



Granta EduPack Technical Paper

MSE Database Property-Process Profiles

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1. Introduction

The properties of materials depend on the way they have been processed. Some of the property-changes are desired (the increase in strength achieved by alloying, for example); others change in ways that may be less desirable (reduced elongation and toughness, lower thermal and electrical conductivities); still others do not change at all. Understanding the ways in which processes change properties is central to the discussion of process, structure, properties and performance (Figure 1).

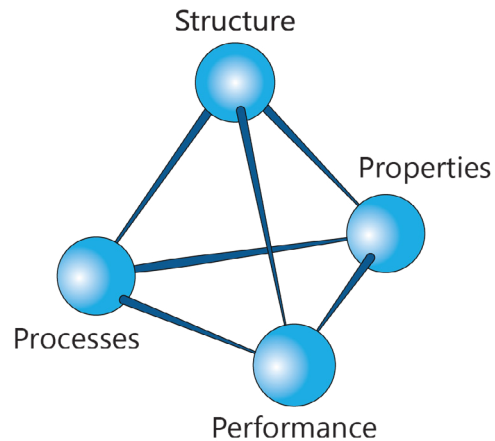


Figure 1. The Process-Structure-Properties-Performance tetrahedron

Experience suggests that learning is better achieved by discovery for oneself than by passive listening. The Ansys Granta EduPack Property-Process Profiles datatable within the Materials Science & Engineering database is a do-it-yourself kit that allows students to explore how the processes it contains change the properties of selected metals, polymers and ceramics.

The datatable stimulates discovery and it poses questions: why does the property change in that way? Why is this other property unchanged? The datatable contains eight sets of records chosen to illustrate how processes influence properties. All the records have a full Level 2 property listing allowing the effect of the process to be explored across the entire list. The eight sets are:

- Alloying and working: copper alloys
- Heat treatment: carbon steels
- Alloying and heat treatment (1): stainless steels
- Alloying and heat treatment (2): aluminum alloys
- Filling and reinforcement: thermoplastic polymers
- Powder processing: sintered ceramics
- Foaming: polymers, metals, ceramics
- Additive manufacturing: metal powder bed fusion

The sections of this report step through this list giving background, details, an illustration of a chart made with the set and suggestions for other informative charts that can be made with it. All the charts that appear here are the output of the datatable, untouched in any way.

2. Using the datatable

Set 1. Alloying, heat treatment and working: copper alloys

Pure, annealed metals are good thermal and electrical conductors but they are soft. They can be strengthened by work-hardening (as in cold rolling, cold forging and wire drawing). They can be strengthened by alloying (as in brass and bronze). And they can be strengthened by precipitation hardening (as in high-strength aluminum alloys and stainless steels) (Figure 2). All three change the properties of metals, but in different ways. This set of records illustrates the effect of solid-solution (alloy) hardening, precipitation hardening and work hardening on the mechanical, thermal and electrical properties of copper.

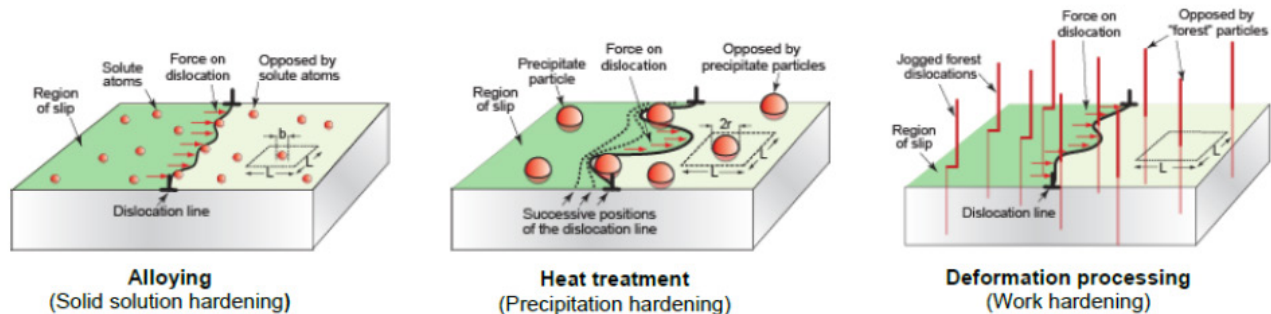


Figure 2.

What's in it?

The folder contains 19 records covering

- Pure copper, in the soft, $\frac{1}{4}$ hard, $\frac{1}{2}$ hard, $\frac{3}{4}$ hard and fully hard condition
- Copper-nickel alloys, ranging in composition from pure copper to pure nickel
- Copper-beryllium alloys in the solution treated, worked, aged, and aged plus worked states.

The symbol “w” means solution heat treated; “wh” means solution heat treated and work hardened; “wp” means solution heat treated and aged to allow precipitation; “whp” means solution treated, work hardened and aged to allow precipitation. What can you do with it? The record set allows you to explore the effect of the three hardening mechanisms on properties. Figure 3 shows an example of their effect on two properties of importance for heat exchangers: strength and thermal conductivity. Increasing cold work increases the yield strength of copper dramatically but has very little effect on conductivity. Solution hardening, by contrast, gives strength but greatly reduces conductivity. Precipitation hardening gives the most desirable combination of high strength with good conductivity.

