the Pugh criterion

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When subject to a tensile test, metals show two distinct types of behaviour:

- for some metals, the tested bar elongates during the test, the bar gets thinner in the middle, and eventually it breaks (right-hand side of the picture). Such metals are called “ductile”.
- for other metals, the tested bar hardly elongates before it breaks (left-hand side of the picture). Such metals are called “non ductile”.

The amount of elongation before rupture is taken as a measure for the degree of ductility of the metal. Being ductile or not is temperature dependent. At very low temperature, all metals become non ductile. The temperature at which they become ductile can be taken as a criterium for ductility too: the higher this temperature, the more non-ductile this material is. This temperature is called the “ductile to brittle transition temperature” or DBTT (a misnomer, because “non ductile” is not the same as “brittle”).

Is there a way to find out whether a metal is ductile or not, without having to do an elaborate tensile test? Can’t we deduce this from simpler properties, that are hopefully tabulated for the considered metal? This was the question tackled by S.F. Pugh, in a paper published in 1954 :

XCII. *Relations between the Elastic Moduli and the Plastic Properties of Polycrystalline Pure Metals*

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Abstract

Relations between the elastic and plastic properties of pure polycrystalline metals are discussed and a systematic relation between shear modulus, Burgers vector and plastic shear strength of metals possessing the same lattice structure is proposed. In addition reasons are given for believing that in a limited temperature range malleability is related to Poisson’s ratio.

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We will focus here on the subset of unary fcc metals. For these metals, Pugh listed the experimental bulk modulus B, shear modulus G and Poisson's ratio ν, together with the elongation-before-rupture in a standard tensile test. Converted into modern units, the table he published in 1954 looks like this:

		G (GPa)	B (GPa)	B/G	elong	ν
Thorium	fcc	31	54	1.741		0.259
Iridium	fcc	210	366	1.743	5	0.259
Rhodium	fcc	150	265	1.765	5	0.262
Strontium	fcc	6	12	1.968		0.283
Calcium	fcc	7	17	2.333	60	0.313
Nickel	fcc	74	185	2.520	30	0.325
Aluminium	fcc	27	73	2.743	50	0.337
Copper	fcc	46	136	2.996	60	0.350
Silver	fcc	29	99	3.435	60	0.367
Paladium	fcc	44	186	4.270	40	0.391
Platinum	fcc	52	273	5.245	40	0.410
Gold	fcc	28	170	6.135	50	0.423
Lead	fcc	6	41	7.368	64	0.435

The materials in this table are listed in order of increasing B/G-ratio, or equivalently, in order of increasing Poisson's ratio ν. This order correlates not too badly with the amount of elongation in a tensile test. Such observations have lead to the Pugh criterion: a metal is expected to be ductile if $B/G>1.75$, $G/B<0.57$ or $\nu<0.26$ (all 3 criteria are equivalent and can be converted into one another).

It would be insightful to inspect the evolution of B/G across the periodic table. This is easier said than done, as not all elements appear in the unary fcc phase. And therefore it is not possible to measure B and G experimentally for those. With DFT, however, this is no problem: you can create a fcc lattice with any element, and do computer experiments to determine B and G. This can then be compared to experimental information about the ductility, either for the fcc phase if it exists, or for another phase if it doesn't.

The hope/expectation is that there will be a clear trend in B/G across the periodic table, which can hint to the physical mechanisms that lead to ductile behaviour.

Step 1

Your team will be assigned 5 elements. Create a fcc lattice for each of them, and do a proper convergence test procedure to find the values for basis size and k-mesh that lead to sufficiently converged results. If you can find one choice of values that gives converged results for all 5 crystals without leading to excessively long computation times for any of them, then proceed with these. If such a single choice does not exist, then continue with a different choice for every element.

Step 2

With your chosen settings, compute the bulk modulus of your 5 crystals (see the chapter on geometry optimization). You can compare your results to (the supplementary information of) this paper (https://dx.doi.org/10.1038/s42254-023-00655-3), in which the equilibrium volume and bulk modulus have been computed for (a.o.) all elements of the periodic table in the fcc structure, and this with extreme precision. If you reproduce these bulk moduli, you can trust you have the proper settings for your calculations.

Step 3

Construct a procedure to compute the shear modulus G of your 5 crystals (see the chapter on elastic constants). If you find computed literature values to which you can compare your results, definitely do so.

Step 4

Compare your computed B and G with experimental values for B and G, either in the fcc structure if it exists, or in the most similar structure you can find.

Step 5

Search experimental information about the ductility of your 5 crystals (or of the same element in another unary structure if the fcc structure does not exist for your element).

Step 6

Compare the experimental ductility information with the Pugh criterion, for your 5 crystals. Does the Pugh criterion hold, based on this info?

Step 7

Based on your computed info or on the experimental info, select one extra element for which you compute and search the same info. Ideally, you take for this an element that can either strengthen or contradict the hypothesis you could derive from your 5 assigned elements.

Optional step 8:

Repeat step 7 as many times as you feel like (if there is time).

The results and interpretation of your calculations should be discussed in a paper and a video, as explained in more detail in the Project tile at www.compmatphys.org. Information about (intermediate) due dates can be found in the Quick Start tile.