.02E+23
	Ω			
Density	g/cm^3	8.96E+00	0.9	1
Molar vol	cm^3/mol	3.24E+00	2.00E+01	1.80E+01
	m^3/mol	3.24E-06	2.00E-05	1.80E-05
Omega	m^3	5.38E-30	3.32E-29	2.99E-29
	nm^3	5.38E-03	3.32E-02	2.99E-02
Omega$^{2/3}$	nm^2	3.07E-02	1.03E-01	9.63E-02
Omega$^{1/3}$	nm	1.75E-01	3.21E-01	3.10E-01
	Angstroms	1.75E+00	3.21E+00	3.10E+00
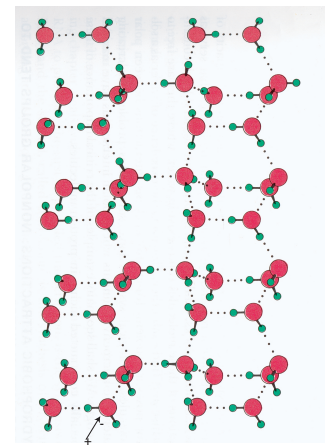
One of the several structures in which water molecules assemble into a crystal. The large atoms are oxygens and the small ones hydrogens. Each H_2O molecule is an effective electrical dipole with lying in the plane of the H_2O molecule with the polarity as shown. The dipoles are arranged in a way that lowers their collective energy.

Ice has an open crystal structure, which exists in many different forms. One example is given just above.

(ii) The microstructural length scale: the grains and grain boundaries.

We will deal mostly (though not exclusively) with crystals which have a regular, periodic structure. All the atoms in a single crystal are arranged in a periodic structure.

There are examples of single crystals that are of engineering significance. Two of the most important ones are single crystals of silicon, used in microelectronics, and single crystals of nickel-base superalloys which are used as the blades in the hot-test section of gas turbines.

In most cases the metals are a collection of small crystallites, which are densely packed.. they are called polycrystals. The picture on right is a cross section of a polycrystal of many grains or crystallites. The nominal length scale of a polycrystal is called the grain size. The grain size can cover a wide range from tens of nm to several micrometers, sometimes to hundreds of micrometers. It is measured by drawing a line across the micrograph and counting the number of grains it crosses.
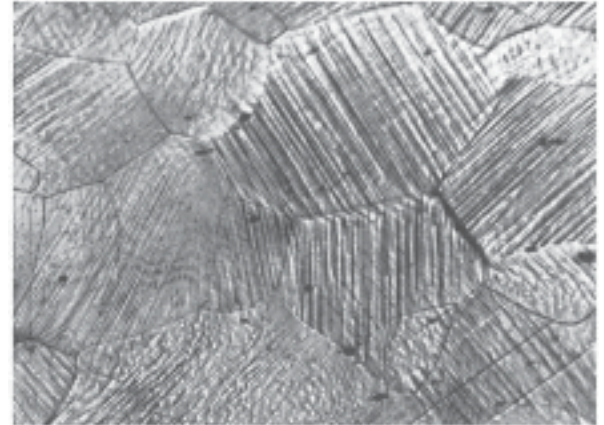
HW - 00A.1
Note how the grains in the polycrystal meet (often) at three grain junctions, the shape of the grains being like hexagons. Can you think about this? Why this is so?

The interfaces where adjacent grains meet are called grain boundaries. As we shall see they have a profound influence on the mechanical properties. At this point is suffices to recognize that the grain boundaries have their own structure, as shown below in schematics and an actual image of a grain boundary obtained in a high-resolution transmission electron microscope. The length scale of the width of the grain boundary is of the same order as the interatomic distance. Most noteworthy is that the crystal structure extends right into the "grain boundary plane". The structure of the boundary can therefore be prescribed by the ledges from both crystals that meet at the grain boundary.

