Materials Selection in Design

The Role of Materials Selection in Design
Exploring relationships - Materials Property Charts
The Materials Selection Process –Design Models
Selecting materials –Materials Indices
Case Studies of Materials Selection using CES
The Role of Materials Selection in Design

- Stiff, Strong, Tough, Light → All OK!
- Not stiff enough (need bigger E)
- Not strong enough (need bigger $\sigma_y$)
- Not tough enough (need bigger $K_{ic}$)
- Too heavy (need lower $\rho$)

The Role of Materials Selection in Design

Materials selection is a **central aspect of design**
In many cases materials represent the **enabling step**
Number of available materials exceeds **100,000**…
Concurrent engineering has re-emphasized the role of materials.

Why Materials Selection?

- **New products.**
- **Remain competitive**

Factors/Criteria?

- **Function**
- **Mechanical Properties**
- **Failure Mode**
- **Manufacturability**
- **Cost**
- **Environmental Considerations**

Materials selection is design-led
Properties of new materials can suggest new products (optical fiber – high purity glass).

Optical Fiber
The need for a new product can stimulate the development of a new material. 

Some Material Properties

- Physical
  - Density
  - Melting point
  - Vapor pressure
  - Viscosity
  - Porosity
  - Permeability
  - Reflectivity
  - Transparency
  - Optical properties
  - Dimensional stability

- Chemical
  - Corrosion
  - Oxidation
  - Thermal stability
  - Biological stability
  - Stress Corrosion
  - ….

- Electrical
  - Conductivity
  - Dielectric constant
  - Coercive force
  - Hysteresis

- Thermal
  - Conductivity
  - Specific Heat
  - Thermal expansion
  - Emissivity

- Mechanical
  - Hardness
  - Elastic constants
  - Yield strength
  - Ultimate strength
  - Fatigue
  - Fracture Toughness
  - Creep
  - Damping
  - Wear resistance
  - Spalling
  - Ballistic performance
  - …..
The goal of design:
“To create products that perform their function effectively, safely, at acceptable cost”….. What do we need to know about materials to do this? More than just test data.

http://www.matweb.com/
The set of properties for a particular material is called the “material attributes”, which includes both structured and non-structured information on the material – materials selection involves seeking the best match between the design requirements and the materials attributes.
Materials Selection Methodology

- Translate the design requirements into materials specifications. It should take into consideration the design objectives, constraints and free variables.
- Screening out of materials that fail the design constraints.
- Ranking the materials by their ability to meet the objectives. (Material Indices).
- Search for supporting information for the material candidates.
1. Defining the Design requirements

<table>
<thead>
<tr>
<th>Function</th>
<th>Objective</th>
<th>Constraint</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;What does component do?&quot;</td>
<td>&quot;What is to be maximized or minimized?&quot;</td>
<td>&quot;What specific requirements must be met?&quot;</td>
</tr>
<tr>
<td>Any engineering component has one or more functions (to support a load, to contain a pressure, to transmit heat, etc.).</td>
<td>The designer has an objective (to make it as cheap as possible, or as light as possible, or as safe as possible or some combination of these).</td>
<td>The objective must be achieved subject to constraints (e.g. the dimensions are fixed; the component must carry the given load without failure, it should function in a certain temperature range, etc.).</td>
</tr>
</tbody>
</table>

Free variables: What is the designer free to change?
2. List the constraints (e.g. no buckling, high stiffness) of the problem and develop an equation for them, if possible.

3. Develop an equation of the design objective in terms of functional requirements, geometry and materials properties (objective function).