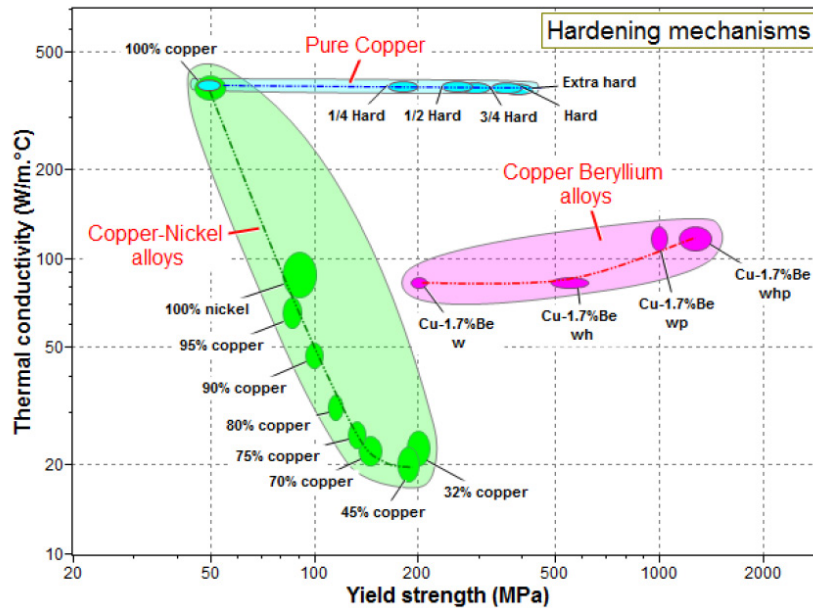


Figure 3. The effect of processing on thermal conductivity and strength of copper

Other charts to explore

- Make a chart of Yield strength plotted against Copper content (choose a linear, not log, scale for the copper content). At what copper content is the strength a maximum?
- Does alloying change Young's modulus or specific heat or thermal expansion? Plot these properties against copper content to find out.
- High speed electric motors and high field magnets both require conductors with high strength and low electrical resistance. Make a chart with these properties as axes and explore the best choice.
- What is the relationship between Thermal conductivity and Electrical resistivity? Make a chart with these two properties as axes to find out.
- Make a chart of Young's modulus plotted against Yield strength. Does work hardening change the modulus? Does solution hardening?
- Make a chart of Elongation plotted against Yield strength. Does work hardening affect elongation more strongly than solution hardening?

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. "Materials Science and Engineering" 9th edition, Chapters 7.9, 7.10, 11.3
- Shackelford, J.F. "Materials Science for Engineers", 6th edition, Chapters 6 and 11.2
- Askeland, D.R. and Phulé, P.P. "The Science and Engineering of Materials", 5th edition, Chapters 10-4 to 10-6
- Ashby, M.F., Shercliff, H. and Cebon, D. "Materials: Engineering, Science, Processing and Design" 3rd edition, Chapters 6.5, 19.5

Set 2. Heat treatment: carbon steels

The properties of carbon steels are controlled by heat treatment. The steel is austenitized at 850 C to dissolve the carbon, quenched to convert the austenite to martensite and tempered at a controlled temperature and time achieve the desired property profile (Figure 4). Heat treatment has a profound effect on structure-dependent mechanical properties (strength, fatigue resistance, elongation, toughness, mechanical damping). These dependencies can all be explored using this data set for two grades of medium carbon steel: a 0.35% C carbon steel and a 0.4% C low alloy steel.

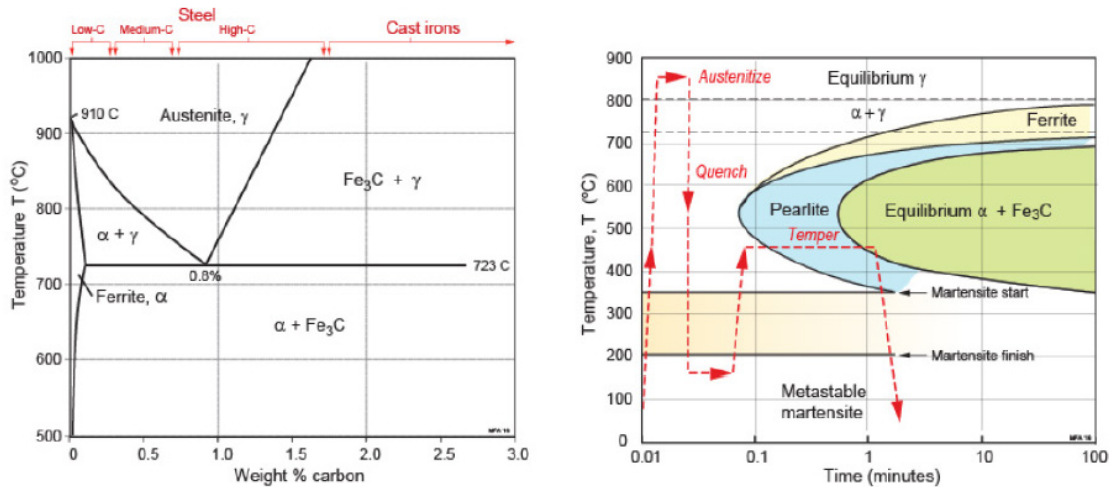


Figure 4. The iron carbon phase diagram and a TTT curve. The chart below is for a 0.35% C carbon steel.

What's in it?