δ_{gb}

effective width of the grain boundary

[1 1 4]

[1 1 0] [2 1 1]

1.0 nm
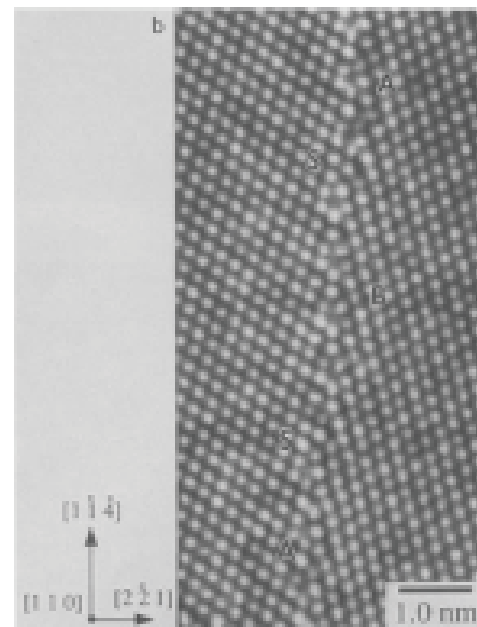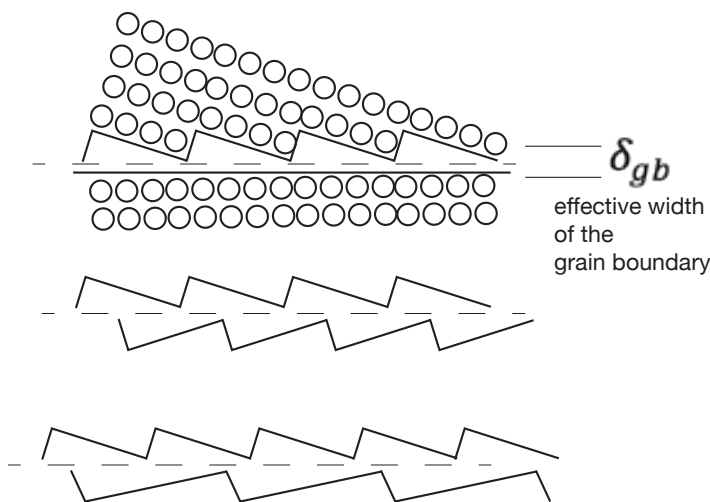
Note that $\delta_{gb} \approx 1.5\Omega^{1/3}$, that is, the effective width of the grain boundary is one and a half times the interatomic spacing.

(iii) Length scales relevant to plastic deformation

When one looks carefully at the grains in a polycrystal, as highlighted below, they have serrations. In a single crystals these serrations can be clearly seen at "steps', also shown below.
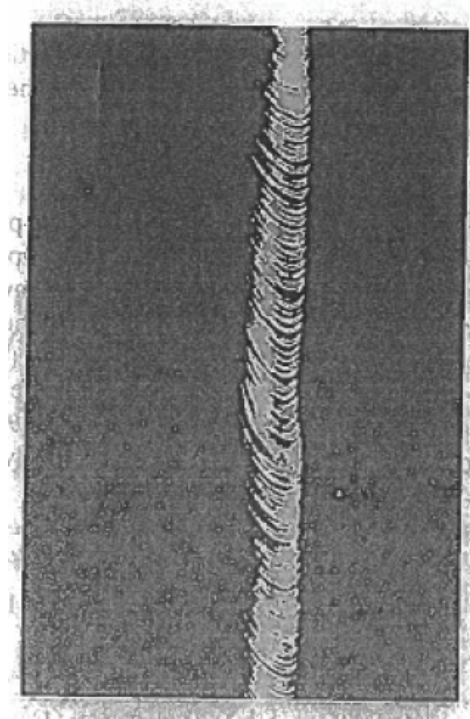

Plastic deformation in crystals occurs by "slip" on these crystal planes, that is the crystal deforms by sliding on specific planes like a pack of cards.

