

# EPFL

PHYSICS SCHOOL

## PHYSICS OF MATERIALS

*Mechanical Properties and Crystal  
Defects in Solids*

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# TABLE OF CONTENTS

<b>INTRODUCTION</b>	<b>1</b>
<b>CHAPTER I Atomic bonds</b>	
<b>1.1 Classes of materials</b>	<b>5</b>
<b>1.2 Atomic bonds</b>	<b>7</b>
1.2.1 Ionic bond	8
1.2.2 Van der Waals interactions	10
1.2.3 Covalent bond	11
1.2.4 Metallic bond	14
1.2.5 Atomic bonds and materials	15
<b>Bibliography</b>	<b>15</b>
<b>CHAPTER II Crystal structure</b>	
<b>2.1 Crystal lattices</b>	<b>17</b>
2.1.1 Historical references	17
2.1.2 Description of a crystal lattice	18
2.1.3 Direct lattice and reciprocal lattice	18
2.1.4 Vector operations: dot product, cross product, metric	21
2.1.5 Crystal systems	22
<b>2.2 Compact structures</b>	<b>23</b>
<b>2.3 Coordination number</b>	<b>27</b>
<b>CHAPTER III Theory of elasticity</b>	
<b>3.1 Simple laws and linear elasticity</b>	<b>29</b>
<b>3.2 Strain tensor</b>	<b>32</b>
<b>3.3 Stress tensor</b>	<b>34</b>
<b>3.4 Thermodynamic review</b>	<b>35</b>
<b>3.5 Thermodynamics and deformation</b>	<b>36</b>
3.5.1 Work	36
3.5.2 Energy	37
3.5.3 Physical origin of elasticity	38
<b>3.6 Hooke's law</b>	<b>39</b>
3.6.1 Deformation of isotropic solids	39
3.6.2 Temperature effects	42

3.6.3	Equilibrium equation of isotropic bodies	42
3.6.4	Generalized Hooke's law	43

## **CHAPTER IV Defects in crystals**

<b>4.1</b>	<b>Introduction</b>	<b>47</b>
<b>4.2</b>	<b>Point defects – an introduction</b>	<b>52</b>
4.2.1	Formation energy for point defects	54
4.2.2	Concentration of vacancies at thermodynamic equilibrium	59
4.2.3	Creation of vacancies	65

## **CHAPTER V Diffusion**

<b>5.1</b>	<b>Fundamental equations of diffusion</b>	<b>69</b>
5.1.1	Phenomenological equations	69
5.1.2	Solution to Fick's second law	71
<b>5.2</b>	<b>Diffusion coefficient and random motion</b>	<b>72</b>
<b>5.3</b>	<b>Self-diffusion</b>	<b>74</b>
5.3.1	The mechanisms of diffusion	74
5.3.2	Vacancy mechanism	75
<b>5.4</b>	<b>Applied force to the diffusing particle: Einstein's equation</b>	<b>76</b>
<b>5.5</b>	<b>Diffusion couple: the Boltzmann-Matano method</b>	<b>78</b>
<b>5.6</b>	<b>The Kirkendall effect</b>	<b>83</b>
<b>5.7</b>	<b>Real solutions</b>	<b>87</b>

## **CHAPTER VI Plastic deformation**

<b>6.1</b>	<b>Phenomenology of plastic deformation</b>	<b>89</b>
6.1.1	Experimental observations	89
6.1.2	Relations between sliding and crystal structure	90
<b>6.2</b>	<b>Elastic yield strength and the dislocation concept</b>	<b>92</b>
6.2.1	Rigid gliding over a plane	92
6.2.2	Localized gliding	93
6.2.3	Creation of a dislocation	100
<b>6.3</b>	<b>General properties of dislocations</b>	<b>104</b>
6.3.1	dislocation loops	104
6.3.2	Properties of the Burgers vector	105

<b>6.4</b>	<b>Dislocation motion</b>	<b>107</b>
6.4.1	Glide plane	108
6.4.2	Climb of a dislocation	109
6.4.3	Relation between dislocation motion and plastic deformation	110
<b>6.5</b>	<b>Multiplication of dislocations</b>	<b>111</b>
6.5.1	Hardening phenomenon	111
6.5.2	Sources of dislocations	113
6.5.3	Other hardening processes	113
<b>6.6</b>	<b>Recrystallization</b>	<b>115</b>
<b>6.7</b>	<b>Crystal growth</b>	<b>115</b>