The folder contains 16 records for

- Pure iron
- Martensite
- Iron 0.35% C, 1.5% Mn steel (AISI1137) in seven states of heat treatment (tempered at the indicated temperature followed by an oil quench)
- A low alloy steel (AISI 4340), 0.4% C, in seven states of heat treatment (tempered at the indicated temperature followed by and oil quench).

What can you do with it?

The chart of Figure 5 shows the trade-off between two key mechanical properties – Fracture Toughness and Yield strength – as the heat treatment schedule is changed. The bubbles are labeled with the tempering temperature. “Annealed” refers to steel heated into the austenite region and the furnace cooled slowly to room temperature. “Normalized” refers to steel heated to austenite then air cooled more rapidly to room temperature.

Other charts to explore.

- Heat treatment changes both hardness and ductility. The changes can be explored by making a chart with Hardness and Elongation as axes.
- Low mechanical damping and high Yield strength are desirable in materials for springs. The way that heat treatment changes these two properties can be explored by making a chart with these as axes.

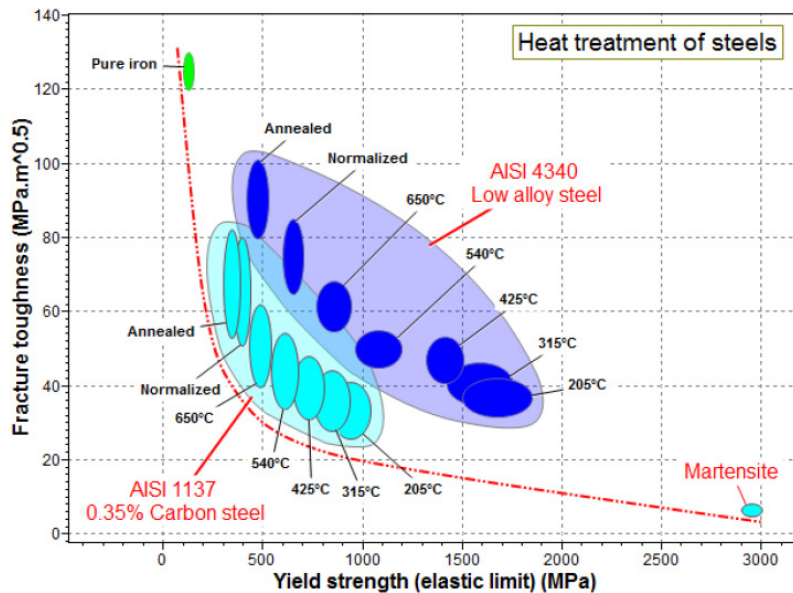


Figure 5. The effect of heat treatment on the strength and fracture toughness of medium carbon steels

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. “Materials Science and Engineering” 9th edition, Chapters 11.2, 11.8
- Shackelford, J.F. “Materials Science for Engineers”, 6th edition, Chapter 11.1
- Askeland, D.R. and Phulé, P.P. “The Science and Engineering of Materials”, 5th edition, Chapter 13-10
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapters 19.4, GL2-60

Set 3. Alloying and heat treatment (1): stainless steels

Stainless steels are remarkable for their strength, toughness and corrosion resistance. There are a number of distinct grades.

- Austenitic (200 and 300 series) stainless steels typically have around 18% chromium and 8% nickel. The nickel stabilizes the non-magnetic austenite (FCC) structure; the chromium gives outstanding corrosion resistance. They are the most widely used of the stainless steels
- Ferritic stainless steels have low nickel content and have a BCC structure. They are stronger than austenitic grades but their corrosion resistance is less good. This set of records does not include ferritic grades.
- Martensitic (400 series) stainless steels are less corrosion-resistant than the previous two classes but are extremely strong and tough and can be heat treated. Typically, they contain 12 – 14% chromium, 0.2 – 1% molybdenum, less than 2% nickel and 0.1 – 1% carbon.
- Precipitation-hardening martensitic stainless steels (also 400 grades) have corrosion resistance comparable to austenitic varieties but can be precipitation hardened to even higher strengths than the other martensitic grades. The most common grades contain 17% chromium and 4% nickel.

What's in it? The folder contains 26 records covering

- Austenitic stainless steels
- Martensitic stainless steels
- Precipitation hardened stainless steels

What can you do with it?

The record set illustrates how solution hardening (the 200 and 300 grades), precipitation and the tempering of martensite (400 grades) change properties. The chart below shows an example: the trade-off between two of the most important mechanical properties – strength and toughness – for three grades of stainless steel.

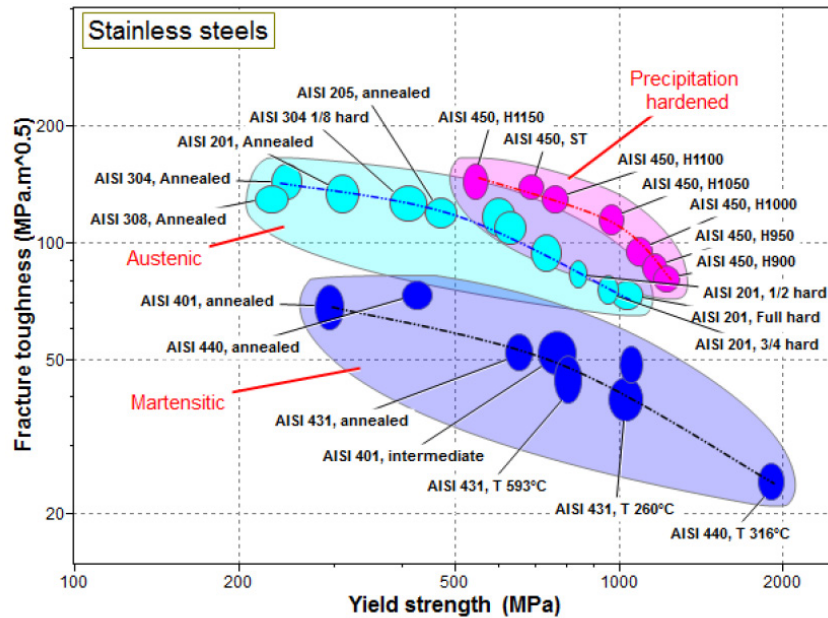


Figure 6. The effect of heat treatment on the strength and fracture toughness of stainless steels.

