PHYSICS SCHOOL

PHYSICS OF MATERIALS

Mechanical Properties and Crystal Defects in Solids

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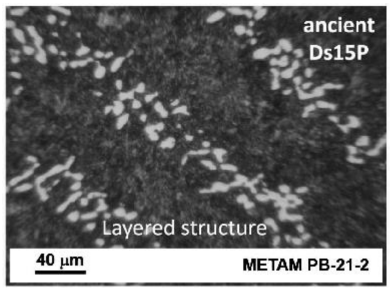
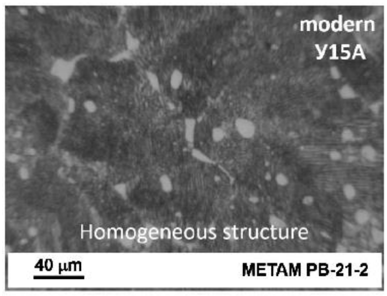
INTRODUCTION

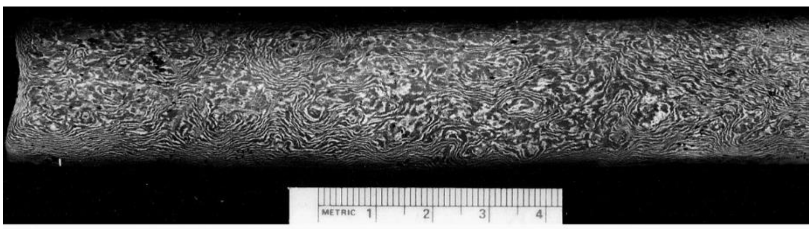
Every evolution of human history is linked to the discovery of new materials, which allowed us to produce tools, structures, and machines with constantly increasing performance. For instance, prehistoric ages are named according to the materials used, e.g., stone, bronze, iron. Some characterize our current era as the information technology and quantum age marked by the discovery of new materials enabling the production of semiconductors and superconductors. For a long time, the discovery of new materials has been driven more by chance and empirical knowledge than by a systematic pursuit of a particular property. For example, the discovery of iron quenching was possible because the iron was heated on a coal fire; the soot deposited on the blade formed an iron-carbon alloy: steel. After rapid cooling of this alloy, a tough and hard structure forms: martensite.

Damascus Steel



Modern Tool Steel





The Figiel blade purchased in Rajasthan India.

The layered microstructure of a Damascus steel sword of antiquity that gives its superior mechanical properties is comparable to those of modern tool steel used in manufacturing.

Damascus Steel is one of the most notable historical references to empirical material processing for weaponry (See Figure 1 above). Swords made of such steel were extremely sharp. They would not bend nor shatter under extreme forces, having extraordinary properties over iron swords of the period, making them fabled to be imbued supernatural powers and invincible (perhaps the famed Excalibur was a Damascus Steel Sword). The first historical references to such swords emerged in regions of modern-day Syria. Writings found in Asia Minor said that to temper a Damascus sword, the blade must be heated until it glows "like the sun rising in the desert. " It then should be cooled to the color of royal purple and plunged "into the body of a muscular slave" so that his strength would be transferred to the sword. Aside from the horrific brutality and cruelty, this macabre account of metallurgy in the Dark Ages has merit from processing and physics of diffusion and phase transformation kinetics. Specific phases are formed by controlling the cooling rate and diffusion of carbon in the steel. Continually heating, folding the steel, and quenching it at optimal rates form a layered microstructure that gives Damascus steel its high hardness, strength, and toughness. Sadly, suppose the Dark Ages societies knew the science of metallurgy and that plant oils and other quench media are far better for making Damascus steel; sword making could have been a less murderous profession. Modern tool steel used for Cutting and other manufacturing applications has similar phase distribution and mechanical properties, which are more performant than Damascus steel and are produced by well-defined processing steps that emerged from the metallurgical research of the 20^{th} century. Chapter XII discusses phase transformation kinetics and continuous cooling curve analysis for producing these desired microstructures.

Previously, every advancement in use and the discovery of new materials had essentially been technological. Only within the past century has the production of new materials left empiricism to become an engineering science. English uses the term "Materials science and engineering" to highlight how fundamental research supports the design of new materials. Materials science is thus a common field for physical engineers. In practice, the term "Materials science and engineering" has been in use since the 1950s, and materials science is a very young discipline.

The question arises about what events marked the transformation of materials technology in science. As R.W. Cahn states in an article in the scientific journal "Nature Materials" (Vol. 1, pp. 34), this transition was achieved when scientists and physicians, in particular, began to be interested in the study of "dirty" matter. Until the 1930s, "good science" had to use the purest substances: just approaching solid matter was considered an incursion into adventurous and mysterious territory.

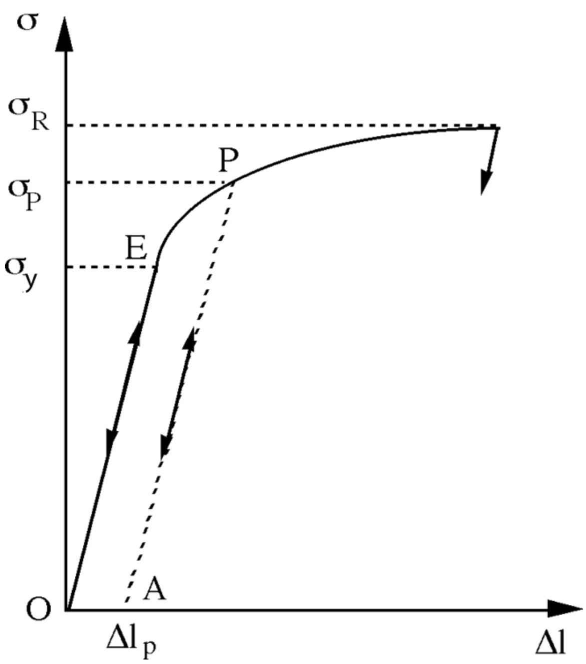
Only in the post-war years did the interest in the effect of impurities in solid conductors pave the way for transistors. Those were the times when a more explicit link between structural defects and mechanical properties of metals was finally drawn. For example, the very peculiar arrangement of carbon within iron gives the steel its characteristic high hardness. Furthermore, due to the dislocation glide (motion), steel can be deformed and shaped into different forms and not shatter due to brittle fracture.