4. Define the unconstrained (free) variables.

5. Substitute the free variable from the constraint equation into the objective function.

6. Group the variables into three groups, functional requirements (F), geometry (G) and materials functions (M), to develop the performance metric (P):
   \[ P \leq f_1(F), f_2(G), f_3(M) \quad \text{or} \quad P \geq f_1(F), f_2(G), f_3(M) \]

7. Read off the materials index, M, in order to maximize the performance metric (P).
Materials Selection Charts

- The performance metric of a design is limited by the materials.
- Performance metric is a function of multiple properties \( f(\text{multiple properties}) \)
- Charts Property 1 versus Property 2 (\( P1 \ vs \ P2 \))
- It can be plotted for classes and subclasses of materials (Classes: metals, ceramics, polymers, composites) (Sub-Classes: engineering ceramics, porous ceramics etc.)
- Combinations of properties are important in evaluating usefulness of materials.
  - Strength to Weight Ratio: \( \sigma/\rho \)
  - Stiffness to Weight Ratio: \( E/\rho \)
- The properties have ranges
  - \( E(\text{Cu}) = \text{few \%} \) (purity, texture, etc.)
  - Strength of \( \text{Al}_2\text{O}_3 \) can vary by a factor of 100 due to (porosity, grain size, heat treatment, etc.)
Modulus vs density

- Density depends on:
  - Atomic weight
  - Atom size
  - Packing
  - Porosity

- Elastic modulus depends on:
  - Bond stiffness
  - # bonds per unit area.

Which one to choose?

Depends on the Performance Metrics

Speed of Sound in a solid, \( \nu \)

\[ \nu = \sqrt{\frac{E}{\rho}} \]
Material Indices

• **Material Indices (MI)** are groups of material properties (including cost) which are useful metrics for comparison of materials.
• Better materials have higher MI’s.
• The form of the MI depends on the functional requirements (F) and geometry (G).

M_I = \frac{E^{1/2}}{\rho}
Materials Indices

Materials indices are specific functions derived from design equations that involve only materials properties that can be used in conjunction with materials selection charts

• e.g. strong, light tie rod in tension–minimize $\rho/\sigma_y$
• e.g. stiff, light beam in bending –minimize $\rho/E^{1/2}$
• e.g. stiff, light panel in bending -minimize $\rho/E^{1/3}$

**Derivation of MI’s**

The derivation of the MI will be illustrated by examples:
Example 1: Strong and light tie-rod

Function
Tie-rod

Objective
Minimize mass

$m = AL\rho$

Constraints
The length (L) is specified
Must not fail under load
Must have adequate fracture toughness

Free Variables
Materials choice

Section Area ($A$) – eliminate using above equations

$m = AL\rho = FL\left(\frac{\rho}{\sigma_y}\right)$

Minimize mass, hence, choose materials with smallest

$\frac{\rho}{\sigma_y}$
**Example 2: Stiff and light beam**

**Function**
Beam of solid square section

**Objective**
Minimize mass \( m = b^2 L \rho \)

**Constraints**
The beam must be stiff, i.e. small deflection (C is a constant)

**Free Variables**
Materials choice
Dimension \( b \) – eliminate using above equations

\[
m = \left( \frac{SL^3}{C_1 E} \right)^{\frac{1}{2}} L \rho = \left( \frac{SL^5}{C_1} \right)^{\frac{1}{2}} \left( \frac{\rho}{E^{\frac{1}{2}}} \right)
\]

Minimize mass, choose materials with smallest \( \frac{\rho}{E^{\frac{1}{2}}} \)
Example 3: Stiff, light panel

**Function**
Panel with given width (w) and length (L)

**Objective**
Minimize mass

**Constraints**
The panel must be stiff, i.e. small deflection (C is a constant)

**Free Variables**
Materials choice
Dimension \( t \) – eliminate using above equations

\[
m = twL\rho\quad t = \text{thickness}
\]

\[
F = (\text{Stiffness})\delta_{\text{Max}}
\]

\[
\text{Stiffness} = S = \frac{CEwt^3}{L^3}
\]

\[
m = \left(\frac{SL^3}{CEw}\right)^{\frac{1}{3}}wL\rho = \left(\frac{SL^6w^2}{C}\right)^{\frac{1}{3}}\left(\frac{\rho}{E^{\frac{1}{3}}}\right)
\]

Minimize mass, choose materials with smallest \( \frac{\rho}{E^{\frac{1}{3}}} \)
Derivation of MI’s: Methodology