Other charts to explore

- Explore the relationship between the elongation (important for metal forming) and the hardness (important as a cause of tool wear) for stainless steels. Use a plot of elongation against hardness to select the four stainless steels look most attractive for making a deep-drawn shape from sheet? Which class do they belong to (Austenitic, martensitic, precipitation hardened)?
- Are tough stainless steels more expensive than those with lower toughness? To find out, make a chart of fracture toughness against price. Add the envelopes to identify the classes.
- Many stainless steel products are expected to resist heat as well as corrosion. Explore the strength and maximum service temperature of stainless steels by making a chart of these two properties. You will find that the austenitic steels have the best resistance to high temperature; the martensitic steels by contrast have a large spread. Why?

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. “Materials Science and Engineering” 9th edition, Chapter 11.2
- Shackelford, J.F. “Materials Science for Engineers”, 6th edition, Chapter 11.1
- Askeland, D.R. and Phulé, P.P. “The Science and Engineering of Materials”, 5th edition, Chapter 13-10
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapter 19.5

Set 4. Alloying and heat treatment (2): Aluminum alloys

Wrought aluminum alloys designed for strength. They are divided into series according to composition:

- 1000 - Pure Al
- 2000 - Cu-alloyed
- 3000 - Mn-alloyed
- 5000 - Mg-alloyed
- 6000 - Mg and Si-alloyed
- 7000 - Zn-alloyed
- 8000 - Li-alloyed and other

Cast aluminum alloys are designed to be fluid so that they flow readily into molds. They too are grouped in series according to composition:

- 1xx.x - Pure Al
- 2xx.x - Cu-alloyed
- 3xx.x - Si, Cu, Mg-alloyed
- 4xx.x - Si-alloyed
- 5xx.x - Mg-alloyed
- 7xx.x - Zn-alloyed

The remarkable range of properties offered by aluminum alloys is illustrated by this set of records.

What's in it?

The folder contains 26 records covering

- Wrought age-hardening aluminum alloys (2000, 6000 and 7000 series)
- Wrought non age-hardening aluminum alloys (1000, 5000 series)
- Cast aluminum alloys (1xx.x, 2xx.x, 3xx.x and 5xx.x series)

What can you do with it?

The figure shows a chart of Fracture toughness against Yield strength made with this record set. Wrought age-hardening alloys (dark green) rely on precipitation hardening. They have the most attractive combinations of toughness and strength. The non age-hardening grades (light green) rely on work hardening and solution hardening. They are slightly less tough than the age-hardening grades. The cast alloys lie in the blue envelope, color coded to show 2xx.x grades in light blue, 3xx.x grades in dark blue and 5xx.x grades in purple. The decrease in hardness with increase in strength is most extreme for the cast grades.

