



Level 3 Industrial Case Study

Materials Selection to Avoid Mechanical Failure

Claes Fredriksson¹, Adeayo Sotayo²

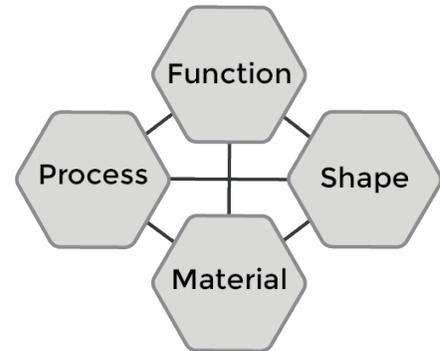
¹Ansys Materials Education Division

² Brunel University, UK

Material selection against failure

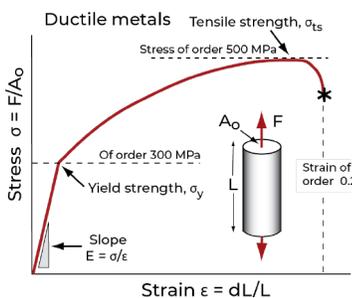
For products involving safety, mechanical failure is completely unacceptable and must be avoided at all cost. This is particularly true for applications in aerospace or bioengineering, as well as for many types of sports equipment. Therefore, extensive testing and analyses are usually needed during product development to prevent failures, economic losses and potential loss of lives from occurring in service.

Failure prevention can and should be considered in early product design or the re-design for critical applications. Mechanical failure might be caused both by insufficient material properties and by badly designed shape for the specific function of the product. Re-design after failure thus involves identifying the cause of failure, such as flaws in the design geometry or inadequate material properties (or both). Material properties can be affected by defects introduced during the manufacturing process or the effect of adverse environmental conditions, but these are usually beyond the designer's control. Here, we are mainly interested in preventing failure by systematic material selection using adequate property data. However, as illustrated schematically to the right, the optimal *material*, its manufacturing *processes* and the *shape* of a product are all interconnected and dependent on the *function* it is designed for.



The best geometry and sufficient dimensions of the design can be found with experience and visual exploration by Finite Element (FE) simulations using, for example, Ansys Discovery, or a more systematic parametric approach. The outcome will, however, depend on the accuracy of the material properties used for analysis. Granta EduPack contains reliable data for a wide range of materials used in product development across all industries. Using this data in combination with accurate material candidates early in the design stage reduces the need for extensive physical testing and therefore saves time, money or even lives. For material failure analysis and re-design of products that risk failure, we provide software tools within Granta EduPack that can help identify materials that perform better in deficient or critical properties (Find similar, Comparison tables). This software can also help determine the minimum material strength for some loading conditions by analytical methods (Engineering solver).

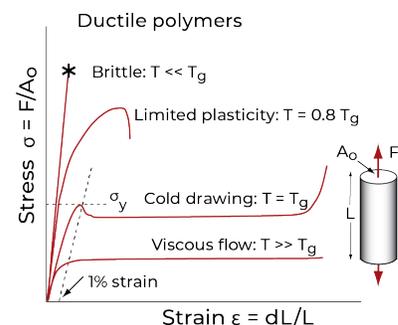
What is the problem?



The material property that first springs to mind when it comes to mechanical failure is the yield strength, σ_y or elastic limit, where the material can no longer return to its original shape after deformation, but is permanently damaged. For metals, such as aluminum, we often identify this with the 0.2% offset yield strength, or proof stress. This is the stress at which the stress-strain curve for axial loading deviates by a strain of 0.2% from the linear-elastic line as shown to the left. It can also be defined by the proportional limit (e.g., in steel). For metals, it is often but not always, the same in tension and compression — notice for instance that wrought aluminum alloys show tension/compression anisotropy.

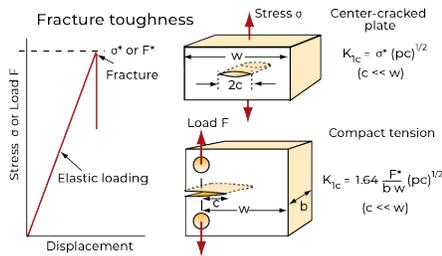
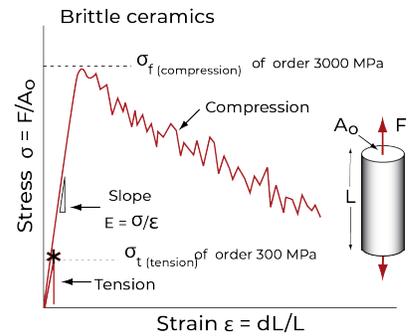
For polymers, however, σ_y is identified as the stress at which the gradient of the stress-strain graph is zero. When such a local maximum is not present, then it is defined as the stress at which the stress-strain curve becomes markedly non-linear, typically, a strain of 1% from linear-elastic behavior. Polymers are a little stronger ($\approx 20\%$) in compression than in tension.

