My view point of Philosophy of Modeling
you may also consider it as the first lesson in modeling

Basic Definitions about Modeling in Materials Science

i- Definition

Simply such phrase "Modeling in Materials Science" means inter-relating the materials properties, physical and chemical quantities in a mathematical formula. Thus, the difference between this philosophy and for ample Newtonian formula of (F = m a) in physics is that in materials science we need to explore at least one materials properties either in atomic (ex. intermolecular bonds) or macro-scale (ex. mechanical or even wetting) in our formula. Some simple examples are the Capillary Height as function of gravity, Partial Pressure as function of temperature, Solubility as function inter-atomic bonds, and so many other topics.

ii- What to Model

We can model two things: a material's property (ex. surface energy) or a material's phenomena (ex. surface melting or even wetting).

iii- Tools for Modeling

For modeling we need a scientific tool which in other words means a phenomenological scientific source of idea. These scientific ideas are Physics, Chemistry, Mechanic, Electric, Magnetic, … and in some special multidisciplinary sciences like Materials Science topics such as Thermodynamics, Fluid Mechanics, and … Practically they are sciences which give us the basic quantities to explain the nature.

Thermodynamics Modeling in Materials Science topics

Here the tool (**iii**) is thermodynamics; therefore, we need to clear what we want to model (**ii**).

As it was mentioned above we either model a

(**ii-a**) material's property

Or

(**ii-b**) material's phenomena (can be a starting point for simulation too)

(**ii-a**) it is obvious that material's property includes the cases which are unknown yet which mostly at this time contains topics related to surface and nano-scale. I rather make them at Ph.D. level.

examples

surface energy of metallic elements (fitting to exp.) (project of me and Dr.Riahifar)
surface energy of ceramics (fitting to exp.)
effect of curvature on surface energy (fitting to exp.)
effect of nano-scale on surface energy (fitting to exp.)
nano-phase diagram (fitting to exp.)
effect of gravity of thermodynamics properties of material
and so on …

(**ii-b**) material's phenomena cases have wider range of topics as they can be divided in two main groups

(**ii-b-1**) total hypothesis which latter fitted to exp. or other models: Here a theory first start and then lead to results and computational algorithms which can be fitted or explain an unknown phenomena

examples

surface melting and over heating (Mr. Jahangir)
effect of nano-scale on chemical and bio activity (partly Mr. Ahmadi)

(**ii-b-2**) correcting or completing the actual theories:

examples

electro wetting on dielectric (Ms. Hadidi)
effect of roughness on wetting transitions (Mr. Esmailian)
reviser electro wetting on dielectric for producing energy (Ms. Gholami)

But what are the steps for modeling in (**ii-b-2**) correcting or completing the actual theories when we deal with (**ii-b**) material's phenomena.

1. study the fundamentals

2. start experiments (if you can) but if your job is total theory then try to gather the others experimental results. (obviously Ms. Hadidi, Mr. Esmailian and Ms. Gholami have to experiment themselves)

3.1. find the singularities and unknown regime of these experimental results

Or

3.2. find the experimental results regime which can not be explained or fitted by actual models

4. chose and find the simplest model or model idea and start with your Modeling Tool (for us Thermodynamics) and try to correct or rewrite the actual models in order to either explain those singularities in a better way or even perfectly.

I tried to write the above, as I think some times students are try to jump section 2 and 3 and fly to section 4. But it is impossible at least in category (**ii-b-2**). Thus, before finishing a series of experiments and finding the singularities there is no scene to talk about the modeling.

Obviously those how study more, are able to chose the experiments in a way that in advance they could lead them to required singularities if an only if those singularities were already mentioned or tried in literatures.

I will put this hand writing in our web-site at Modeling Section too.

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