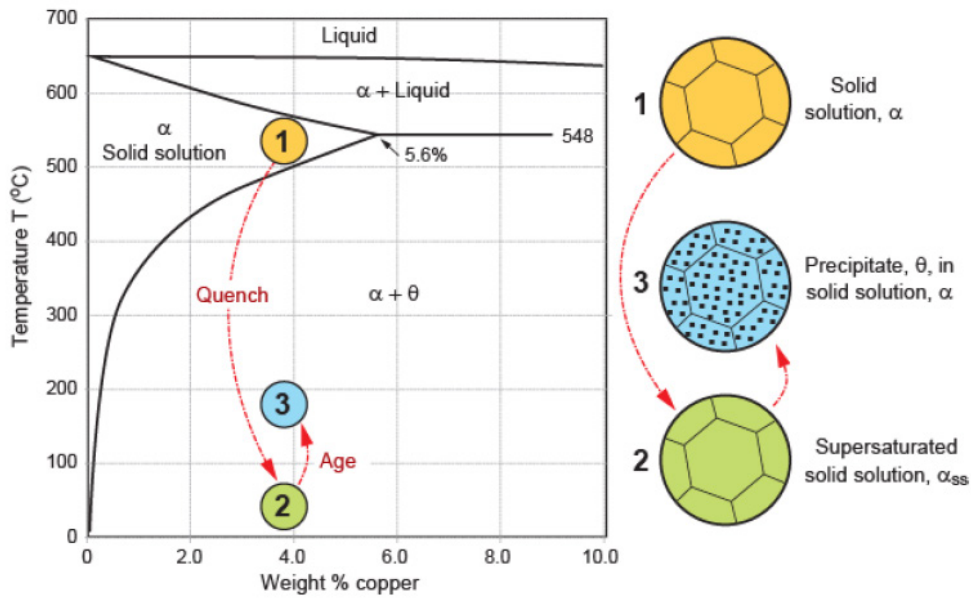


Figure 7. The heat treatment of an aluminum 4% copper alloys

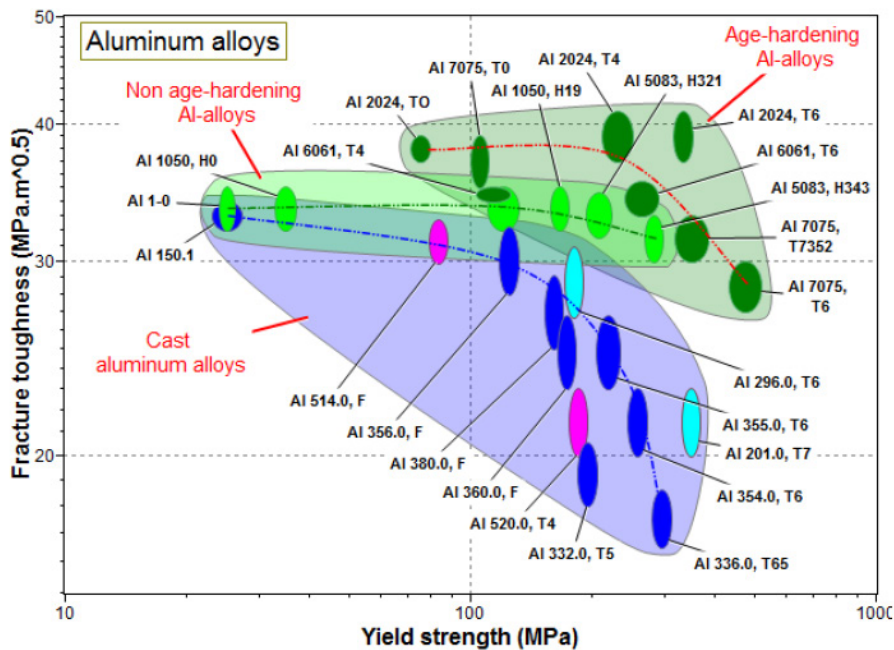


Figure 8. A chart for the three types of aluminum alloy

Other charts to explore

- Heat exchangers require materials with high thermal conductivity and – if pressurized – high strength. A chart of Thermal conductivity against Yield strength guides selection of aluminum grades for this application.
- The Wiedemann-Franz law states that the thermal conductivity for metals is inversely proportional to the electrical resistivity. Does it hold for aluminum alloys? A chart of Thermal conductivity against Electrical resistivity allows this to be explored.
- Does ductility (Elongation) fall with increasing strength? A chart of Elongation against Yield or Tensile strength shows that it does.

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. “Materials Science and Engineering” 9th edition, Chapters 11.3, 11.9
- Shackelford, J.F. “Materials Science for Engineers”, 6th edition, Chapter 11.2
- Askeland, D.R. and Phulé, P.P. “The Science and Engineering of Materials”, 5th edition, Chapter 14-1
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapter 19.2

Set 5 – Filling and reinforcement of thermoplastic polymers

Polymers have low elastic moduli and only moderate strength. They can be stiffened (raising the modulus) by blending them with fillers such as talc, calcium carbonate or other minerals; and they can be both stiffened and strengthened by blending with chopped or long fibers of glass or carbon. The fillers and reinforcements affect not only the stiffness and strength, but all the other properties as well. This set of records allows the effect of fillers on polymer properties to be explored.

What’s in it?

The folder contains a record for the mechanical, thermal and electrical properties of Polypropylene homopolymer and for the same polypropylene filled with:

- Four weight fractions of talc (hydrated magnesium silicate, $Mg_3 Si_4 O_{10} (OH)_2$) particles
- Four weight fractions of calcium carbonate (chalk) particles
- Six weight fractions of glass fibers, chopped and long-fiber
- Two weight fractions of EPDM (an elastomeric ethylene propylene diene, an elastomeric terpolymer)

What can you do with it?

The figure shows the way in which Yield strength and Young’s modulus of polypropylene homopolymer change with filler type and content. All the fillers raise the modulus; only glass fibers significantly increase the strength as well.



Figure 9. A polymer with particulate and fiber fillers

Other charts to explore

- Fillers increase the modulus but they also increase the density. What happens to the specific stiffness (modulus/density)? A chart of yield strength/density and Young's modulus/density reveals how these combinations of properties change with filler content.
- What do fillers do to the thermal properties of polymers? A chart of Thermal conductivity against Thermal expansion coefficient shows what happens.

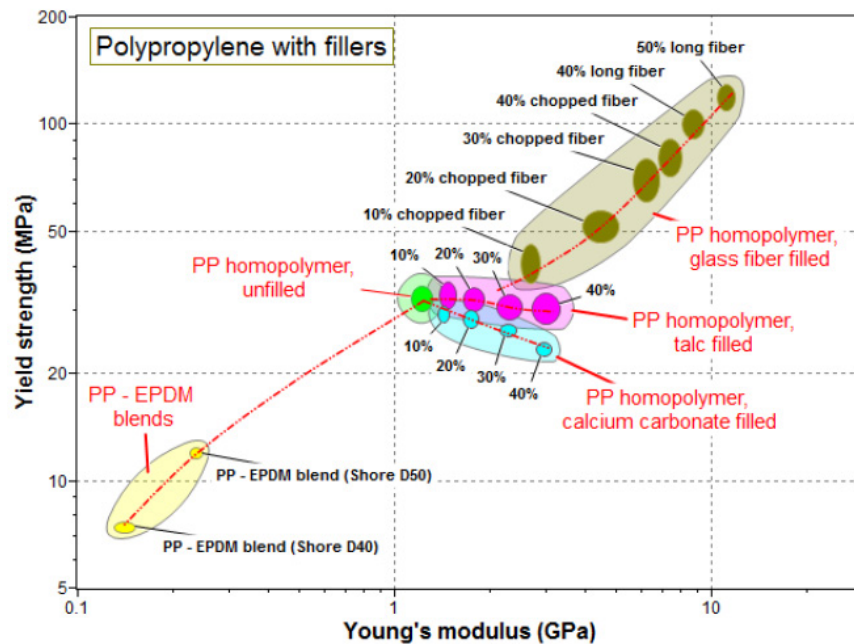


Figure 10. Polypropylene, shown in green, with particulate and fiber fillers.