## CHAPTER VII Elastic theory of dislocations

<b>7.1</b>	<b>Introduction</b>	<b>119</b>
7.2	Stress field around a dislocation	120
7.2.1	Screw dislocation	120
7.2.2	Edge dislocation	123
<b>7.3</b>	<b>Elastic energy</b>	<b>124</b>
7.3.1	Screw dislocation	124
7.3.2	Edge dislocation	125
7.3.3	Mixed dislocation	126
7.3.4	The problem of the dislocation core	127
<b>7.4</b>	<b>Interaction energy between dislocations</b>	<b>128</b>
<b>7.5</b>	<b>Force of a dislocation</b>	<b>129</b>
7.5.1	Definition	129
7.5.2	Applications	130
7.5.3	interaction with surfaces: image forces	132
7.5.4	The concept of line tension	133
7.5.5	Interpretation of the line tension	133
7.5.6	Application: Frank-Read sources	135
<b>7.6</b>	<b>Dislocations in FCC metals</b>	<b>137</b>
7.6.1	Shockley partial dislocations	137
7.6.2	Thomson tetrahedron. Frank partial dislocation, Lomer-Cottrell dislocation	140
7.6.3	observation after quenching of samples at high and low stacking fault energy	145
7.6.4	Measure of the energy for a stacking fault	147
7.6.5	Cross-slip	149

## **CHAPTER VIII Dislocation kinetics**

<b>8.1</b>	<b>Relation between shear and macroscopic deformation</b>	<b>153</b>
<b>8.2</b>	<b>Strain curve</b>	<b>154</b>
<b>8.3</b>	<b>Interactions of dislocations with the crystal lattice</b>	<b>157</b>
<b>8.4</b>	<b>Propagation regulated by the interaction with other dislocations</b>	<b>159</b>
8.4.1	Long distance stresses due to the Frank network	159
8.4.2	Short distance interactions	164
<b>8.5</b>	<b>Propagation controlled by the interaction with a solid solution</b>	<b>164</b>
8.5.1	Types of interaction between dislocations and atoms of the solute	164
8.5.2	Propagation of the dislocation through a distribution of point defects	165
<b>8.6</b>	<b>Interactions with moving impurities</b>	<b>168</b>
8.6.1	Portevin - Le Châtelier effect (qualitative description)	169
<b>8.7</b>	<b>Interaction with precipitates</b>	<b>170</b>
8.7.1	cutting of a precipitate	170
8.7.2	Bypass mechanism	170
8.7.3	Competition between the bypass and cutting mechanisms	171
<b>8.8</b>	<b>Interaction with the grain boundaries: Hall-Petch law</b>	<b>172</b>

## **CHAPTER IX Thermal activation of the dislocation motion**

<b>9.1</b>	<b>Introduction</b>	<b>175</b>
<b>9.2</b>	<b>Strain rate</b>	<b>176</b>
<b>9.3</b>	<b>Gibbs free energy calculation during the crossing of an obstacle</b>	<b>177</b>
9.3.1	Analysis in terms of applied stress	177
9.3.2	Analysis in terms of effective stress	182
<b>9.4</b>	<b>Measure of thermodynamic quantities</b>	<b>184</b>
<b>9.5</b>	<b>Climb of dislocations</b>	<b>187</b>
9.5.1	Introduction	187
9.5.2	Geometric aspect of the climb	188
9.5.3	Forces on a dislocation	189
9.5.4	Bardeen-Herring sources	191
9.5.5	Velocity of the climb of a dislocation	192
9.5.6	Climb governed by diffusion in the crystal	196
9.5.7	Application to stationary creep	196

## **CHAPTER X Electron Microscopy characterization of Dislocations**

<b>10.1</b>	<b>Transmission Electron Microscope (TEM)</b>	<b>198</b>
10.1.1	A Brief History and Background	198
10.1.2	Spatial Resolution of TEMs	199
10.1.3	TEM construction	201
10.1.4	Interactions of fast electrons with TEM samples	203
10.1.5	Diffraction and Imaging Modes	204
<b>10.2</b>	<b>Howie Whelan Equations</b>	<b>206</b>
10.2.1	Kinematical and Dynamical Diffraction	207
10.2.2	Using the Howie -Whelan equations to interpret dynamical diffraction contrast around defects	209
<b>10.3</b>	<b>Characterization of Dislocations Using TEM Imaging Techniques</b>	<b>212</b>
10.3.1	Brightfield Imaging	212
10.3.2	Dark-Field Imaging	213
10.3.3	Weak-Beam Dark-Field Imaging	213
10.3.4	Determination of Burgers Vector and Line Direction	214
<b>10.4</b>	<b>Scanning TEM dislocation imaging</b>	<b>215</b>
10.4.1	High Angle Annular Darkfield Imaging	217
10.4.2	Fourier Filtering	218
<b>10.5</b>	<b>Geometric Phase Analysis (GPA)</b>	<b>219</b>

