Current Opinion in Solid State & Materials Science xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Current Opinion in Solid State & Materials Science

journal homepage: www.elsevier.com/locate/cossms

Predicting whether a material is ductile or brittle

R.P. Thompson*, W.J. Clegg

Department of Materials Science and Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge CB3 0FS, United Kingdom

ARTICLE INFO

Keywords:
Ductility
Ductility criteria
Fracture
Yield
Dislocations
Lattice resistance
Crystal structure

ABSTRACT

In this paper we discuss the various models that have been used to predict whether a material will tend to be ductile or brittle. The most widely used is the Pugh ratio, G/K, but we also examine the Cauchy pressure as defined by Pettifor, a combined criterion proposed by Niu, the Rice and Thomson model, the Rice model, and the Zhou-Carlsson-Thomson model. We argue that no simple model that works on the basis of simple relations of bulk polycrystalline properties can represent the failure mode of different materials, particularly where geometric effects occur, such as small sample sizes. Instead the processes of flow and fracture must be considered in detail for each material structure, in particular the effects of crystal structure on these processes.

1. Elastic ductility criteria

1.1. The Pugh ratio

Many models exist that try to predict the plastic behaviour of materials. By far the most widely used, no doubt due to the ease with which elastic constants can be measured or calculated by density functional theory, is that of Pugh [1].

The Pugh ratio, G/K where K is the bulk modulus and G is the shear modulus, represents the competition between two processes, plasticity and fracture. If plasticity is easier then a material will tend to be ductile, whereas if fracture is easier then a material will tend to be brittle.

Pugh assumed that the yield stress, i.e. a measure of the difficulty of plastic deformation, scales with the shear modulus, as the Orowan bowing [1] stress is:

$$\sigma_y = \frac{Gb}{\lambda} \tag{1}$$

where σ_y is the yield stress, G is the shear modulus, b is the Burgers vector, and λ is the size of the Frank-Read source [2]. Pugh assumed that λ does not vary between metals, i.e. any work hardening can be neglected. Pugh associated this with the Brinell hardness number:

$$B.\ H.\ N. = \frac{Gb}{c} \tag{2}$$

where $B.\ H.\ N.$ is the Brinell hardness number and c is a constant for a particular crystal structure, which is not explicitly defined by Pugh, but presumably relates to available slip systems and average Schmid factors.

The fracture stress of a material can also be linked to elastic constants. Pugh noted that fracture stress scales with the Young modulus, E [3], and that the surface energy of a material, to which some of the work of fracture must be converted [4], was shown to correlate with E by Elliott [5]; however Pugh neglects the fact that during the fracture of ductile materials such as aluminium, the energy dissipated by dislocations is much larger than the surface energy. The surface energy, and therefore the stiffness, only has a small influence on the fracture stress of ductile materials.

Pugh suggested that the particular constraints on strain state at the crack tip will cause the relevant elastic modulus to vary between two limiting cases: the Young modulus, E, and the bulk modulus, K. Since these constants generally scale together, Pugh used the bulk modulus for convenience, and took the fracture stress to obey:

$$\sigma_* \propto Ka \tag{3}$$

where a is a lattice parameter.

If this is true, then the ratio of the yield stress, as characterised by the Brinell hardness, and the fracture stress will follow the expression:

$$\frac{B.\ H.\ N.}{\sigma_*} \propto \frac{Gb}{cKa} \tag{4}$$

As noted by Pugh the crystal structure will affect this criterion, however these are usually neglected to enable easy comparison of materials. If the effects of crystal structure are neglected, b/ac is constant, the relative difficulty of plastic flow and fracture is represented by:

$$\frac{B.\ H.\ N.}{\sigma_*} \propto \frac{G}{K}. \tag{5}$$

Hence the ratio G/K provides a measure of the likely nature of a

* Corresponding author.
E-mail addresses: rpt26@cam.ac.uk (R.P. Thompson), wjc1000@cam.ac.uk (W.J. Clegg).

https://doi.org/10.1016/j.cossms.2018.04.001
Received 16 January 2018; Received in revised form 23 March 2018; Accepted 8 April 2018
1359-0286/

material's failure: a high value of G/K implies brittle failure, while a low value implies ductile failure. This assumes that the changes in crystal structure affect both processes to the same degree.

Thermal effects were neglected for metals like iron, for which the homologous temperature is low at room temperature (~ 0.16 for iron). However, it is well documented that the yield stress of iron falls by almost three orders of magnitude between absolute zero and room temperature [6,7] due to the thermally activated nature of the lattice resistance. This is much greater than the change in the shear modulus, which falls by just over 5% over the same temperature range [8].

Pugh collated a large amount experimental data to support his ideas [9–11]. The yield stress was estimated from the Brinell hardness across a large range of metals with body- and face-centred cubic, and hexagonal crystal structures. The data presented are generally consistent, though there are discrepancies, notably Ca, Pt, Be, and, perhaps surprisingly given its isotropy, W. These discrepancies are associated with twinning [1] or solute drag [12,13].

The Brinell hardness number is measured using a spherical indenter. This has the complication that the indents are not necessarily self-similar. The hardness therefore depends on the load, W and the diameter of the ball, D, and is given by [9]:

$$B.\,H.\,N. = \frac{2W}{\pi D^2 [1 - \sqrt{1-(d/D)^2}]} \tag{6}$$

where d is the diameter of the indent.

The Brinell hardness number of two indents, in the same material, will be the same if the indents are geometrically similar, i.e. if d/D is constant. However there is no indication in Pugh's sources [9–11] that the quoted values were obtained under this condition, so that the experimental support for this idea cannot be conclusive.