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. "Materials Science and Engineering" 9th edition, Chapter 15.9
- Shackelford, J.F. "Materials Science for Engineers", 6th edition, Chapter 13.6

- Askeland, D.R. and Phulé, P.P. “The Science and Engineering of Materials”, 5th edition, Chapter 16-5
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapter 19.6

Set 6 – Powder processing: sintered ceramics

Ceramic shapes are usually made by the compaction and sintering of powders. The porosity of the resulting ceramic body depends on the temperature and time of sintering and on the pressure under which this takes place. The properties of the end-product depend strongly on the extent of this porosity. This set of records allows exploration of how the properties of the most widely used ceramic – alumina (Al_2O_3) – depend on porosity.

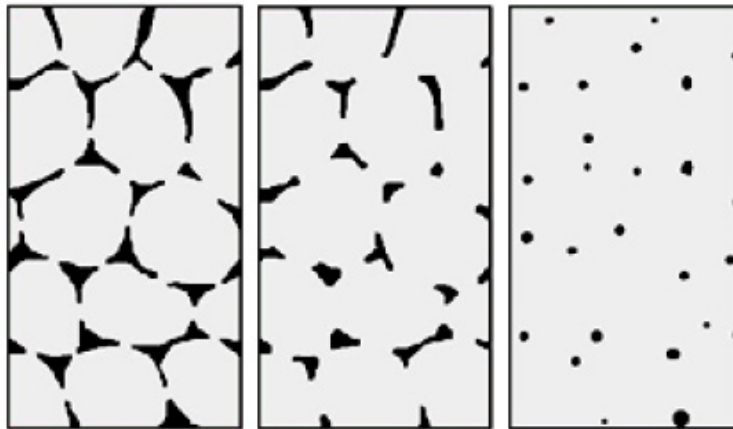


Figure 11. Porosity in sintered alumina

What's in it?

The folder contains seven records for

- Alumina with relative densities ranging from 55% to 99.5% (porosities between 0.05% and 45%). What can you do with it? The chart of Figure 12 shows how the Yield strength and Young's modulus of alumina fall as the relative density ($1 - \text{porosity}$) decreases. Almost all the mechanical, thermal and electrical properties of alumina depend on relative density. The set of records allow this to be explored.

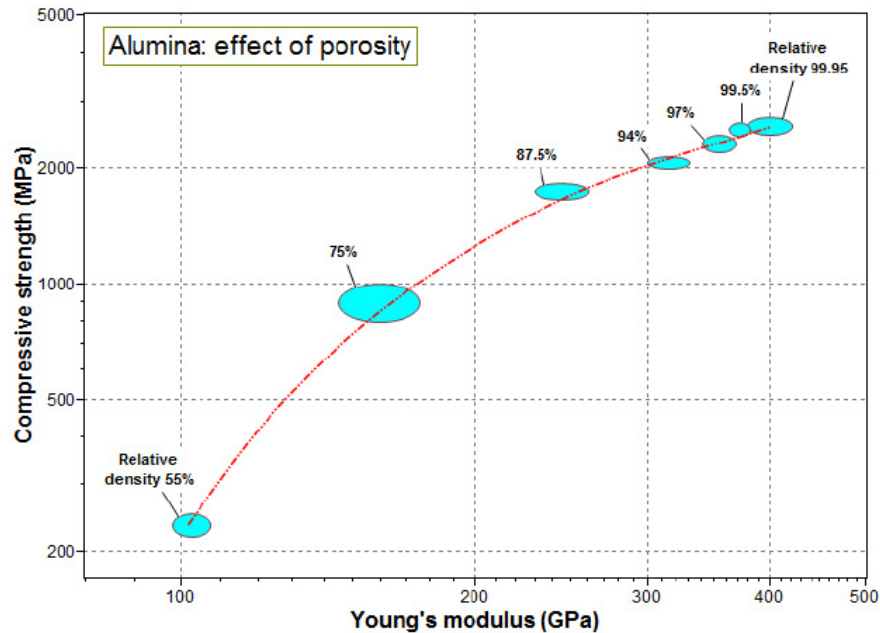


Figure 12. The effect of residual porosity on the modulus and compressive strength of alumina.

Other charts to explore

- The fracture toughness of ceramics decreases steeply with increasing porosity. A chart of Fracture toughness against Relative density illustrates this well.
- Alumina is frequently used as an electrical insulator. The AC losses in an insulator depend on the product of the Dielectric constant and the Dielectric loss factor. A chart with these two quantities as axes shows how they change with porosity.
- How does the thermal conductivity of a ceramic like alumina depend on porosity? Is the relationship a linear one or is it stronger than linear? Devise a chart to answer the question.