## **CHAPTER XI Phase transformations I: solidification**

<b>11.1</b>	<b>Introduction</b>	<b>222</b>
<b>11.2</b>	<b>Thermodynamics background</b>	<b>222</b>
11.2.1	Calculation of the mixing entropy (ideal solid solution)	223
11.2.2	Formation heat or mixing enthalpy $\Delta H_m$ calculation (real solution)	223
11.2.3	Chemical potential and activity	226
<b>11.3</b>	<b>Binary phase diagrams</b>	<b>227</b>
11.3.1	Chemical potential	227
11.3.2	Free energy of a mixture of phases	227
11.3.3	Construction of binary phase diagrams	228
<b>11.4</b>	<b>Solidification</b>	<b>233</b>
11.4.1	Nucleation	236

11.4.2	Statistics of nucleation	239
11.4.3	TTT curves (Time-Temperature-Transformation diagrams)	241
11.4.4	Crystal growth	242
11.4.5	Dendritic growth in pure metals	243
<b>11.5</b>	<b>Solidification of binary alloys</b>	<b>247</b>
11.5.1	Thermodynamic equilibrium	248
11.5.2	Thermodynamic equilibrium in the liquid - no diffusion in the solid	248
11.5.3	Solidification controlled by diffusion in the liquid phase	250
<b>11.6</b>	<b>Solidification structures of alloys</b>	<b>252</b>
11.6.1	Cellular texture	252
11.6.2	Dendritic texture	253
11.6.3	Eutectic solidification	254
<b>11.7</b>	<b>Solidification of a bar</b>	<b>258</b>
11.7.1	Crystallization of the bar	258

## **CHAPTER XII Phase transformations II: Solid state transformations**

<b>12.1</b>	<b>Introduction</b>	<b>260</b>
<b>12.2</b>	<b>Transformations with diffusion</b>	<b>261</b>
12.2.1	Homogeneous nucleation	261
12.2.2	Heterogeneous nucleation	267
<b>12.3</b>	<b>Transformation kinetics: Avrami-Johnson-Mehl equation</b>	<b>268</b>
<b>12.4</b>	<b>Examples of TTT diagrams</b>	<b>271</b>
12.4.1	CCT diagrams (Continuous cooling transformation)	272
<b>12.5</b>	<b>Transformations without diffusion</b>	<b>273</b>
<b>12.6</b>	<b>The martensitic transformation</b>	<b>274</b>
12.6.1	Crystallography of the martensitic transformation	275
12.6.2	Thermodynamic of the martensitic transformation	278
<b>12.7</b>	<b>Thermoelastic alloys: memory effect and pseudoelasticity</b>	<b>282</b>
12.7.1	Shape memory effect	282
12.7.2	Pseudoelasticity	283

# INTRODUCTION

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The discovery and mastery of new materials and technologies have marked every significant stage of human history. Prehistoric ages are even named after them: Stone, Bronze, and Iron Ages. The development of tools, structures, and machines has always relied on our ability to shape materials into stronger, sharper, lighter, or more durable forms. Today, some describe our era as the information and quantum age, enabled by the development of semiconductors, superconductors, and advanced alloys. As in the past, the properties of these materials define the frontiers of technology.



*Figure 1: Man has learned to harness nature and progress through material science and engineering and the development of new materials and technologies.*

For millennia, progress in metallurgy and materials processing relied more on chance and empirical observation than on scientific understanding. The discovery of quenching steel illustrates this: when iron, heated in a coal fire, absorbed carbon from the soot and was rapidly cooled, it transformed into a hard phase known as martensite. Another legendary example is Damascus steel, renowned for its exceptional sharpness, resilience, and toughness in swords. They would not bend or shatter under extreme forces, possessing extraordinary properties compared to iron swords of the period. Ancient blacksmiths achieved this through repeated heating, folding, and quenching of steel, unknowingly creating a layered microstructure comparable to modern tool steels. Folklore attributed mystical powers to these weapons, although their superiority stemmed from microstructural control — specifically, the diffusion of carbon, phase transformations, and controlled cooling rates. Perhaps the famed Excalibur was a sword made of Damascus steel.