The important length scale is the spacing of these "glide planes" or "slip planes". This distance varies from a few micrometers to tens of micrometers.

(iv) The length scale relevant to the study of Fracture

We shall be concerned mainly with brittle or semi-brittle fracture in this course. Brittle fracture as in silica glass or as in optical fibers is initiated from a pre-existing flaw, which is like a microcrack. The stress concentration at the sharp tip of the crack propels that crack causing complete fracture.

Thus, the length scale of the microcrack determines the propensity to fracture. These microcracks can range from a few tens of micrometers to millimeters or more, depending on the size of the workpiece. A micrograph of a flaw in glass which is the focal point for crack propagation is show in the figure just below.

Griffith's Failure Strength Vs. Diameter of Glass Fibers
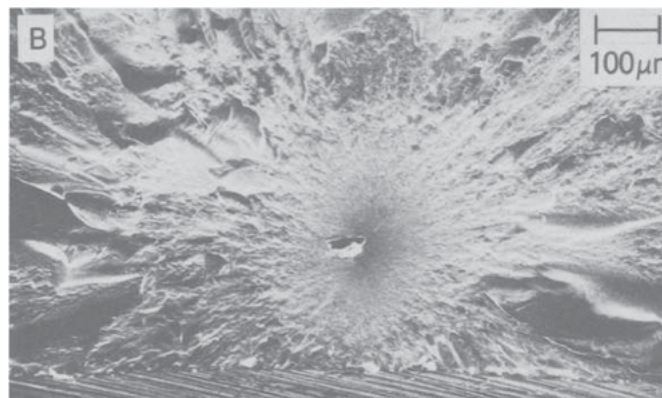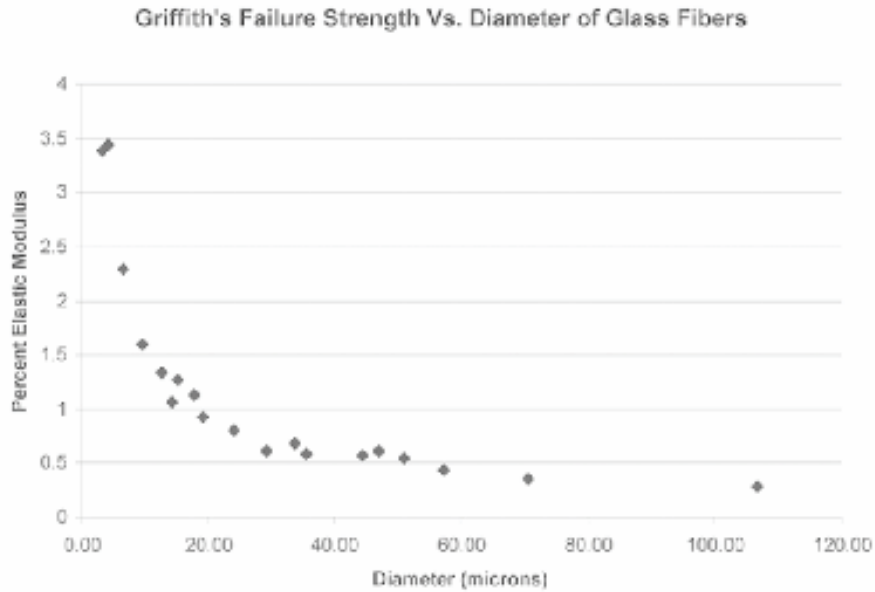
Brittle facture is probabilistic. The chance of finding a flaw in a specimen of small dimensions, such as an optical-fibers. Since the flaw must be significantly smaller than the size of the specimen, the fracture strength of glass fibers rises with smaller fiber diameter as shown just above,

HW 00A.2
In 50 words or less explain why the fracture strength of optical glass fibers increases for smaller fiber diameters.
HW 00A.3
How would you expect the strength of the fibers, testing in uniaxial tension, to change with the length of the fibers