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. “Materials Science and Engineering” 9th edition, Chapter 13.12
- Shackelford, J.F. “Materials Science for Engineers”, 6th edition, Chapter 12.1
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapter 19.6

Set 7 – Foaming: polymers, metals and ceramics

Polymers, metals and ceramics can all be made with cellular, foam-like structures. Nature makes extensive use of cellular structures (“foams”) for light-weight mechanical and thermal efficiency – examples are wood, cork, pith, trabecular bone and coral. The cell shape and size of natural foams have evolved to maximize the effective use of materials. Man-made foams have clumsier, less efficient shapes, but they are useful none-the-less. This set of records allows the effect of foaming on material properties to be explored.

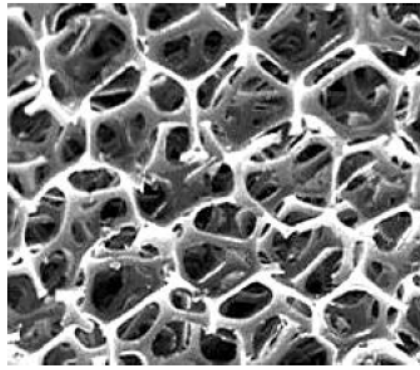


Figure 13. A polymer foam

What's in it?

The folder contains records for:

- Solid polyethylene and eight polyethylene foams,
- Solid Al-SiC alloy (an alloy that is foamable) and six foams based on the alloy.
- Solid zirconia (ZrO₂ ceramic) and three zirconia foams.

What can you do with it?

The chart of Figure 14 shows how Young's modulus decreases roughly as the square of the density. Almost all properties change with foam density, most in a non-linear way.

Other charts to explore

- Many foams are used for thermal insulation. A chart of thermal conductivity against density shows how the conductivity falls, flattening out at the conductivity of air at 20 C and atmospheric pressure, 0.025 W/m.°C.
- Do foams have a higher mechanical loss coefficient, and thus damp vibrations, than the solid from which they are made? Devise a chart to explore this.
- Most properties change when a solid is foamed. Is this true of the specific heat capacity? Create an appropriate chart to find out.
- A chart of Embodied energy against Density reveals how much additional energy is needed to create a foam from a solid.
- Foams are crush when compressed, absorbing energy. The energy U absorbed per unit volume is where σ_y is the Yield strength and E is Young's modulus. A chart with these two properties as axes allows a comparison of foams for energy-absorbing applications.

$$U = \frac{1}{2} \frac{\sigma_y^2}{E} \text{ J/m}^3$$

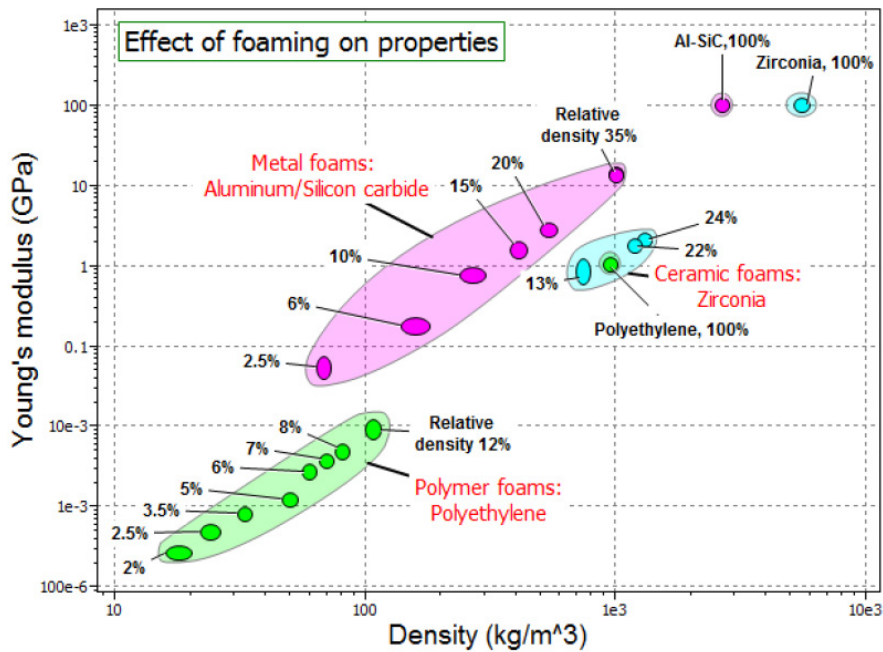


Figure 14. The effect of fillers and fibers on the strength and modulus of a single grade of polypropylene.

Where can you learn more?

- Callister, W.D and Rethwisch, D.G. “Materials Science and Engineering” 9th edition, Chapter 15.18
- Askeland, D.R. and Phulé, P.P. “The Science and Engineering of Materials”, 5th edition, Chapter 16.10
- Ashby, M.F. Shercliff, H. and Cebon, D. “Materials: Engineering, Science, Processing and Design” 3rd edition, Chapter 4.5

Set 8-Additive manufacturing: metal powder bed fusion

Laser Powder Bed Fusion (LPBF) is a metal additive manufacturing process that involves selectively melting layers of metal powder using a high-energy laser beam. It enables the creation of complex, intricate, and customized metal parts. Optimizing LPBF processing parameters is crucial for achieving high-quality parts and minimizing potential defects like porosity. Parameters such as laser power, scan speed, hatch spacing, and powder layer thickness directly influence the melting and solidification behavior of the metal powder. By carefully controlling these parameters, porosity (which can weaken the structural integrity of the part) can be minimized.