Only in the 20th century did metallurgy evolve from craftsmanship into a science. Systematic research on atomic bonding, crystal structures, defects, and phase transformations established Materials Science and Engineering as disciplines. For a long time, the discovery of new materials has been driven more by chance and empirical knowledge than by a systematic pursuit of specific properties. Modern tool steel used for cutting and other manufacturing applications has a similar phase distribution and mechanical properties, which are more performant than Damascus steel and are

produced by well-defined processing steps guided by **phase transformation kinetics** and **continuous cooling curve analysis** (see Chapter XII), which emerged from the metallurgical research of the 20<sup>th</sup> century, producing these desired microstructures.

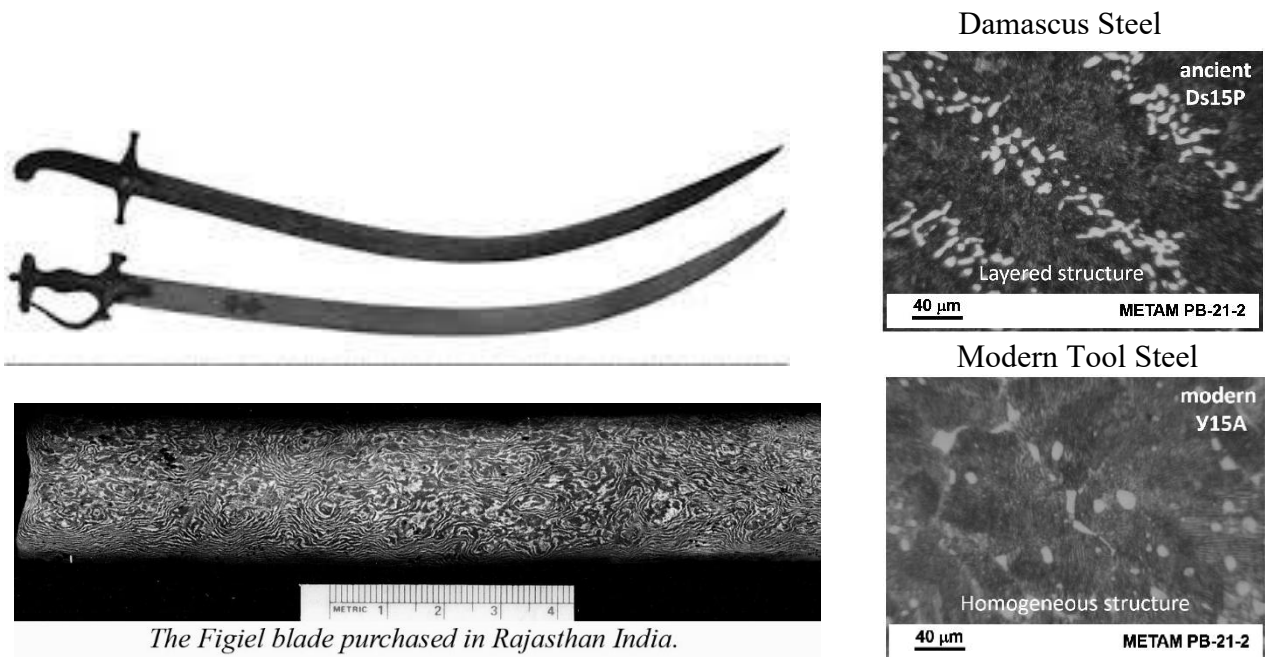


Figure 2: The layered microstructure of a Damascus steel sword of antiquity that gives its superior mechanical properties is comparable to those of modern tool steel used in manufacturing.

Previously, every advancement in use and the discovery of new materials had essentially been technological in nature. 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. 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 the mechanical properties of metals was finally drawn. For example, the very peculiar arrangement of carbon within iron gives the steel its characteristic high hardness. Moreover, due to dislocation glide (motion), steel can be deformed and shaped into different forms without shattering due to brittle fracture. As R.W. Cahn noted, a decisive turning point occurred when scientists began studying "dirty" matter — real solids with impurities and defects — rather than focusing exclusively on pure substances. This shift led to fundamental discoveries:

- The link between **defects in crystals** and **mechanical properties**.
- The role of **impurities** in semiconductors, paving the way for **transistors**.
- The relationship between **dislocation motion** and the ductility of metals.

These insights connected atomic-scale structure to macroscopic performance, laying the foundation of much of modern theoretical understanding in materials science.

