3.14 Physical Metallurgy
3.40J/22.71J Modern Physical Metallurgy

Structures – Properties – Processing – Functions

theory

Acta Materialia (1996-present)
Materials Processing

**Thermomechanical:** “Heat and Beat”

**Chemical:** alloy chemistry, doping, corrosion, oxidation

**Radiation:** exposure to light, electron beam, $\alpha$ particles, neutrons

During processing, the material is often put in excited states, to achieve structural changes. These structural changes are preserved as the materials “cools down”, and taken advantage of (“properties”) during use. The whole process requires free-energy dissipation & varying degree of out-of-equilibriumness.
Mechanical metallurgy: “Just beat, No heat”

Creates compressive residual stress on the surface to delay fatigue crack initiation
Structure-property relationship

Electronic structure: \[ i\partial_t \Psi(x_1, x_2, \ldots, x_N) = \mathcal{H} \Psi(x_1, x_2, \ldots, x_N) \]

Atomic structure: FCC, BCC, HCP, diamond cubic, liquid, glass, gas, …

Molecular structure: double stranded helical DNA, protein

Nanostructure: ZnO nanowire, Pt nanoparticle, …

Microstructure: grain boundaries, dislocation tangle, …

Mesostructure: pile of sand, …

Macrostructure: bicycle, Great Wall, …
"microstructure controls properties" - old-school metallurgists

"One nanometer (one billionth of a meter) is a magical point on the dimensional scale. Nanostructures are at the confluence of the smallest of human-made devices and the largest molecules of living systems..." - U.S. National Science Foundation, 2001, Nanoscale Sci. & Eng. Center program
http://tu-freiberg.de/fakult4/imfd/cms/Multiscale/multiscale.html
Dao et al, "Toward a quantitative understanding of mechanical behavior of nanocrystalline metals," Acta Mater. 55 (2007) 4041: Fig. 1. (a) Grain size dependence of strength of Cu. The strength (or hardness) is plotted vs. $d^{-1/2}$. Literature data on hardness (solid symbols) and yield strength (multiplied by 3) from compression tests (empty symbols) are included in (a), and tensile yield strength are included in (b). The straight lines represent the H–P relation extrapolated from mc Cu. Note that most ultrafine crystalline Cu samples (with $d$ in the submicron regime) exhibit higher hardness and tensile strength than the H–P expectation. The possible reason may be related with the fact that the ufc samples were prepared via severe plastic deformation, in which dense dislocation walls, tangles, cell walls or even subgrain boundaries are formed.
Microstructural **Evolution** versus Darwin’s **Evolution**?


Carnot ideal heat engine efficiency:

\[ \frac{T_1 - T_2}{T_1} \]

Cosmic radiation background: 2.7K

In terms of quantity: \( E_{in} \approx E_{out} \)

But in terms of quality or free energy, earth enjoys (spends) huge drop
Residual Stress

Self-equilibrating body

\[ \nabla \cdot \sigma = 0 \]

does not mean \( \sigma(x) = 0 \)
### Table 1.1 Crystal Structure of Some of the More Important Metallic Elements

<table>
<thead>
<tr>
<th>Face-Centered Cubic</th>
<th>Closed-Packed Hexagonal</th>
<th>Body-Centered Cubic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron (911.5 to 1396°C)</td>
<td>Magnesium</td>
<td>Iron (below 911.5 and from 1396 to 1538°C)</td>
</tr>
<tr>
<td>Copper</td>
<td>Zinc</td>
<td>Titanium (882 to 1670°C)</td>
</tr>
<tr>
<td>Silver</td>
<td>Titanium (below 882°C)</td>
<td>Zirconium (863 to 1855°C)</td>
</tr>
<tr>
<td>Gold</td>
<td>Zirconium (below 863°C)</td>
<td>Tungsten</td>
</tr>
<tr>
<td>Aluminum</td>
<td>Beryllium</td>
<td>Vanadium</td>
</tr>
<tr>
<td>Nickel ferromagnetic</td>
<td>Cadmium</td>
<td>Molybdenum</td>
</tr>
<tr>
<td>Lead</td>
<td>Cobalt ferromagnetic</td>
<td>Alkali Metals (Li, Na, K, Rb, Ca)</td>
</tr>
<tr>
<td>Platinum</td>
<td>graphite</td>
<td></td>
</tr>
<tr>
<td>Palladium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Iridium</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**Fig. 1.1** (A) Body-centered cubic unit cell. (B) Eight unit cells of the body centered cubic lattice. (C) Cut view of a unit cell.