The strength of a composite is best defined by a set deviation from linear-elastic behavior: a strain deviation of 0.5% is sometimes taken for this. Composites that contain fibers (e.g., natural composites like wood) are a little weaker (up to 30%) in compression than tension because fibers buckle. This is converse to the behavior of polymers, described above.



Strength, for ceramics and glasses, depends strongly on the mode of loading. In tension, “strength” means the fracture strength - this value is taken as both the ultimate tensile and yield strength (elastic limit) for ceramics. In compression, it means the crushing strength, which is much larger, by a factor of 10 to 15, than that in tension. All the cases above can be handled by design.

Failure by fracture is technically predictable and can be related directly to a material property; the fracture toughness. Failure by yield, i.e., irreversible plastic deformation which may or may not lead to ultimate failure is also in principle predictable; it occurs in metals when the stress within the material exceeds the yield strength at some point inside the part.

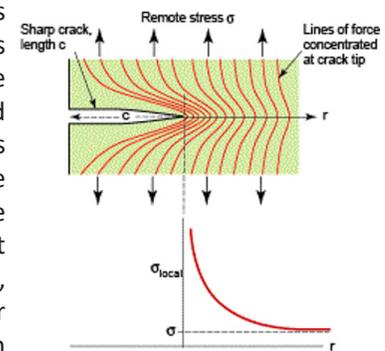


In the Science Notes, found via the attribute of any material record in Granta EduPack, the following definition is given: The fracture toughness, K_{Ic} (units: $\text{MPa m}^{1/2}$ or $\text{MN/m}^{1/2}$) measures the resistance of a material to the propagation of a crack. It is measured by loading a sample containing a deliberately-introduced contained crack of length $2c$ or a surface crack of length c , recording the tensile stress, s^* , or the bending load, F^* , at which the crack suddenly propagates. The quantity K_{Ic} is then calculated, as shown in the Figure to the left.

Measured in this way, K_{Ic} has well-defined values for brittle materials (ceramics, glasses, and brittle polymers). In ductile materials, like metals, a plastic zone develops at the crack tip. If this is small compared to all dimensions of the test sample the measurement remains valid; if not, a more complex characterization is required. If the plastic zone size exceeds the sample thickness, the crack does not propagate at all; the sample yields before it breaks.

Even when nominally pure, most metals contain tiny inclusions or foreign particles, often formed by the reaction of the metal with oxygen or impurities. Within the plastic zone, plastic flow around these inclusions causes them to debond, leading to elongated cavities that grow and link to give a ductile fracture. The plasticity also blunts the crack, and the stress concentration effect of a blunt crack is less severe than that of a sharp one, so that at the crack tip itself, the stress is just sufficient to keep plastically deforming the material there, resulting in potential failure by yield.

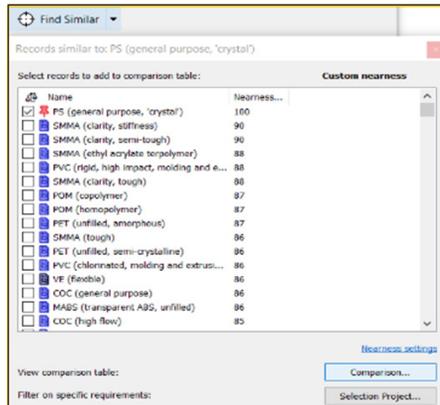
Cleavage, or fast fracture, is much more dangerous than one that is ductile: it occurs without warning or any prior plastic deformation. At low temperatures, some metals and all polymers become brittle and the fracture mode switches to one of cleavage - in fact, only those metals with an FCC structure (copper, aluminum, nickel, and stainless steel for example) remain ductile to the lowest temperatures. All others have yield strengths that increase as the temperature falls, with the result that the plastic zone at any crack they contain shrinks until it becomes so small that the fracture mode switches, giving a ductile-to-brittle transition. For some steels that transition temperature is as high as 0°C (though for most it is considerably lower), with the result that steel ships, bridges, and oil rigs are more likely to fail in winter than in summer. Polymers, too, have a ductile to brittle transition, a consideration in selecting those that are to be used in freezers and fridges.