This criterion is also often justified by considering the properties of the f.c.c. metals [14]. As shown in Fig. 1, soft ductile metals, such as Au and Ag have low values of G/K, while more brittle metals, particularly Ir, have high values of G/K. However despite the fact that Ir is often considered brittle, plastic flow occurs before fracture [15], and the failure mode is strongly dependent on grain boundary properties, particularly impurity levels [16].

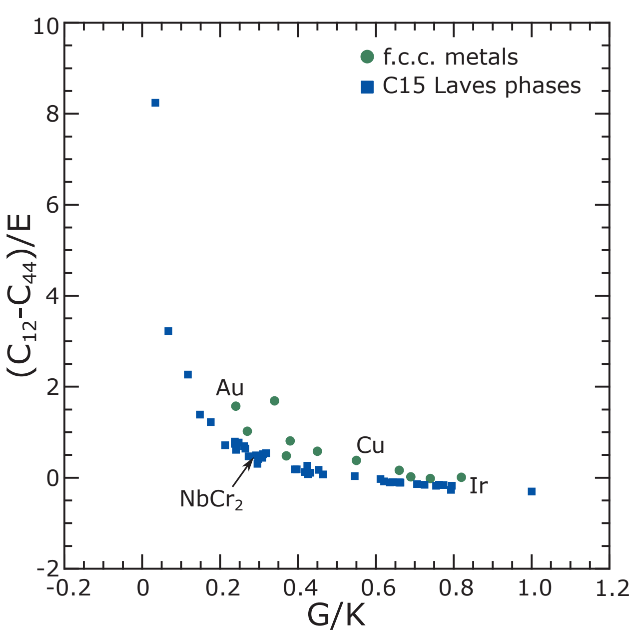

Fig. 1. The variation of two ductility criteria, that of Niu et al. [18] and Pugh [1], for the f.c.c. metals and the C15 Laves phases. As can be seen the Laves phases cover a similar range of values for both the criteria and overall fall on the ductile side of the f.c.c. metals. Data from [14,21–33].

1.2. Cauchy pressure

As metals tend to be more ductile than non-metals, another possible criterion is the Cauchy pressure, as discussed by Pettifor [17]. The Cauchy pressure is defined, in terms of the single crystal elastic constants of a cubic material, as $C_{12}-C_{44}$, and can be used to describe the nature of the bonding in a material. A material with a high resistance to bond bending, such as a covalently bonded solid, will have a negative Cauchy pressure, i.e. $C_{44} > C_{12}$. In contrast materials with metallic bonding exhibit a positive Cauchy pressure.

It is worth noting that Pettifor states this is a metric for the nature of bonding and appeals to the Pugh ratio when commenting on ductility. It seems likely that the use of the Cauchy pressure as a ductility criterion [18–20] is due to its relative ease of calculation with density functional theory, as with the Pugh ratio. A positive Cauchy pressure is considered to indicate ductile behaviour, while a negative pressure implies brittle behaviour.

Niu et al. [18] have shown that one can draw lines where Pettifor's criterion, that the Cauchy pressure should be greater than zero, intersects that of Pugh's criterion at $G/K = 0.571$. This is close to the critical value of 0.6, suggested by Gilman [14]. Pugh, himself, does not actually give a critical value for the ratio dividing brittle from ductile materials, although he does state that he expects the transition to be sharp.

It was found that materials followed a broadly hyperbolic trend when the Pugh ratio was plotted against the Cauchy pressure, normalised by the Young modulus [18]. This is plotted for some of the f.c.c. metals and some of the cubic Laves phases in Fig. 1. The Laves phases are describing a different hyperbola to f.c.c. metals, one that is generally lower in G/K. Without a theoretical underpinning it is not clear what significance can be attached to this trend.

The low values of G/K and high positive values of the Cauchy pressure in some Laves phases do not correspond to ductile behaviour. While dislocation motion has been observed in micropillars of the Laves phases [34], these phases are brittle [35]. For example the Laves phase $NbCr_2$ has a Pugh ratio of 0.28 and a normalised Cauchy pressure of 0.56. These values both lie between those of copper and gold, but experimentally the fracture toughness of $NbCr_2$ is found to be around $1.5\,\mathrm{MPa}\sqrt{\mathrm{m}}$ to $2\,\mathrm{MPa}\sqrt{\mathrm{m}}$ [24,36], which is clearly brittle. This is comparable with ceramics such as borosilicate glass, which have a toughness of about $1.5\,\mathrm{MPa}\sqrt{\mathrm{m}}$ [37], and lower than alumina, for which the toughness is approximately $3.5\,\mathrm{MPa}\sqrt{\mathrm{m}}$ [38].

In this case, the change of crystal structure has violated an assumption of the Pugh model. The crystal structure has made the Laves phases brittle by increasing the difficulty of plastic flow, i.e. the yield stress, without a corresponding increase in the difficulty of fracture, i.e. the fracture stress. Since this is an effect of the crystal structure, it cannot be captured by the ratio of elastic constants alone.

Another effect that is often overlooked is that of geometry. In particular the effect of size is known to be significant. For instance, in small micropillars cracking is suppressed and even very brittle materials, such as silicon, will plastically deform [39–41]. The size effect is also significant in indentation where the hardness is known to increase markedly as indent depths become small [42]. As the elastic properties are unchanged, criteria such as the Pugh ratio or the Cauchy pressure cannot account for these phenomena.

At best the Pugh ratio might provide a general indication of behaviour across materials with the same or similar crystal structure and deformation mode. Other changes in the balance between the competing processes could prevent even that; for example a change in the nature of dislocations, such as dissociation into partial dislocations. This would not change G/K but would alter the yield stress of the material with no corresponding change in the difficulty of fracture. Certainly the Pugh model and Cauchy pressure cannot provide a basis for the prediction of the behaviour of novel materials.