**Fig. 1.2** (A) Face-centered cubic unit cell. (B) Cut view of a unit cell.
Coordination = 12

**FIG. 1.4** (A) Face-centered cubic unit cell (hard-ball model). (B) Same cell with a corner atom removed to show an octahedral plane. (C) The six-face diagonal directions

Coordination = 8

**FIG. 1.3** Hard-ball model of the body-centered cubic unit cell
**FIG. 1.16** The four coordinate axes of a hexagonal crystal
FIG. 1.5 Atomic arrangement in the octahedral plane of a face-centered cubic metal. Notice that the atoms have the closest possible packing. This same configuration of atoms is also observed in the basal plane of close-packed hexagonal crystals.
Miller Index for Crystallographic Direction

\[ \text{[hkl]} \equiv h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3 \]

\(<hkl> \equiv \text{all symmetry permutations of } [hkl]\)

**FIG. 1.11** The [111] and [101] directions in a cubic crystal; directions \(m\) and \(n\), respectively
Miller Index for Crystallographic Plane

\((hkl)\) are planes parallel to the plane that goes through three points \(h^{-1}a_1, k^{-1}a_2, l^{-1}a_3\)

\(\{hkl\} \equiv \text{all symmetry permutations of } (hkl)\)

**FIG. 1.13** The intercepts of the (623) plane with the coordinate axes
FIG. 1.17 The (1012) plane of a hexagonal metal
\[(X, Y) = \left( \frac{x}{1-z}, \frac{y}{1-z} \right), \]

\[(x, y, z) = \left( \frac{2X}{1 + X^2 + Y^2}, \frac{2Y}{1 + X^2 + Y^2}, \frac{-1 + X^2 + Y^2}{1 + X^2 + Y^2} \right). \]
\[ \frac{n}{|n|} = (\sin \theta)(\sin \phi)e_x + (\cos \theta)e_y + (\sin \theta)(\cos \phi)m \]
FIG. 1.20 Stereographic projections of several important planes of a cubic crystal. (A) The (100) plane, line of sight along the [100] direction. (B) The (110) plane, line of sight along the [100] direction. (C) The (111) plane, line of sight along the [100] direction.
**FIG. 1.21** Cubic system, the (120) plane, showing the stereographic projections from both hemispheres, line of sight the [100] direction.
**FIG. 1.22** Cubic system, the (101) plane and the two $\langle 111 \rangle$ directions that lie in this plane, line of sight [100]
FIG. 1.23 Cubic system, zone of planes the zone axis of which is the [111] direction. The three \{110\} planes that belong to this zone are illustrated in the figures.
FIG. 1.24 The \{112\} and \{123\} planes that have [111] as their zone axis
FIG. 1.25 Stereographic projection of the zone containing the 12 planes shown in Figs. 1.23 and 1.24. Only the poles of the planes are plotted. Notice that all of the planar poles lie in the (111) plane.
\[
\frac{n}{|n|} = (\sin \theta)(\sin \phi)e_x + (\cos \theta)e_y + (\sin \theta)(\cos \phi)m
\]

Polar angle \( \theta \) "latitude"

Azimuthal angle \( \phi \) "longitude"

**FIG. 1.26** Wulff, or meridional, stereographic net drawn with 2° intervals
**Fig. 1.27** Rotation about the center of the Wulff net. 