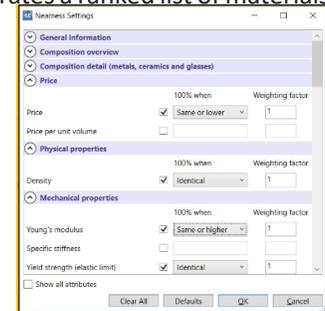
The vast majority (up to 90%) of mechanical failures in metals occur by fatigue, however, this is tricky to design against, since it is caused by loads below the tensile or yield strength. Fatigue is initially caused by small cracks that propagate progressively over a long period of time as a consequence of repeated but relatively small cyclic loads, exceeding the material’s fatigue strength, until a sudden catastrophic failure takes place. The cracks are nearly always initiated at surface defects or other sites of stress concentration. This makes the surface smoothness an important property, and scratches should be avoided.

What can Granta EduPack do?

Firstly, Granta EduPack is equipped with most of the relevant materials data needed to prevent failure in early design. This includes mechanical properties like yield strength or fracture toughness, of course, but also a great wealth of other related and useful attributes, such as durability to UV radiation and for different environments, maximum and minimum service temperatures etc. Some properties which are pertinent only for specific material families are also included, for example, temperature-dependent strength and corrosion resistance for metals or glass transition temperature for polymers.

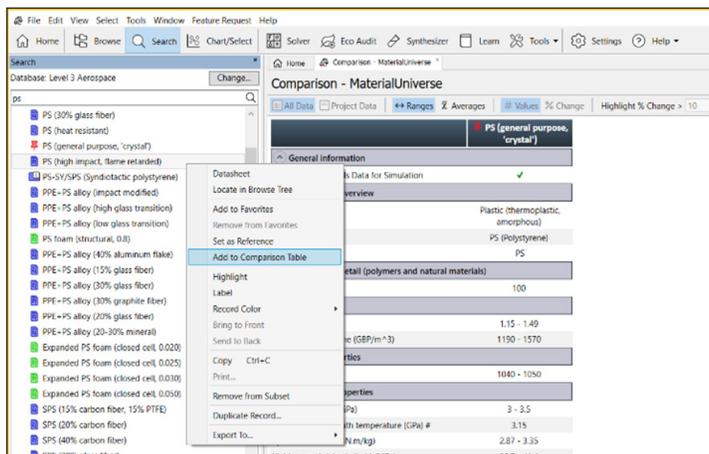
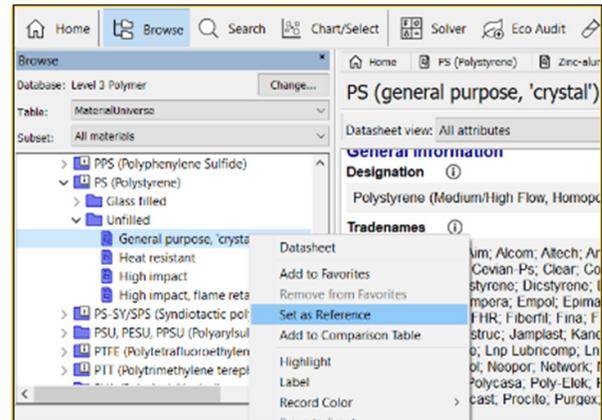


In this case study, we will explore the materials selection tools “Find Similar” and “Comparison Tables” as well as the “Engineering Solver” in Granta EduPack in order to prevent material failure. These can be seen as complementary to FE simulations which are used to promote safe shape design. The Find Similar functionality is activated from within a material record that will be made a reference. This generates a ranked list of materials that resembles the reference according to a set of nearness criteria. The criteria are given percent values (0-100%) and are controlled by setting conditions to *Identical*, *Same or lower*, or *Same or higher*. The default is to screen for Identical values for: Price, Density, Young’s modulus, Yield strength (elastic limit),



Fracture toughness, Thermal conductivity as well as requiring same or higher values for: Maximum service temperature and Durability in water (salt).

Find Similar opens up the possibility to rank or ultimately select materials based on a reference and to improve one or more of the properties. In our case, the one whose deficiency has caused or might cause failure. This is a more powerful way to select improved material than to simply introduce limit stages, since it allows a tailored and weighted set of requirements in replacement or re-design. The *Set as reference* function introduced in Granta EduPack 2020, can also be reached directly via a right-click on the material name or from the Chart/Select menu option. When a reference material is set, it can easily be used to compare properties from other materials side by side, by right-clicking and choosing *Add to Comparison Table*, as shown below.