Each combination of
- Function
- Objective
- Constraint
- Free variable

Has a characterising material index

INDEX
\[ M = \left[ \frac{\rho}{E^{1/2}} \right] \]

Minimise this!
**Demystifying Material Indices**

### Material properties --

- Cost, $C_m$  
- Density, $\rho$  
- Modulus, $E$  
- Strength, $\sigma_y$  
- Endurance limit, $\sigma_e$  
- Thermal conductivity, $\lambda$  
- T-expansion coefficient, $\alpha$

### Material indices --

**Objective: minimise mass**

<table>
<thead>
<tr>
<th>Function</th>
<th>Stiffness</th>
<th>Strength</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tension (tie)</td>
<td>$\rho/E$</td>
<td>$\rho/\sigma_y$</td>
</tr>
<tr>
<td>Bending (beam)</td>
<td>$\rho/E^{1/2}$</td>
<td>$\rho/\sigma_y^{2/3}$</td>
</tr>
<tr>
<td>Bending (panel)</td>
<td>$\rho/E^{1/3}$</td>
<td>$\rho/\sigma_y^{1/2}$</td>
</tr>
</tbody>
</table>

*Minimise these!*
Using Materials Indices with Materials Selection Charts

Index \[ M = \frac{\rho}{E^{1/2}} \]

\[ E = \frac{\rho^2}{M^2} \]

\[ \log(E) = 2\log(\rho) - 2\log(M) \]

Contours of constant \( M \) are lines of slope 2 on an \( E-\rho \) chart.

## Commonly used Materials Indices (MI’s)

<table>
<thead>
<tr>
<th>Function, objective, and constraints</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tie, minimum weight, stiffness prescribed</td>
<td>$E$</td>
</tr>
<tr>
<td></td>
<td>$\rho$</td>
</tr>
<tr>
<td></td>
<td>$E^{1/2}$</td>
</tr>
<tr>
<td>Beam, minimum weight, stiffness prescribed</td>
<td>$\rho$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_y^{2/3}$</td>
</tr>
<tr>
<td>Beam, minimum weight, strength prescribed</td>
<td>$\rho$</td>
</tr>
<tr>
<td></td>
<td>$E^{1/2}$</td>
</tr>
<tr>
<td></td>
<td>$C_m \rho$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_y^{2/3}$</td>
</tr>
<tr>
<td></td>
<td>$C_m \rho$</td>
</tr>
<tr>
<td>Beam, minimum cost, stiffness prescribed</td>
<td>$\rho$</td>
</tr>
<tr>
<td></td>
<td>$E^{1/2}$</td>
</tr>
<tr>
<td>Column, minimum cost, buckling load prescribed</td>
<td>$C_m \rho$</td>
</tr>
<tr>
<td>Spring, minimum weight for given energy storage</td>
<td>$\sigma_y^{2/3}$</td>
</tr>
<tr>
<td></td>
<td>$E \rho$</td>
</tr>
<tr>
<td>Thermal Insulation, minimum cost, heat flux prescribed</td>
<td>$1$</td>
</tr>
<tr>
<td></td>
<td>$\lambda C_p \rho$</td>
</tr>
<tr>
<td>Electromagnet, maximum field, temperature rise prescribed</td>
<td>$C_p \rho$</td>
</tr>
<tr>
<td></td>
<td>$\rho_e$</td>
</tr>
</tbody>
</table>

$\rho$ = density; $E$ = Young’s modulus; $\sigma_y$ = elastic limit; $C_m$ = cost/kg; $\lambda$ = thermal conductivity; $\rho_e$ = electrical resistivity; $C_p$ = specific heat.
The nature of material data

- **Numeric:** properties measured by numbers: density, modulus, cost ...other properties

- **Non-numeric:** properties measured by yes - no (Boolean) or poor-average-good type (Rankings)

- **Supporting information, specific:** what is the experience with the material?

- **Supporting information, general:** what else do you need to know?

