

THERMODYNAMIC CRITERION FOR PREDICTING THE BRITTLENESS AND PLASTICITY OF METALS

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A brief comparative analysis of the various methods of evaluating the brittle fracture of metals is given. A plasticity index for metals is proposed and substantiated, and the relation describing its effect on the relative contraction at rupture is obtained.

Among the scientific concepts of the fracture strength of a metallic crystal lattice that have been established to date, one can distinguish the following two basic trends: the mechanistic approach (the Born model) and the thermodynamic approach.

In their fracture model, Born and Huang [1] assume that fracture occurs when the elastic or shear moduli of a tensile specimen vanish at the moment the strain energy reaches a limiting value. In this model, the temperature dependence of the strain modulus is of significance. In most cases, especially for "pure" metals, the strain modulus obeys the formula [2]

$$E/E_0 = 1 - (T/T_{\text{melt}})^2, \quad (1)$$

where E_0 is the strain modulus at absolute zero, T is the temperature, and T_{melt} is the melting point.

However, there are considerable peaky deviations (toward decrease) from relation (1), especially for metals with impurity [2, 3]. In our opinion, in these cases there is a second-order phase transition in which the isothermal coefficient of cubic expansion (compression) of the material, and, hence, the strain modulus, undergo a discontinuity. As follows from the propositions of thermodynamics, second-order phase transformations are accompanied by discontinuous changes in one or several physical quantities, for example, the specific heat, the temperature coefficient of cubic expansion, and the bulk modulus.

Larionov and Semenov [3] established the abnormal behavior of the physical characteristics of steel alloys, in particular the temperature coefficient of cubic expansion, magnetic susceptibility, and electric resistance, near the temperature of tough-brittle fracture transition. This phenomenon is explained by replacement of the metallic bond by a covalent bond, which occurs with a decrease in temperature in a narrow region of tough-brittle fracture transition. Abrupt transitions from one dominant bond to another can be accompanied by softening of the metal due to a change in the forces of attraction between atoms in the crystal lattice.

According to the mechanistic approach, fracture occurs when the elastic or shear moduli vanish either as a result of supply of mechanical energy or as a consequence of the second-order phase transition due to a temperature change. This indicates the necessity of developing the thermodynamic model of fracture.

The increased attention to the development of thermodynamic models of fracture is due to the fact that the specific work of deformation due to fracture has the same order of magnitude as the specific heat of melting of metals, and the fracture strain is comparable to the thermal expansion of the fracture region upon heating from the initial temperature to the melting point. Thus, Stepanov [4] gives a simple relation between

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the specific work of fracture and the latent heat of melting for zinc and cadmium, which, in his opinion, may be universal for metals:

$$\rho \dot{W}/L = 0.19 = \text{const.}$$

Here W is the deformation work in fracture of 1 g of a metal, ρ is the density, and L is the specific latent heat of melting.

In discussing the value of the effective surface energy for steel in the Griffith formula, which is 2 or 3 orders of magnitude lower in brittle fracture than in tough fracture, Zener [5] put forward an interesting idea. He explained this phenomenon by the fact that with occurrence of rupture, shear becomes more and more adiabatic, and the associated local heating, which is enhanced as the specific heat decreases with decrease in temperature (below the Debye temperatures), lowers the fracture work.

An analogy between mechanical failure and melting of metals after attainment of the critical energy density is drawn by Osipov [6] and in the more recent work of Ivanova and Terent'ev [7]. An important step in the development of the thermodynamic view on the fracture process were the papers of Zhil'mo [8] and D. Sih [9]. Zhil'mo [8] states that of the entire work required for fracture, it is necessary to distinguish only the work in an elementary volume located in a cross section that is critical from the viewpoint of fracture. The work on fracture of a certain microvolume is a characteristic constant quantity for a particular material. According to [8], for construction steels similar in chemical composition and strength properties to domestic construction low-carbon steels, this quantity, called the limiting deformation work, is 650–850 J/cm³.

The failure concept of Sih is based on the local (near the concentrator) and global (along the entire cross section of the member) critical energy densities, i.e., on a two-parameter fracture criterion. In this case, the fraction of tough and brittle fractures can be established from the ratio of the energy density of shape change (distortion) to the energy density of volume change (dilatation).

Developing the ideas of Zhil'mo and Sih, Ivanova believes that the critical energy densities of distortion W_{cd} and dilatation W_{cv} are $W_{cd} = L$, where L is the latent heat of melting and $W_{cv} = H$, where H is the enthalpy of the metal heated from the initial temperature to the melting point [7].