Finally, the Engineering Solver tool is a way to connect a particular function (shape and load situation) analytically to required mechanical properties in order to stay within deflection limits. This helps eliminate materials with insufficient performance from the candidates in question for the selection. By choosing one of the available standard load situations, including point or distributed applied force, as well as specifying dimension, safety factor and maximum deflection, the minimum required mechanical properties in terms of Young’s modulus and yield strength are generated.

Three types of mechanical failure

1. Fracture

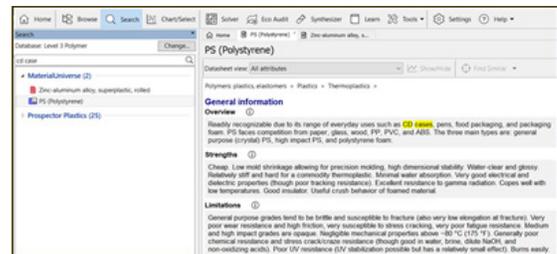


Let us consider an example from a classic design failure due to flawed material selection, the *Jewel* case for compact discs (CDs). It is not related to safety but very easy to grasp, since the problems arise mainly from insufficient fracture toughness. This results in cracks forming even by normal handling or dropping the case to the floor. The hinges are also susceptible to breaking, which might be due to a combination of bad shape and brittleness.



The first generation of CD cases were made from polystyrene, which is a transparent thermoplastic that was utilized in similar cases for magnetic cassette tapes used in the 1970s and 80s. It is also common for household products, such as pens. We can assume that the original design from the early 1980s was conceived looking for a, transparent lid, for the CD sleeve to be seen from the outside. The hinge construction required manufacture by molding and the main objective being low cost.

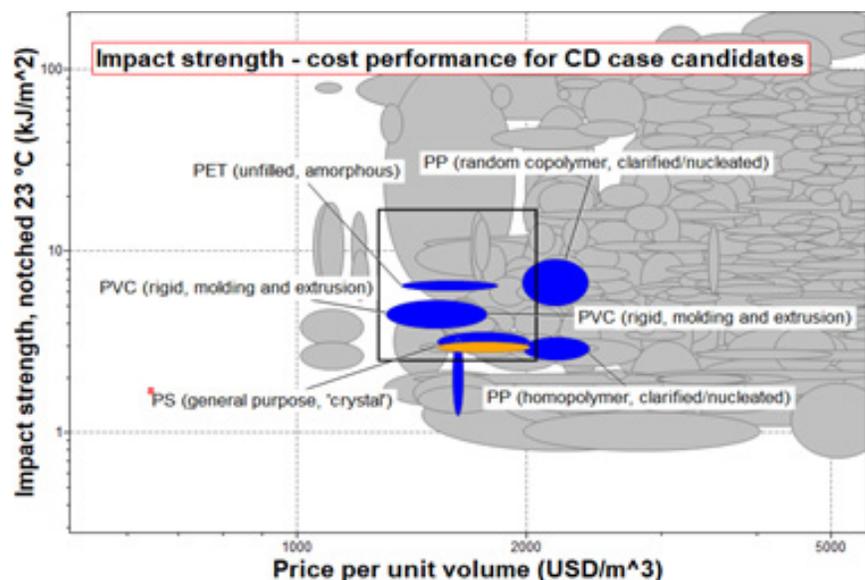
A simple search for “CD case” in the software gives two results, but only the polystyrene folder-level record is relevant. It shows the main features of the material, typical uses and limitations. Indeed, it confirms that “General purpose grades tend to be brittle” and, hence, “susceptible to fracture”. See also below. We can find out more about fracture properties by clicking the *Impact strength* attribute.