"Structured" and "Unstructured" data

- Handbooks, data sheets
- Reports, papers, the Web
### Other Materials Selection Charts

| Modulus | Relative Cost | Modulus | Strength | Specific Modulus | Specific Strength | Fracture Toughness | Modulus | Fracture Toughness | Modulus | Conductivity | Diffusivity | Expansion | Conductivity | Diffusivity | Expansion | Modulus | Strength | Expansion | Expansion | Modulus | Strength | Temperature | Wear Rate | Hardness | Environmental Attack Chart |
|---------|---------------|---------|----------|------------------|------------------|-------------------|------------------|---------|-------------------|---------|--------------|-------------|-----------|--------------|-------------|-----------|---------|----------|-----------|-----------|---------|----------|-------------|-----------|---------|---------------------------|
| Modulus | Relative Cost | Modulus | Strength  | Specific Modulus | Specific Strength | Fracture Toughness | Modulus | Fracture Toughness | Modulus | Expansion | Conductivity | Diffusivity | Expansion | Modulus | Strength | Expansion | Expansion | Modulus | Strength | Temperature | Wear Rate | Hardness | Environmental Attack Chart |
Summary: Material Indices

• A method is necessary for translating design requirements into a prescription for a material
• Modulus-Density charts
  – Reveal a method of using lines of constant
    \[ \frac{E^{1/n}}{\rho} \quad n = 1,2,3 \]
    to allow selection of materials for minimum weight and deflection-limited design.
• Material Index
  – Combination of material properties which characterize performance in a given application.
• Performance of a material:
  \[ p = f \left[ \left( \frac{Functional}{Needs, F} \right), \left( Geometric Parameters, G \right), \left( Material Characteristics, M \right) \right] \]
  \[ p = f_1(F)f_2(G)f_3(M) \]
2. Strength – density

Metals, polymers: yield strength
Ceramics, glasses: crushing strength

Lines of $\frac{\sigma_y}{\rho} = C$ and $\frac{\sigma_y^{2/3}}{\rho} = C$.
Modulus - Strength

- Metals and polymers: yield strength
- Ceramics and glasses: MoR
- Elastomers: tensile tear strength
- Composites: tensile failure

- Yield before buckling

Non-technical ceramics

- Foams
- Rigid polymer foams

Young's modulus, $E$ (GPa)

Strength, $\sigma_f$ (MPa)

Specific modulus - Specific strength

- Metals and polymers: yield strength
- Ceramics and glasses: MoR
- Elastomers: tensile tear strength
- Composites: tensile failure

Yield before buckling

Non-technical ceramics

Concrete
Stone
Brick
Silica glass
Soda glass

Technical ceramics

Al₂O₃
Si₃N₄
B₂C

Composites

CFRP

Metals

Al alloys
CERAMICS
Stainless steels
Magnesium alloys
Titanium alloys

Polymers

PMMA
PA
Elastomers

Elastomers: tensile tear strength

Silicones

Foams

Rigid polymer foams

EVA
Polyurethane

Buckling before yield

Design guide lines

Fracture toughness - Modulus

Toughness $G_c = \frac{\left(K_{1C}\right)^2}{E}$ kJ/m²

Design guidelines

Polymers and elastomers

Natural materials

Composites

Metals

Non-technical ceramics

Technical ceramics

Foams

Young's modulus, $E$ (GPa)

Fracture toughness, $K_{1C}$ (MPa.m¹/²)
Fracture toughness - Strength

Yield before fracture
Guidelines for safe design

Elastic limit, \( \sigma_f \) (MPa)

(process zone size, mm)

Metals
- Low alloy steels
- Stainless steels
- Carbon steels
- W alloys
- Ni alloys
- Cast irons

Composites
- GFRP
- SiC
- Si3N4

Technical ceramics
- Lead alloys
- Mg alloys
- Al alloys
- Cu alloys
- Ni alloys
- Stainless steels
- Low alloy steels

Non-technical ceramics
- Zinc alloys
- Leather
- Ionomers
- Blown polyethylene
- PTFE
- PE
- PP
- PS
- PMMA
- Phenolic
- Silica glass
- Silicon

Polymers and elastomers
- Butyl rubber
- Neoprene
- Isoprene
- Polyurethane
- Polyethylene
- Polypropylene
- Polyvinyl chloride