(v) The length scale relevant to deformation at high temperatures

Deformation at high temperatures depends on temperature. At high temperatures atoms move, thereby leading to deformation as shown in the schematic just below
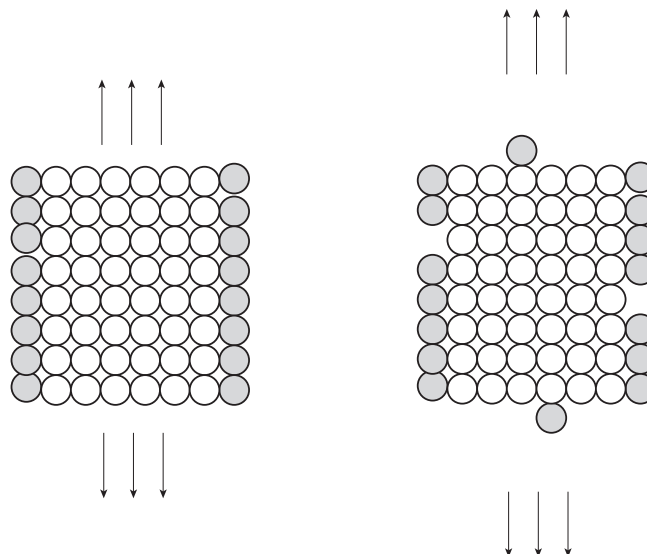
As you can imagine the movement of atoms through the crystal would be difficult.. the atoms would have to squeeze through the small spaces in between the atoms. This method of atom jumps therefore requires an activation barrier. As shown below the atoms are always jumping back and forth, but in the presence of a "driving force", there is a net flow of atoms in the direction of the driving force, illustrated below
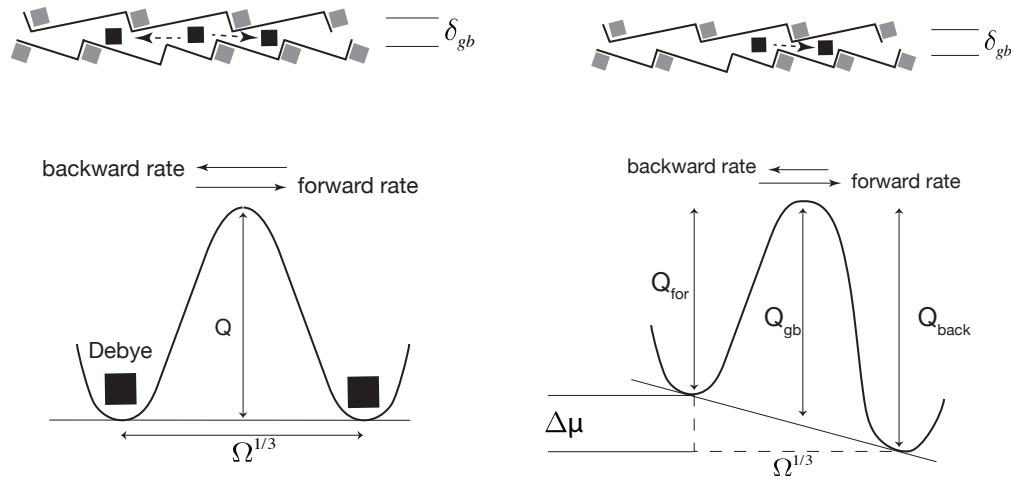
Therefore, the critical length scale in high temperature deformation is the jump distance of the atoms which is equal to $\Omega^{1/3}$.

In a polycrystal the atoms are transported from one grain boundary to another. Therefore the diffusion distance which determines the rate of high temperature deformation is equal to the grain size. Thus the grain size plays a critical role in the rate of deformation

As a note, according to above high temperature deformation can be, and is, suppressed in single crystals. That is why the turbine blades for gas turbines are made from single crystals.