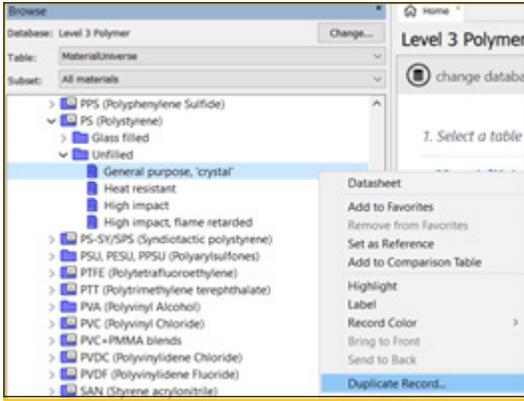


kJ/m²	ft.lbf/in²	Typical description	Example material
<5	<2.5	Brittle plastics	Polystyrene (PS)
10-40	5-20	Toughened plastics	Polypropylene co-polymer ABS
>50	>24	Tough plastics	Polypropylene impact copolymer Polycarbonate (PC)
590-600	280-285	Rubbery- ‘no break’ <i>i.e.</i> maximum value	Low density polyethylene (PE-LD) Elastomers

This table from the Science Notes shows values for Impact strength, which is widely used for ranking the toughness of materials. The notched test indicates the susceptibility of breakage on fast impact, for example, a drop on a hard floor, where the material has notches, sharp corners, cracks, and other ‘stress concentrating’ features. The unnotched test, sometimes called ‘practical toughness’, is mainly used for objects designed without those.

To mimic the conditions for the original material selection, the price per unit volume, is plotted on the X-axis of an Ashby chart using the Polymer Level 3 database. Transparency with *optical quality* or *transparent*, and *unfilled* polymer are introduced as constraints via a limit stage and a tree stage is used to include only the *thermoplastics*. Here, the Impact strength is plotted on the Y-axis for an overview and a box selection is used to limit the selection to materials cheaper and tougher than *unfilled General purpose ‘crystal’ polystyrene*, which can be set to be the reference material.



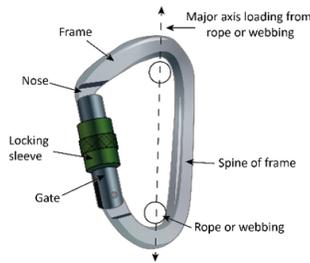


The fracture toughness can also be plotted as a benchmark for brittleness in a similar chart as above. If so, right-click *Polystyrene, Unfilled General purpose 'crystal'* in the database. This enables one to Duplicate Record and introduce a value of 0.7-1.1 for fracture toughness, which is in line with a CD case. This record can now be named, e.g., “CD case Polystyrene” and made a reference. From either reference material record, a Find similar operation results in a ranked list of similar materials (or better). The nearness settings can be adjusted to fit the improvements desired. Here, the default setting can be modified by *Price: same or lower and Impact strength, notched 23 °C: same or higher instead of Fracture toughness: Identical*. The *Thermal conductivity* can be canceled.

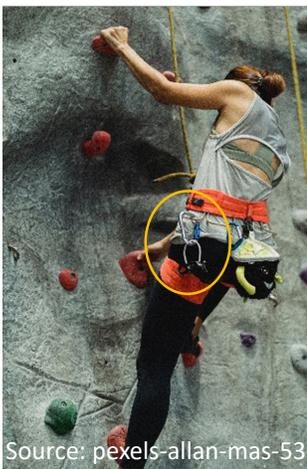
When it comes to re-design in Granta EduPack, using Level 3 databases, interesting candidates can now be compared side-by-side. In this case, we can make use of the Result list ranked by nearness and tick the most relevant materials from the chart, e.g., PVC, PET, and PP. In this example, PET appears to be a good option. Following this methodological demonstration, a display of actual alternative materials is given at the end.

Comparison - MaterialUniverse				
	PS (general purpose, 'crystal')	PVC (rigid, molding and extrusion)	PET (unfilled, amorphous)	PP (homopolymer, clarified/nucleated)
General Information				
Included in Materials Data for Simulation	✓	✓	✓	✓
Price				
Price per unit volume (USD/m ³)	1530 - 2010	1310 - 1770	1370 - 1830	1980 - 2410
Impact & fracture properties				
Impact strength, notched 23 °C (kJ/m ²)	2.86 - 3.15	3.8 - 5.4 ↑	6.19 - 6.83 ↑	2.53 - 3.39
Optical, aesthetic and acoustic properties				
Transparency	Optical quality	Transparent ↓	Optical quality	Transparent ↓

2. Yield



One example of an application where yield failure is a potential safety risk, is a Carabiner (Karabiner), which is a special type of shackle used to connect ropes or other components quickly and reversibly. Carabiners are used, for instance, in mountaineering, caving, construction, rescue or yachting. The vast majority of Carabiners are made from aluminum alloy 7075 T6, because of low specific weight. In situations where weight is not important, such as in fixed anchors or fire rescue, stainless steels are used, due to their higher wear resistance and tensile strength. Main alternatives include X2CrNiN23-4 or even a regular C45 carbon steel.