For each material, optimizing the LPBF processing parameters typically starts with melting single tracks (using different processing parameters) on a layer of the powder material and characterizing the resulting melting pool, as a first step. The depth, width, and length of these melt pools can be a good indicator of whether a specific set of processing parameters may result in different types of porosity (lack of fusion, keyholing, and balling). This step helps in narrowing down the range of processing parameters being investigated. In the second step, the remaining sets of processing parameters are used to manufacture small specimens (typically cubes). Characterization of the porosity of these specimens determines which set of processing parameters are optimal for the material of interest, as they would yield minimal or no porosity in LPBF manufacturing of this material. This approach can be

expanded to consider other forms of structural defects like micro-cracks and/or aim to find processing parameters that would yield a microstructure of interest as well.

This set of records (new in the 2024R1 release of Ansys Granta EduPack) allows for exploration of the influence of laser power, laser speed, and laser energy density on the resulting melt pool sizes and porosities of four metallic alloys, namely Nickel-chromium alloy INCONEL 625, Stainless steel AISI 316L, Aluminum alloy Al₁₀SiMg, and Titanium alloy Ti₆Al₄V ELI.

What's in it?

This folder contains 35 records for additively manufactured metal alloys using the selective laser melting process. The metals are as follows:

- Nickel-chromium alloy INCONEL 625
- Stainless steel AISI 316L
- Aluminum alloy Al₁₀SiMg
- Titanium alloy Ti₆Al₄V ELI

What can you do with it?

Figure 15 shows the different ways in which (within the range depicted) laser energy density influences porosity for the four metallic alloys. In the case of INCONEL 625 and AISI 316L, increased laser energy density results in decreasing porosity and can be attributed to eliminating the possibility of production of lack of fusion porosity. For Ti₆Al₄V ELI, increased laser energy density yields higher porosity which can be attributed to an increasing formation of keyholing porosity and higher values of laser energy density. In the case of Al₁₀SiMg, a combination of these two effects can be seen, where increasing laser energy density first eliminates lack of fusion porosity and then contributes to the formation of keyholing porosity at higher energy density levels.

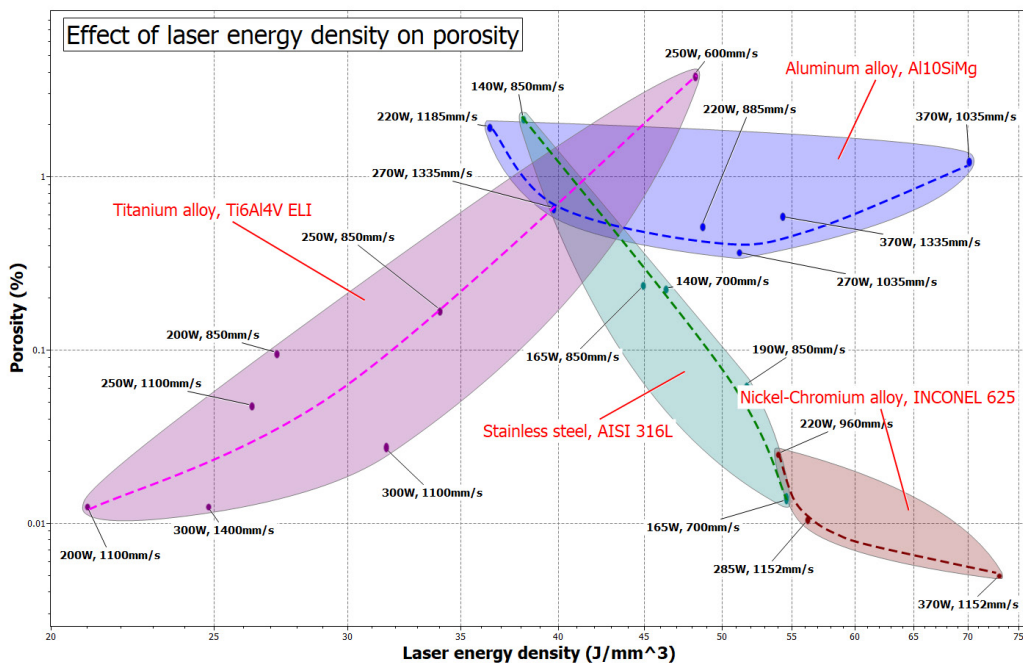


Figure 15. The effect of laser energy density on porosity for four metallic alloys

Other Charts to Explore

- Laser power plotted against melt pool width. Is there a relationship?
- Porosity plotted against melt pool depth. Melt pool dimensions are assumed to provide a preliminary indication of whether a set of processing parameters would result in high porosity (and the type of porosity). Does this plot reaffirm this when compared with the energy density vs. porosity plot?

Where can you learn more?

- Gibson, I. Rosen, D. Stucker, B. Khorasani, M. “Additive Manufacturing Technologies” 3rd edition Chapter 5-5
- Toyserkani, Y. Sarker, D., Ibadode, O., Liravi, F., Russo, P., Taherkhani, K. “Meal Additive Manufacturing” 1st edition, Chapters 2-3, 2-4, 10-2-1
- Milewski, J.O., “Additive Manufacturing of Metals: from Fundamental Technology to Rocket Nozzles, Medical Implants, and Custom Jewelry” 1st edition, Chapter 10

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