Foams
- Flexible polymer foams
- Rigid polymer foams
- Closed cell foams
- Open cell foams

The diagram illustrates various materials plotted on a graph that shows thermal expansion (α) vs. thermal conductivity (λ). The materials are categorized into five main groups: Foams, Polymers and elastomers, Natural materials, Composites, and Technical ceramics. Each category is represented by a region on the graph, with specific materials indicated by white dots. The graph also highlights a region labeled 'Small thermal strain mismatch' in grey, and another labeled 'Large thermal strain mismatch' in red. The axis labels are: Thermal expansion, α (μstrain/K) on the vertical axis, and Thermal conductivity, λ (W/m.K) on the horizontal axis.
Wear rate - Hardness

Dimensionless wear constant \( K = k_a H \)

Hardness, \( H \) (MPa)

Wear-rate constant, \( k_a \) (1/(MPa))

Materials:
- Metals
  - Cu alloys
  - Al alloys
  - Low carbon steels
  - Medium carbon steels
  - Stainless steels
  - High carbon steels
  - Tool steels
  - WC
- Polymers and elastomers
  - PTFE
  - PE
  - PP
  - PMMA
  - PC
  - Filled thermoplastics
- Technical ceramics
  - SiC
  - Al₂O₃

Modulus - Relative cost/vol

- Technical ceramics
- Metals
- Composites
- Polymers
- Elastomers
- Foams
- Natural materials
- Non-technical ceramics

Guidelines for minimum cost design

Case 1: Materials for Table legs

Design a slender, light table legs that will support the applied design load and will not fracture if struck.

**Function**
Column, supporting compressive loads.

**Objective**
Minimize mass and maximize slenderness

**Constraints**
Specified length,
Must not buckle
Must not fracture if struck

**Free Variables**
Diameter of the legs
Choice of materials

The weight is minimized by selecting materials with the greatest value of the materials index:

\[ m = \pi r^2 L \rho \]  \hspace{1cm} (1)

Maximum elastic buckling load:

\[ F_{\text{crit}} = \frac{\pi^2 EI}{L^2} = \frac{\pi^3 E r^4}{4 L^2} \quad \text{where} \quad I = \frac{\pi r^4}{4} \]  \hspace{1cm} (2)

Solving for \( r \):

\[ m \geq \left( \frac{4F}{\pi} \right)^{1/2} L^2 \left( \frac{\rho}{E^{1/2}} \right) \]  \hspace{1cm} (3)

\[ M_1 = \left( \frac{E^{1/2}}{\rho} \right) \]  \hspace{1cm} (4)
Inverting equation (2) gives an equation for the thinnest legs which will not buckle:

$$r \geq \left( \frac{4F}{\pi^3} \right)^{1/4} L^{1/2} \left( \frac{1}{E} \right)^{1/4}$$  \hspace{1cm} (5)

to yield the second materials index (maximize):

$$M_2 = E$$  \hspace{1cm} (6)

Set $M_1$ to be minimum of 5 and $M_2$ to be greater than 100 (an arbitrary choice—it can be modified later if a wider choice of materials to be screened is desired). Candidate materials include some ceramics, CFRP:

• engineering ceramics are not tough—legs are subjected to abuse and this makes them a bad selection for this application

Selection = CFRP

must consult designer wrt cost—expensive
Case 2: Materials for Flywheels

Flywheels are rotating devices that store rotational energy in applications such as automotive transmissions. An efficient flywheel stores maximum energy per unit volume/mass at a specified angular velocity.

The kinetic energy the device can store is limited by the material strength.

**Function**

Flywheel for energy storage.

**Objective**

Maximize kinetic energy per unit mass.