Source: pexels-allan-mas-5384157

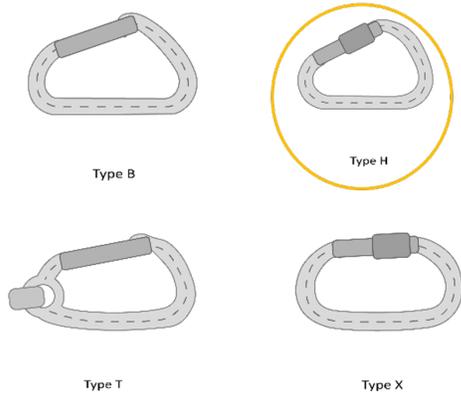


pexels-riccardo-bresciani-303040

Some of the most important factors to be considered in selection of materials for mountaineering equipment are:

- | | |
|--|--|
| <ul style="list-style-type: none"> • Low weight | <ul style="list-style-type: none"> • Durability to water and sunlight-UV resistance |
| <ul style="list-style-type: none"> • High strength (static/dynamic loading) | <ul style="list-style-type: none"> • Service temperature (-40°C to +50°C) |
| <ul style="list-style-type: none"> • Hardness/abrasion resistance | |

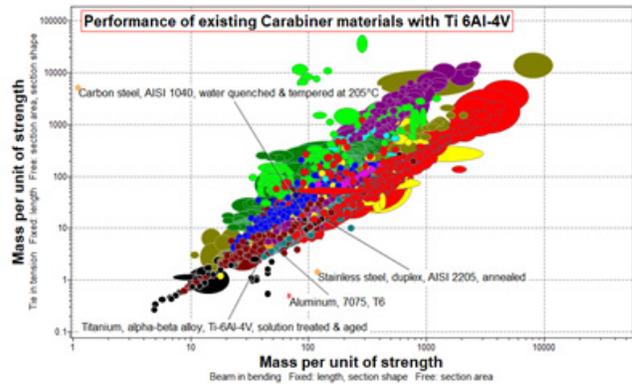
Furthermore, there is a European standard (EN 12275) for Carabiners, which specifies the loading requirements for different types of carabiners. Carabiners are classified into several types, some of which are shown below. An axial load of a minimum of 6 kN must be sustained for type H Carabiners with an open gate and 20 kN for a closed gate.



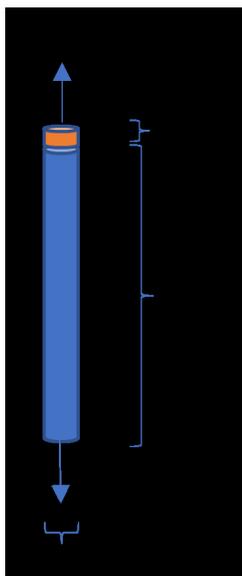
HMS Carabiner (type H):



Here, we assume that Al 7075 T6 is a good option but want to compare the safety performance with stainless and carbon steel, while also exploring improving the strength-to-weight performance. A chart is created in Level 3 Aerospace and the reference material is set to Al 7075 T6. C45 carbon steel is approximated with AISI 1040 in the *MaterialUniverse*, assuming water quenched & tempered at 205°C. The X2CrNiN23-4 stainless steel is approximated with Duplex (semi austenitic) AISI 2205 annealed, which has a similar composition and chromium content.



All three are set as *Favorites* by right-clicking and the Performance Index Finder is used to plot the performance of a beam in bending on the X-axis and a tie in tensile stress on the Y-axis. Since this is mountaineering equipment, the objective is to minimize mass in strength limited design. From aerospace applications and others, it is well known that some titanium alloys exhibit superior specific strength and thermal stability. A solution treated and aged alloy Ti-6Al-4V is therefore chosen as a potential candidate to challenge Al 7075 T6. As can be seen from the plot above, it has very similar mechanical performance.



The Engineering solver can be used to estimate the required stiffness and strength needed for the given load, 6 kN and maximum deflection, say 1%. Assuming a spine of 100 mm that translates to 1 mm. Using dimensions from an actual Carabiner and a typical safety factor of 4, the solver calculates the minimum Young's modulus to 25.3 GPa, in order not to exceed 1 mm extension. The Yield strength required from the material given these parameters is calculated to 253 MPa. Both these values are met by all four materials considered in the chart shown above, which can easily be verified in a comparison table (not shown).