Global Variables (the concept of energy)

Energy is a constant feature of modeling in materials science. It is a thermodynamic parameter, and therefore, can be used to find equivalence between thermal energy, mechanical energy and, indeed, electrical energy (important in the study of batteries, for example).

Thermal energy is the output of energy into the environment (exothermic) of absorption of energy into the system from the environment (endothermic) when something changes. An obvious event is the evaporation of a solid into vapor, which is expressed as the heat of evaporation.

Some values are:

copper: 300 kJ/mol

water: 2.26 kJ/g or 41 kJ/mol

Heat of evaporation of ice: 46.2 kJ/mol

First we look up the latent heat of melting of ice into water (334 J/g) and water into vapor (2230 J/gm), adding them gives the of evaporation as given just above, i.e. 2564 J/gm * molecular weight of ice (18 g/mol).

In work in mechanical systems is related to force and displacement. For example, consider a simple uniaxial experiment shown as above,

The data is obtained by applying a displacement and measuring the load in the drive train which gives
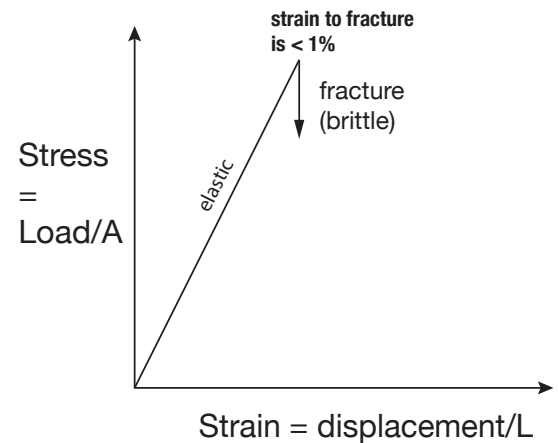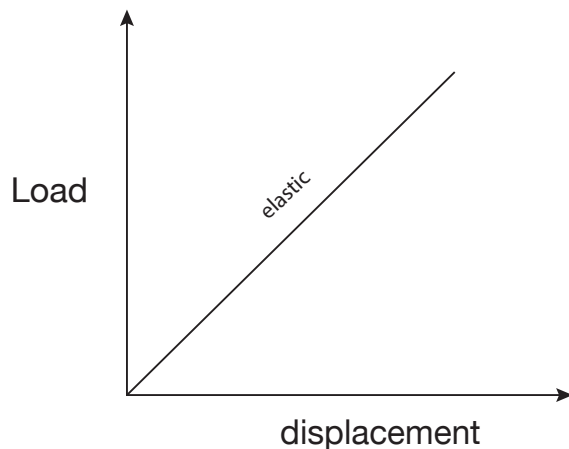
Symbols and units:

Stress $\quad \sigma = \dfrac{F}{A}$ MPa or MN m^{-2}. $\hspace{3cm}$ (00.1)

Strain $\varepsilon = \dfrac{\delta}{L}$ (dimensionless) $\hspace{3cm}$ (00.2)

Note that stress also has units of J m–3, that is energy per unit volume since,

N m–2 is the same as (Nm)m–3. Since product of force and displacement is work done, that is mechanical energy, stress may also be given the units of J m–3.

Small Strain versus Large Strain

When a specimen is deformed (for example in uniaxial tension) the length and the cross-sectional area are continuously changing. Therefore the stress and the strain are changing continuously as the specimen is pulled in tension.

In elastic deformation we approximate the strain as given in (00.2). This is an approximation that applies at small strains.

Strictly speaking the strain is accurately described as follows

$$\varepsilon_{uniaxial} = \ln\frac{L}{L_o}$$ (00.3),

which may also be written as

$$\varepsilon_{uniaxial} = \ln\left[1+\frac{\Delta L}{L_o}\right]$$

where ΔL is the physical lengthening of the sample.

