01_Surface_to_Volume

Relevance to NS&E

Small objects have a high surface to volume ratio; therefore, this topic is of general interest to our course. The shape, the size and the surface area of the objects can determine the functionality of Nanoscale objects. For example, the application of graphene sheets is enhanced by their high surface area. However, the high mechanical strength of thin films and optical fibers is dependent on the probability of finding small defects within the bulk, although often emanating from the surface. The color of small particles of semiconductors such as CdSe depends on their size. The size of the embryo that we shall consider in the section on Cloud Seeding depends on the volume of the embryo, that is the number of molecules contained within it.

The surface-to-volume ratio

It is useful to recognize that surface to volume ratio, by definition, has units of m^{-1} , or nm^{-1} , etc. The surface to volume ratio of small objects is always "inversely" proportional to the smallest dimension in the shape of the object. For spheres this length scale is the diameter, in fibers is the also the diameter, and in thin films it is the thickness of the film.

Sphere

$$\frac{S}{V} = \frac{4\pi r^2}{(4/3)\pi r^3} = \frac{3}{r} = \frac{6}{d}$$

Wire

 $\frac{S}{V} = \frac{2\pi rL}{\pi r^2 L} = \frac{2}{r} = \frac{4}{d}$

Thin Films (consider just one surface is exposed since the film is on a substrate - for example a thin film of a metal grown silicon)

 $\frac{S}{V} = \frac{A}{At} = \frac{1}{t}$

Here A is the surface area of the film, t is its thickness.

Porous Materials

The high-surface-area property of the porous material cannot be surmised by surface to volume ratio. Instead, it is given by

-SSA

-specific surface area,

-it has units of $m^2 g^{-1}$, that is, the total surface area of the pores contained within one gram of the material. Typical numbers -for SSA are 10 m²/g to 1000 m² g⁻¹.

The value of SSA is related to the size, that is the surface area of each pore, and the number density of pores contained within the object. These individual pores can be nanoscale which a high surface area.

A simple way to calculate this number theoretically is to visualize the pores to be distributed in a cubic lattice, with cubes stacked next to one another, in all three directions, with each cube containing one pore per-cube. Now it is possible to calculate the weight of the cube from its effective volume and the true density of the material (remember to subtract the volume of the pore from the physical volume of the cube). The surface area within the cube is given by the surface area of one pore (usually a spherical shape is assumed).

Parameters:

Number density of pores: n (# pores per m³), pore size is d

$$n = \frac{1}{L^3}$$
, where L is the edge length of the cube.

Surface area within one cube = $4\pi \left(\frac{d^2}{4}\right)$ units m²

Weight of one cube = (volume of the cube - volume of the pore)* ρ in g

Mass of the cube =
$$\left[L^3 - \frac{4}{3}\pi \left(\frac{d}{2}\right)^3\right]\rho$$

$$SSA = \frac{4\pi \left(\frac{d^2}{4}\right)}{\left[L^3 - \frac{4}{3}\pi \left(\frac{d}{2}\right)^3\right]\rho} \qquad m^2 g^{-1}$$

$$= \frac{6}{d\rho \left[\frac{6}{n\pi d^3} - 1\right]}, \text{ check units,}$$

$$n\pi d^3$$

the upper term is dimensionless

the lower term (dp) cm*g/cm³ --> g/cm² which then gives the units for SSA.

Convert $n\pi d^3$ into the volume fraction of the pores.

Note: that experimentally we measure the volume fraction of the pores by simple measurements of the physical density of the body, that is, the density is the ideal value (we call is unity) when there are no pores and less than "unity" in the presence of pores.

 $v_f = n^*$ (volume per pore)

$$= n\frac{4}{3}\pi \left(\frac{d}{2}\right)^3 = \frac{\pi}{6}nd^3$$

SSA
$$= \frac{6}{d\rho \left[\frac{6}{n\pi d^3} - 1\right]} = \frac{6}{d\rho \left(\frac{1}{v_f} - 1\right)}$$

SSA
$$= \frac{6v_f}{d\rho (1 - v_f)}$$

(Answer)

Check the limits in the equation. (i) If the volume fraction is zero then SSA = 0. (ii) If the material is all pores then the SSA blows up because the material has no weight.

v_f	0.5
d	10 nm
	0.0000001m
density	3g/cm ³
	3000000g/m^3
SSA	200m^2/g

The excel sheet will be posted on the web (where the pdf files are uploaded). You can put in different values in the equation to check how the SSA varies with pore size for example.

In ceramics processing (called sintering) we are often interested in the SSA of a powder-pressed compact made by compaction of ceramic powders (having a diameter of few tens of nanometers upto a few μ m). In these instances the SSA is simply the surface area of one powder particle (using the average sized particle) divided by its weight. Generally small particle sizes, that is high SSA values are conducive to easier processing.