Engineering Solver

Tie in tension Change situation ?

Estimates the minimum strength and stiffness values required for a tie with the specified geometry and load conditions.

Assumptions:

- Bar is straight with uniform cross section
- Material is homogeneous
- Uniform stress distribution is achieved

Geometry

Cross-section:

Radius (R): mm

Length (l): mm

Design parameters

Load: kN

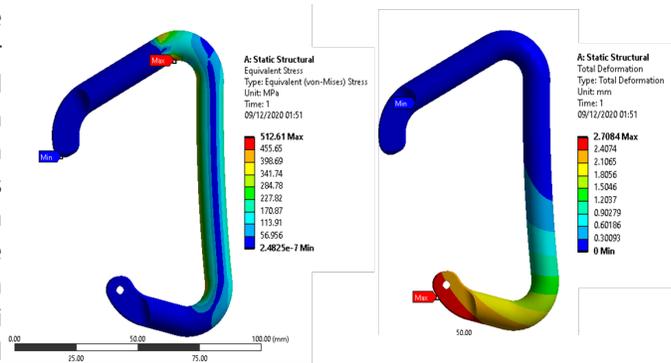
Safety factor:

Maximum extension: mm

Results

Young's modulus	Yield strength
<input type="text" value="25.3"/> GPa	<input type="text" value="253"/> MPa

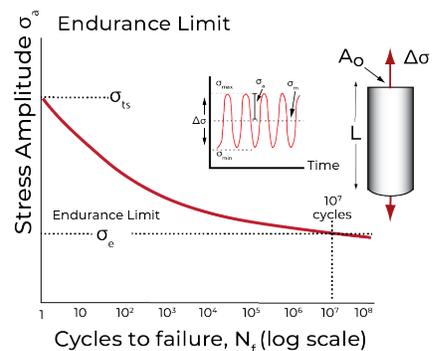
Once the material is chosen, a FE simulation can be performed to optimize the geometry of the Carabiner or analyze the predicted deformations and internal stress distribution. Here is an example taken from an 11 mm diameter CAD model using material data from Al 7075 T6. In this example, it shows a maximum stress (von Mises) of 513 MPa near the end of the spine and a visualization of the deformations at 6kN axial load. The spine is extended by around 1 mm and the maximum deformation (bending) is 2.7 mm. If acceptable, the Ti 6Al-4V (827-1070 MPa) has sufficient strength but the Al 7075 T6 (460-530 MPa) might not.



Comparison - MaterialUniverse				
	Aluminum, 7075, T6	Titanium, alpha-beta alloy, Ti-6Al-4V, solution treated & aged	Stainless steel, duplex, AISI 2205, annealed	Carbon steel, AISI 1040, water quenched & tempered at 205°C
Computed Properties				
Mass per unit of strength	5.28 - 6.09	4.14 - 5.36	15.3 - 17 ↑	10.8 - 13.2 ↓
Mass per unit of strength	42.7 - 47	42.4 - 50.3	122 - 131 ↑	96.8 - 111 ↑
Physical properties				
Density (kg/m ³)	2770 - 2830	4410 - 4450 ↑	7800 - 7820 ↑	7800 - 7900 ↑
Mechanical properties				
Yield strength (elastic limit) (MPa)	460 - 530	827 - 1070 ↑	460 - 510	595 - 730 ↑
Flexural strength (modulus of rupture) (MPa)	460 - 530	827 - 1070 ↑	460 - 510	595 - 730 ↑