The log-term can be expanded as a power series for example $\ln(1+x) = x + \frac{x^2}{2} + \frac{x^3}{3}.....$

Therefore for small strain

$$\varepsilon_{uniaxial} = \ln\left[1+\frac{\Delta L}{L_o}\right] \approx \frac{\Delta L}{L_o}$$ (00.4)

Mechanical Energy

Now let us calculate the work done in elastic deformation:

$$Work = \int_0^\delta F\,d\delta$$

Writing F as stress and δ as strain we have

$$Work = AL\int_0^\varepsilon \frac{F}{A}d\frac{\delta}{L} = V\int_0^\varepsilon \sigma\,d\varepsilon$$

Therefore energy stored per unit volume = Work/(A*L)

$$U = \frac{Work}{AL} = \int_0^\varepsilon \sigma\,d\varepsilon$$

	copper	ice
E	1.21E+11 Pa	1.00E+10
strain	0.01 i.e. 1%	0.01
molar vol	3.24E-06 m³	2.00E-05
U	6.05E+06 J/m³	5.00E+05
U_{molar}	1.96E+01 J/mol	1.00E+01
	1.96E-02 kJ/mol	1.00E-02

which is equal to the area within the triangle in the figure above on the right.

Let us apply the above equation to copper which is strained to 1%. We can calculate the stress from Youngs equation that is

$$\sigma = E\varepsilon$$

where E is the Youngs modulus. Note that it has the same units as stress, that is MPa or GPa.

Substituting above in the work equation

$$U = \int_0^\varepsilon \varepsilon E\,d\varepsilon = \frac{E\varepsilon^2}{2} \quad \text{or} \quad \frac{\sigma^2}{2E}$$ (00.3)

Let us now apply to copper.

$E_{Copper=} = 121$ GPa, or 121×10^9 Pa

U has units of energy per unit volume. We must convert it into energy per mole to compare with the heat of vaporization. Therefore, $U_{molar} = U * (molar\ volume)$, where the molar volume for copper from the Table above is 3.24E-06 m³

A comparison of chemical and elastic energy

Here we shall compare the elastic and chemical energy in ice in the following way:

(i) Chemical Energy

Here we use the handbook value for the heat of evaporation of ice, as given in one of the table above,

46.2 kJ/mol.   (00.4)

This value represents the work done to separate the bonds completely from one another.

(ii) Mechanical Energy

Assuming a fracture strain of 1%, we calculate how much mechanical work (that is the elastic strain energy stored in ice when it fractures) is needed to break the bonds.

The Youngs Modulus of ice is

10 GPa

From equation (00.3) the strain energy is given by

$$U = \int_0^\varepsilon \varepsilon E\, d\varepsilon = \frac{E\varepsilon^2}{2} \quad \text{Per Unit volume}$$

The molar volume of ice (see table further up) is 2×10^{-5} m³/mol. Therefore, the elastic energy at 1% strain is given by

$\dfrac{10 GPa * 0.01^2}{2} * 2 x 10^{-5}$. Converting GPa into Pa, we obtain the mechanical energy at the point of fracture to be

0.01 kJ/mol   (00.5)

Upon comparing Eqns. (00.4) and (00.5) we see that the chemical energy is 4,620 times greater than the mechanical energy.

Important Note: mechanical energy is usually much weaker than chemical energy. Think about how a small amount of gun powder (a chemical) can send a 100 kg shell to distances of one or two miles! Think about a small seedling can break through a road surface made from concrete. How one gallon of gasoline and power a car for 30 miles or more? It is said that the Yorkshire Cathedral which rests on iron beams at its base is lifted up when iron rusts and expands.

HW 00A.4
One gallon of gasoline has 33.7 kWh (kilo Watt hours). Convert this number into kJ.
Now calculate with reasonable approximations the work done to drive a 6000 lb car up hill at a grade of 2%, adding to it wind resistance (approximately) and the efficiency of the gasoline engine (please get this information from open sources. How far would one gallon of gasoline be able to propel this car.