The 21<sup>st</sup> century has ushered in remarkable advancements in materials science, focusing on the development of materials with superior performance and properties optimized for specific

applications. The current century has introduced a new paradigm: **materials-by-design**. Instead of relying on decades of empirical trial and error, scientists use computational modeling, artificial intelligence, and high-throughput experiments to design alloys, composites, and nanomaterials with tailored properties. Applications are broad:

- **Aerospace**: high-strength, lightweight alloys for extreme environments.
- **Nanotechnology**: nanocomposites in electronics, energy, and sports.
- **Shape memory alloys**: medical devices, robotics, and actuators.
- **Renewable energy**: steels for wind turbines, materials for solar cells, and advanced battery components.
- **Biomedicine**: biocompatible metals for implants and prosthetics.

At the same time, metallurgy faces new challenges: **sustainability**, **resource scarcity**, and the demand for **eco-friendly processes**. 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.. Despite these advancements, challenges such as sustainability, resource scarcity, and environmental concerns persist. Materials science research remains essential, with a continued emphasis on developing stronger, lighter, and more environmentally friendly materials and processes. Green metallurgy, recycling, and circular materials economy are now as critical as mechanical performance.

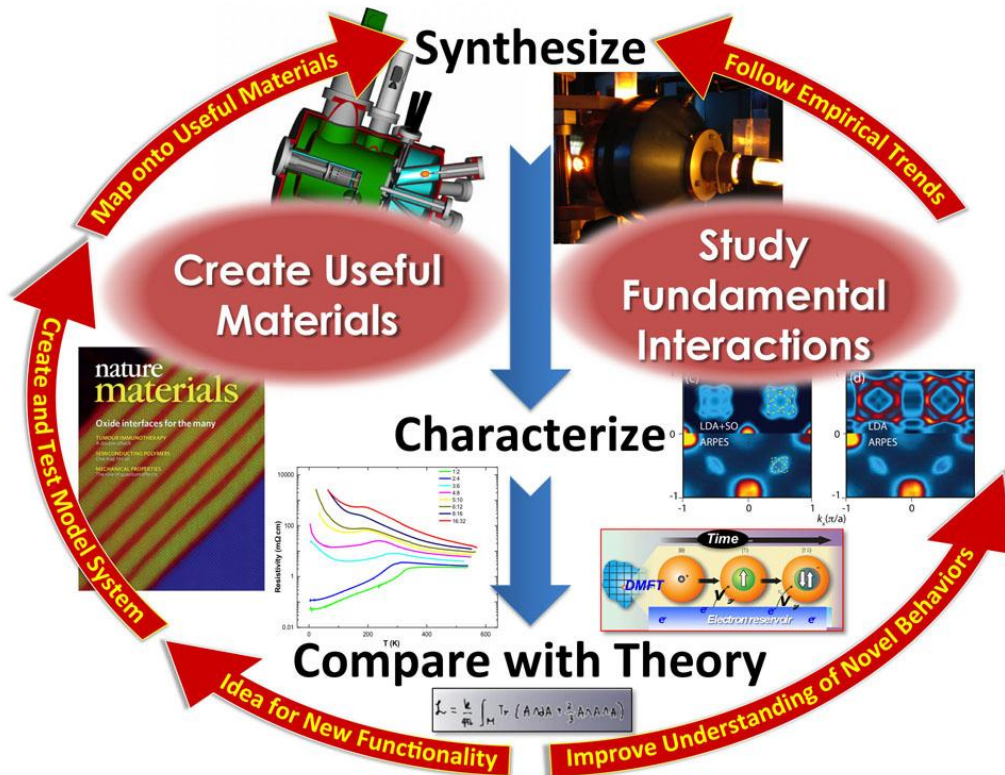


Figure 3: The Materials-by-Design Concept.

The 21<sup>st</sup> 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, which is far 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 employ materials-by-design strategies to enhance fundamental understanding and develop tools for addressing critical materials issues. These efforts help identify gaps and improve material characterization tools and models at various length scales, from the atomic level to bulk properties, thereby 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 builds a bridge from atomic-scale structure to macroscopic properties:

- **Chapters I–II:** Foundations — atomic bonds and crystal structures.
- **Chapter III:** Theory of elasticity, linking atomic interactions to macroscopic deformation.
- **Chapters IV–X:** Defects in crystals, defect diffusion kinetics, dislocation theory, and experimental characterization, explaining how imperfections govern plasticity, strength, and toughness.
- **Chapters XI–XII:** Phase transformations — solidification, martensite, and recrystallization — showing how processing controls microstructure and performance.

By the end of this course, students will be able to interpret the **mechanical behavior of solids** from their **atomic structure**, understand the role of **defects and microstructure**, and appreciate the central role of materials in technology and innovation.