(A) The effect of the desired rotation on the cubic unit cell. Line of sight [100].

(B) Perspective view of the (111) plane before and after the rotation.

(C) Stereographic projection of the (111) plane and its pole before and after rotation. Rotation clockwise 45° about the [100] direction.
**FIG. 1.29** The rotation of the pole of the $(1\bar{1}0)$ plane is given here. The diagram on the left shows the rotation in a perspective figure, whereas that on the right shows the motion of the pole along a latitude line of a stereographic projection which, in this case, is the equator.
FIG. 1.30 A 100 standard stereographic projection of a cubic crystal
FIG. 1.31 A 100 standard stereographic projection of a cubic crystal showing additional poles
High index plane in zone of [111]; Smaller $d_{\text{min}}$

Low index plane in zone of [111]; Larger $d_{\text{min}}$

If $ZA=[111]$ then all planes with indices on the equator will light up (approximately)

**FIG. 1.32** A 111 standard projection of a cubic crystal
Relationship between stereographic projections and diffraction patterns

Orientation relationship between bcc [110] diffraction pattern at left, and [110] stereographic projection at right. Angles between the vectors are the same on the left and right sides.
FIG. 1.34 When it is necessary to compare the orientations of a number of crystals, this often can be done conveniently by plotting the crystal axes in a single stereographic triangle, as indicated in this figure.
**FIG. 1.9** An iron crystal is much easier to magnetize along an *a* direction of Fig. 1.8 than along a *b* or *c* direction. The opposite is the case for nickel$^{2,3}$.
BCC Fe-4wt% Si soft magnet: by a complex rolling / heat treatment procedure, it is possible to produce texture (B)
Three Euler angles \((\alpha, \beta, \gamma)\)

“random” rotations:
\[
\alpha: \left[0, 2\pi\right]
\]
\[
\cos \beta: \left[-1, 1\right]
\]
\[
\gamma: \left[0, 2\pi\right]
\]

Fig. 5—Illustration of orientation imaging in as-cast 1100 aluminum at three different scales of inquiry (2.5, 10, and 30 μm).
Fig. 12—Orientation imaging of a section parallel to the rolling plane in as-cast and 40 pct channel-die compressed 1100 aluminum. Boundaries are highlighted with dark lines for minimum disorientations \( \omega > 20 \) deg. Coloring of the grains according to their orientation corresponds to the code given in Fig. 11.
Fig. 13 — [111], [200], and [220] pole figures obtained in 7544 measurements in fully recrystallized high-purity aluminum.

equilibrium is however yet a bit more subtle:

It is possible to reach equilibrium among a subset of the degrees of freedom (all atoms in a shot) or subsystem, while this subsystem is not in equilibrium with the rest of the system.

This is why engineering & material thermodynamics are still useful in cars.
Imagine a car going 80 mph on highway: the car is *not in equilibrium* with the road the axel is *not in equilibrium* with the body the piston is *not in equilibrium* with the engine block …

But we may apply material thermodynamics to steel in piston, hydrogen in tank, rubber in tire… because there is a *separation of timescales*: atoms in condensed phases collide with each other $\sim 10^{12}$ times per second, so atoms can reach equilibrium with adjacent atoms before macro scale components reach equilibrium with each other.
In this course, we will mainly study type A non-equilibrium phenomena, where temperature can be locally defined: $T(x)$.
Equilibrium state $\rightarrow T, S$

**type B** non-equilibrium state: no $T, S$

Far-from-equilibrium ions in Tokamak plasma:

Equilibrium Maxwellian distribution:

$$\frac{d^3v}{(2\pi k_B T / m)^{3/2}} \exp\left( -\frac{m |v - v_0|^2}{2k_B T} \right)$$

Bimodal distribution: thus no concept of temperature!