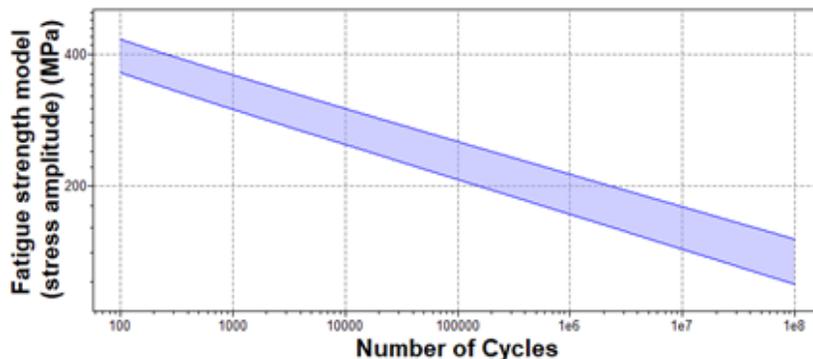
3. Fatigue

The last of the three examples of failure is fatigue, which is initially caused by small cracks that propagate progressively over a long period of time as a consequence of repeated but relatively small loads (in comparison to the yield load) until a sudden catastrophic failure takes place. The cracks are nearly always initiated at surface defects or other sites of stress. This makes the surface smoothness important and to avoid scratches on it. Material subjected to repeated stress cycles may fail even when the peak stress is well below the tensile strength, or even below that for yield. That is the reason why this kind of failure is so challenging for the designer. Fatigue data are measured and presented as $\Delta\sigma - N_f$ or S-N curves, where $\Delta\sigma$ is the range over which the stress varies and N_f is the number of cycles to failure.



Fatigue strength at 10 ⁷ cycles	152	-	168	MPa
Fatigue strength model (stress amplitude)	143	-	179	MPa

Parameters: Stress Ratio = -1, Number of Cycles = 1e7cycles



To aid designers in preventing fatigue, the fatigue strength (for 10⁷ cycles) and a simple model of strength vs number of cycles are available for many metal alloys in the advanced databases. The graph for Al 7075 T6 is shown to the left. Note that Al does not have a fatigue limit, i.e., an asymptotic value for the strength as the number of cycles approaches infinity.

Reality check

In this case study, we have considered failure by fracture, yielding and fatigue. In the first case, polystyrene was found to be too brittle for normal use and was riddled with failures. The black part, made of high impact PS (HIPS), was also criticized. The case re-design was tackled with modified both shape and material. A new thicker hinge design, the Super Jewel box (see below), with supports as well as a tougher quality polystyrene containing recycled material. The CD case design has since evolved, however, by “thinking outside of the box”. Subsequent solutions include polypropylene cases (like VHS or DVD boxes) but translucent (cloudy), or cardboard sleeves, where information was printed on the outside, instead of inside, or hybrids with plastic.



1 Super Jewel Box (still PS) 2. Slimline (translucent PP) 3 Digisleeve (cardboard) 4 Digipak (HIPS/cardboard)

Even thin paper sleeves lined by spunbonded polyethylene is now marketed (Tyvek, not shown) but mostly used for other digital media than music, where marketing is not a priority. Ironically, music CDs with the original mechanically failing cases are often sold wrapped in shrink-wrap that have been criticized for being too tough to open (not failing easily enough).



	Aluminum, 7075, T6	Titanium, alpha-beta alloy, Ti-6Al-4V, solution treated & aged
Computed Properties		
Mass per unit of strength	5.28 - 6.09	4.14 - 5.36
Mass per unit of strength	42.7 - 47	42.4 - 50.3
Processing properties		
Metal casting	Unsuitable	Excellent ↑
Metal cold forming	Acceptable	Limited use ↓
Metal hot forming	Excellent	Acceptable ↓
Metal press forming	Acceptable	Acceptable
Metal deep drawing	Acceptable	Limited use ↓
Machining speed (m/min)	76.2	11.6 ↓
Weldability	Unsuitable	Good ↑

On the questions of improved Carabiners (lighter, stronger), the option of titanium or perhaps Magnesium appears attractive. Most mechanical properties are better for titanium. However, there are few, if any, such products on the market. That is partly because the material price is 5-8 times higher for Ti 6-4 than Al 7075 and partly because of poor manufacturing properties, that makes it difficult to product defect-free Carabiners made of titanium. Although Ti is readily cast, cold or hot forming to carabiner shapes is not favorable.



Source: v Commons (Imperial War Museum)

In the final example of actual failure, we consider the tragic but extensively studied De Havilland Comet I, which was the first passenger jet airliner in commercial operation, introduced in service 1952 by British Overseas Airways Corporation (BOAC). Following a number of accidents, two aircraft were lost in similar circumstances 1954, airliners breaking-up in mid-flight.

Metal fatigue was recognized as being the cause of the issue; a concept that was not fully understood at this time. This led to a court of inquiry that tasked the Royal Aircraft Establishment in Farnborough, UK to investigate the cause of these accidents. Their report concluded that structural failure, brought about by fatigue was responsible. Fatigue is considered as the most common cause of failures in aircraft metal structures. The occurrence of fatigue in aircraft is partly due to the stress cycle from pressurization of the fuselage occurring every flight. For the design and construction flaws, including improper riveting and dangerous concentrations of stress around some of the square windows, were ultimately identified. As a result, the Comet was extensively redesigned, with oval windows, structural reinforcements and other changes.

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