- Mass of the disc: \( m = \pi R^2 t \rho \)
- Kinetic energy (\( J \) is the mass moment of inertia) for a solid round disc around its rotation axis: \( J = \frac{1}{2} m R^2 \)
- \( KE = \frac{1}{2} J \omega^2 \)

\( \sigma = \frac{\rho R^2 \omega^2}{2} \)

Material Strength \( \sigma \)

Stress

Burst shield

Material Density \( \rho \)

Density

Material Strength \( \sigma \)
The quantity to be maximized is the energy per unit mass

\[
\frac{KE}{m} = \frac{1}{4} R^2 w^2
\]

**Constraints**

- The outer radius is fixed.
- It must not burst.
- It must have adequate toughness (crack tolerance)

**Free Variables**

**Choice of materials**

The maximum radial stress (principal stress) is given by the equation:

\[
\sigma_{r,\text{Max}} = \frac{3 + \nu}{8} \rho \omega^2 R^2 \approx \frac{\rho \omega^2 R^2}{2}
\]

The stress must not exceed the yield stress:

\[
\frac{KE}{m} = \frac{1}{2} \left( \frac{\sigma_y}{\rho} \right)
\]

Hence, the material index to maximize is:

\[
M = \frac{\sigma_y}{\rho}
\]
The choices are some composites (CFRP), some engineering ceramics and high strength Ti and Al alloys
• engineering ceramics eliminated due to lack of toughness
• further selection must be made on the basis of cost and energy storage capacity for specific materials
  – e.g. CFRP can store 400kJ/kg
Case 3: Materials for Passive Solar Heating

A simple way of storing solar energy for residential heating is by heating the walls during the day and transferring heat to the interior via forced convection at night. Need to diffuse heat from the outer to inner surface in 12h. For architectural reasons, the wall thickness (W) cannot exceed 0.5m.

<table>
<thead>
<tr>
<th>Function</th>
<th>Heat storage medium</th>
</tr>
</thead>
<tbody>
<tr>
<td>Objective</td>
<td>Maximize thermal energy storage per unit material cost.</td>
</tr>
<tr>
<td>Constraints</td>
<td>Heat diffusion time through wall time (t) ~12h</td>
</tr>
<tr>
<td></td>
<td>Wall thickness ( w &lt; 0.5m )</td>
</tr>
<tr>
<td></td>
<td>Working temperature ( T_{\text{Max}} \sim 100^\circ C )</td>
</tr>
<tr>
<td>Free Variables</td>
<td>Wall thickness ( w ).</td>
</tr>
<tr>
<td></td>
<td>Choice of materials</td>
</tr>
</tbody>
</table>

What material will maximize the thermal energy captured by the wall while retaining the required heat diffusion time of up to 12h?
For a wall of thickness $w$, the heat ($Q$) per unit area of wall heated through $\Delta T$ is given by:

$$Q = w \rho c_p \Delta T$$

For the heat diffusion distance in time $t$:

$$w = \sqrt{2Dt}$$

where $\Delta$ is the thermal diffusivity, $\lambda$ is the thermal conductivity and $\rho$ is the density

$$D = \frac{\lambda}{\rho c_p}$$

The heat capacity of the wall is maximized by choosing a material with a high value of:

$$\frac{\lambda}{\sqrt{D}}$$

The restriction on the wall thickness ($w$) and diffusion time ($t$) yield the constraint:

$$D \leq \frac{w^2}{2t} \leq 3 \times 10^{-6} \text{ m}^2/\text{s}$$
$a = 3 \times 10^{-6} \text{ m}^2/\text{s}$

- High volumetric specific heat
- Search region
- Non-technical ceramics
- Polymers and elastomers
- Foams
- Technical ceramics
- Metals

$M = \lambda / a^{1/2}$

Guidelines for thermal design

Low volumetric specific heat
Cost must be a significant consideration in this selection because the application is for housing, where cost is always a significant factor. Taking cost into consideration, the most likely choice is concrete, with stone and brick as alternatives.
Literature Resources

M.F. Ashby, “Materials Selection in Mechanical Design, 2ndEd.”
  • multiple sources listed in appendices of the book
  • materials selection charts in lecture Appendix
Other references:
  • ASM Metals Handbook
  • Perry’s Chemical Engineering Handbook
  • CRC Handbook of Mathematics and Physics
  • ASM Handbook of Ceramics and Composites