The 21^{st} century has ushered in remarkable advancements in metallurgy research, focusing on developing materials with superior performance and designed properties optimized for applications. One of the key areas of exploration is advanced materials, where high-strength alloys, nanomaterials, and shape memory alloys are gaining prominence. High-strength alloys, particularly for aerospace, are engineered to be lighter, more fuel-efficient, and capable of withstanding extreme conditions, which is vital for commercial and defense aviation. Meanwhile, integrating nanotechnology in metallurgy has opened up new possibilities for creating nanomaterials and nanocomposites, which can be found in electronics, sports equipment, and more. Shape memory alloys, which have the unique ability to return to their original shape after deformation, are making strides in medical devices, robotics, and actuators, demonstrating the versatility of metallurgical innovations in modern technology.

Sustainability is another crucial focus in 21st-century metallurgy research, driven by growing environmental concerns. Researchers are increasingly exploring green materials that reduce carbon footprints and contribute to a circular economy. Additionally, metallurgy plays a critical role in renewable energy, particularly in developing components for wind turbines, solar panels, and batteries, which are essential for a sustainable energy future. The advent of advanced manufacturing techniques, such as additive manufacturing and 3D metal printing, is further revolutionizing the field by enabling the production of complex metal components with enhanced properties and reduced waste. Moreover, incorporating artificial intelligence in material discovery accelerates innovation, allowing for more efficient design and development of new materials. As the field progresses, metallurgy contributes significantly to biomedical advancements by developing biocompatible metals for implants and prosthetics. Despite these advancements, challenges such as sustainability, resource scarcity, and environmental concerns persist. Metallurgical remains important, with a continued emphasis on creating stronger, lighter, more eco-friendly materials and processes.

The 21st century of material physics also marks a paradigm shift away from empirical research, making explicit links between applications and specific alloys or compounds. The empirical research method takes decades to develop new materials for applications and is much too slow. The Material by Design concept was formed from large-scale initiatives and the need to design new materials with tailored properties for specific applications. Researchers use materials-by-design strategies to improve fundamental understanding and develop tools for critical materials issues. These efforts help to identify gaps and improve material characterization tools and models at different length scales, from the atomic level to bulk properties, advancing computational tools for designing better materials. This new modality of materials design is essential for developing nanotechnology and quantum materials and technologies. This course provides a fundamental background of structural defects in crystal solids and their link to their structural and mechanical properties. Solid-state physics courses broadly discuss transport, magnetic, optical, and electrical properties. This course aims to provide basic notions and a general method enabling physicists to interpret the mechanical properties of solid materials typically encountered during their career as professional engineers and may form the basis to drive new avenues of research in their academic careers.

The scientific method's first stage is based on observing natural phenomena. For example, the figure below represents the stress-strain curve of a crystalline sample undergoing a tensile test with fixed elongation velocity. If the tensile test is interrupted before the sample breaks and the stress is brought back to zero, two cases may arise:



Schematic representation of a stress-strain curve of a metallic sample in a tensile test at imposed Velocity.

1) If the maximum stress was lower than a value σ_y, the unloading curve overlaps with the loading curve. In this case, the sample has the same shape at the end of the unloading as before the stress was applied (absence of permanent deformation). The temporary deformation is called elastic strain. The stress σ_y is the **yield stress** of the material. The elastic behavior of a solid body is defined by the return to the initial zero deformation once all applied stresses vanish. Solid materials - as opposed to liquids and gases - show this behavior under lower stresses.

2) If the maximum actual stress σ_a has peaked to a higher value than the yield strength σ_p, then the stress-strain curve is no longer reversible, and the sample has a residual deformation Δl_p, called plastic strain. Moreover, if another stress is applied, the loading will follow line A-P as in the previous unloading, a line parallel to the initial elastic slope O-E. The new yield strength will be in point P at a stress value of σ_p, which is called plastic flow stress and has the same role that σ_y had before the solid has thus strengthened.

3) Suppose the deformation is continued until the stress σ_R, the sample breaks, and the ultimate tensile strength is defined as the maximum stress on the stress-strain curve before rupture, the fracture strain being the maximum plastic strain that occurs at this point. This behavior can be explained through models of the material's microstructure and its evolution under the Application of stresses.

In this sense, the elastic behavior should be related to the crystal structure and the type of atomic bonding. The first three chapters of this course discuss elastic theory and its relation to materials' structure and mechanical behavior. The non-linearities and the permanent deformations observed beyond the elastic yield limit can be explained by the presence of defects in the crystal structure: point and line defects called dislocations. From Chapter IV to Chapter X, we discuss the motion of these defects and the methods to measure them. Finally, the last part of the course focuses on the structural changes (solidification, phase transitions) that arise during the fabrication and processing of actual materials.