

Class 1: Introduction

This course is aimed at Undergraduate students majoring in Metallurgical and Materials Engineering. An attempt is made to ensure that the contents presented are quite complete in the sense that a typical undergraduate student may be able to read it in a continuous fashion, without having to interrupt the process to read additional background information.

Although the course is primarily aimed at students in the Metallurgical and Materials Engineering stream, the material presented in this course will largely be accessible to most undergraduate engineering students.

While this is a bit of oversimplification, pursuing a career as a materials engineer or materials scientist, broadly results in two types of jobs – that of an engineer in an industry focused on a single product, or that of a scientist in a university/laboratory setting.

An engineer in an industry setting usually faces several technical trouble shooting challenges. Such challenges, with stiff timelines, require substantial familiarity with information databases, and characterization techniques, to be successfully addressed. Addressing trouble shooting challenges are often based on the selection and use of the best available resources and substitutes. The types of questions the engineer is faced with include questions of the sort:

Is there a lighter material readily available which can replace the existing material in the product?

Why is a specific batch of the product not as good as another batch?

Will it be possible for this product to function with lesser parts than it currently has?

Answers to such questions enable the industry meet the demands of their customers at lower costs and with greater reliability.

A scientist in a university or laboratory setting faces a different kind of challenge. The questions the scientist wishes to answer are:

“Why is the value of any specific property of a material what it is?”

“What is the fundamental science behind the property?”

“What are the limits, if any, to this property?”

Answers to such questions enable one to design new materials and to push the capabilities of existing materials.

Based on the professional setting a materials specialist ends up in, he/she will likely get pulled into one of the above types of activities. However having both - a good feel for the fundamental sciences, as well as an understanding of the engineering approach to relate to the real world, can greatly enhance the value of a materials scientist/engineer to his or her organization.

However, it usually takes considerable experience to fully understand, appreciate, and make use of the linkages between fundamental sciences and the world of engineering. Experience and systematic studies provide us with the insight to make the connections

between the real world inventions and the science behind them. Such insight helps us truly appreciate the contributions of the scientist as well as the engineer in shaping our interactions with the world around us. Such insight, also enables us to take our technical pursuits to greater heights and wider reaches, and hence is desirable.

In this course we shall focus on trying to understand the science behind material properties. One of the approaches used for this is to model materials. The idea behind this approach can be described as follows: The constituents of the material, atoms, electrons etc. are assumed to follow specific rules. The set of rules we assume for the constituents together constitute the 'model' we propose for the material. These rules are selected by us based on our best guess of what is reasonable to assume for these constituents. Assuming that the constituents follow these rules, the material is then 'built up' based on these constituents. Based on the rules that we have assumed, predictions are now made on what the material properties are likely to be and how these properties will respond to external influences. These predictions are then compared with experimental data. If the experimental data and trends in experimental data match the predictions, we conclude that our 'model' is correct. In case we have incorrect predictions, the model needs to be changed or corrected till we can get predictions to match the experimental data.

In this activity we accept the hierarchy that experimental data is supreme. A model, no matter how sophisticated it may appear at first glance, is of value, if it is unable to predict experimental data. At the same time, it must also be noted that when a failure is noted for a model, in a sense the failure identifies limits to be placed on the model's capabilities. For example, if a model correctly predicts experimental data between two temperatures T_1 and T_2 , but makes incorrect predictions at temperatures outside this range, it is not correct to dismiss the model as 'useless'. A more appropriate reaction is to say that the model may need further refinement, and specifically, as long as the temperatures of interest lie between T_1 and T_2 , the model is still very usable. Further refining the model may require us to add additional details into the model or perhaps recognize and incorporate new phenomena and processes that come into operation when specific threshold values of temperature, or other experimental parameters, are crossed.

In the literature as well as in many industries models are used which are entirely empirical. This often means that there is no firm understanding of the science behind the response of a system, maybe because the system is too complicated, yet there is an empirical formula or curve fit that matches the experimental data from the system very well. Such models are of practical value since it does enable some predictions of what is likely to happen when specific parameters change in value, even though there may be little understanding of why the response is changing the way it is.

In this course we will broadly look at the following:

- 1) Properties of materials
- 2) Relationships between some of the properties of materials
- 3) Theories for the behavior of metallic systems
- 4) Quantum mechanics
- 5) Understanding material properties based on the theories developed.

The focus of much of this course will be on electronic properties of materials, and relatively less on the other properties, although initially an overview of the properties and some relationships between them will be considered and discussed.

This course will cover material equivalent to 40 lectures and will contain sections that are descriptive, and other sections that rely heavily on theory and derivations.

It is also noteworthy that many of the topics discussed in this course as well as the corresponding equations and insights, resulted in the associated researchers receiving Nobel Prizes. It is therefore not entirely surprising to face some initial difficulties in understanding the topics covered.