However, an essential contradiction in the failure model of Ivanova is the assumption that brittle fracture is controlled by microshear after attainment of the critical shear stress τ_c , which is related to the critical energy density of distortion by

$$W_{cd} = L = \tau_c^2/(2G). \quad (2)$$

In turn, tough, i.e., high-power-consuming fracture, is determined by microrupture after attainment of the critical normal stress σ_c , which is related to the critical energy density of volume change by

$$W_{cv} = H = \sigma_c^2/(2E). \quad (3)$$

Comparing the left and right sides of expressions (2) and (3), Ivanova obtained the quantity Δ , which she called the universal fracture constant:

$$\tau_c/\sigma_c = \Delta^{0.5} = \sqrt{LG/(HE)}. \quad (4)$$

In expression (4) for the majority of metals, $G/E \approx 0.35$ – 0.40 and $L/H \approx 0.4$. Therefore, the values of the universal fracture constant are within $\Delta \approx 0.12$ – 0.16 . It should be noted that the criterion Δ does not reflect the tendency of metals to brittle or tough fracture and the plastic metal workability (change in shape). Thus, according to the results of [7], the values of Δ for ductile materials such as pure aluminum and gold are markedly different and are equal to 0.225 and 0.153, respectively. At the same time, for brittle and hard-to-work beryllium, $\Delta = 0.18$, which is larger than that for gold, iron, nickel, and other ductile metals. The moment of transition from tough to friable fracture is determined by the condition of equal intensities of tangential and normal stresses in local volumes of the metal:

$$\tau_c \sqrt{\Delta_t} = \sigma_c \sqrt{\Delta_\sigma}. \quad (5)$$

Condition (5) and expression (4) allow one to define the physical meaning of the universal constant as the ratio of the fractions of a metal failed by normal and tangential stresses.

The condition of transition from tough to brittle fracture is determined from the relation

$$W_{cd} = W_{cv} = L. \quad (6)$$

In our opinion, conditions (5) and (6) do not have sufficient theoretical grounding. This follows from an analysis of the limiting strain energy densities in fracture and fracture stresses. Thus, for steels, irrespective of their chemical composition, the latent heat of melting is equal to 2120 J/cm³, and the enthalpy for heating of steels from room temperature to the melting point is 8380 J/cm³. At the same time, the volume density of strain energy at the moment of fracture has the same numerical values as the fracture stress σ_{fr} . This follows from the equation for the limiting value of the specific energy consumption W_c of the process of deformation and fracture of the crystal lattice, in which stresses are related to displacements of atoms by the well-known sinusoidal law

$$W_c = \int_0^d \sigma_c \sin \frac{\pi x}{d} d\left(\frac{x}{d}\right) \approx \sigma_c, \quad (7)$$

where σ_c is the maximum strength of the crystal and d is the atomic lattice period.

For the majority of constructional steels, $\sigma_{fr} = 650\text{--}850$ MPa, which is close to the above limiting energy density 650–850 J/cm³. From relations (6) and (7), the theoretical limiting stresses in steels should be numerically comparable to the latent heat of melting and approximately equal to 2120 MPa. This, however, does not agree with the theoretical strength of steels ($\sigma_{theor} = 13,000$ MPa). The more so as for many constructional steels, for example, ShKh15 and ShKh15SG, $\sigma_{fr} > 2120$ MPa. In addition, there is also a considerable difference between the theoretical rupture strengths of steel determined from the enthalpy (8380 MPa) and using the Frenkel procedure ($\sigma_{fr} = E/10 = 21,000$ MPa).

More accurate calculations of the theoretical strength and limiting strain energy density for fracture of metals are given by Fedorov [10]. Developing the thermodynamic model of fracture, he assumed that the specific volumetric internal energy absorbed by a metal at the moment of fracture can be written as the sum of the enthalpy of a metal heated from absolute zero to the melting point and the latent heat of melting:

$$W = \int_0^{T_{melt}} C_p dT + \frac{V_{fr}}{V} L.$$

Here C_p is the specific isobaric heat, V_{fr} is the volume of the failed metal, and V is the entire volume of the metal. Depending on the structure of the metal and deformation and fracture conditions, the value of V_{fr}/V varies from 0 to 1. The maximum fracture energy density is thus 10,500 J/cm³, and the theoretical strength is 10,500 MPa, which is close to the true value.

We hold to the idea that the processes of melting, limiting thermal expansion, and mechanical failure of metals are energetically equivalent. In this connection, we propose a model of brittle and tough fracture that assumes, as the models of Sih and Ivanova, that the hazard of brittle fracture depends on the physical properties of materials and on the accumulated energies of shape and volume changes in structural members. These energies have two different critical values. If the critical dilatation energy in a microvolume of a material is reached earlier than the critical distortion energy, fracture is mainly brittle; otherwise, it is tough.

These conditions can be written as

$$\begin{aligned} W_v = W_{vc}, \quad W_d < W_{dc} \quad \text{for brittle failure;} \\ W_v < W_{vc}, \quad W_d = W_{dc} \quad \text{for tough fracture,} \end{aligned} \quad (8)$$

where W_v and W_d are the specific energies of dilatation and distortion. In the elastic region of the work of the material, the components of the total strain energy density are given by

$$W_v = (1 - 2\mu)/(6E)(\sigma_1 + \sigma_2 + \sigma_3)^2 \quad \text{for dilatation;} \quad (9)$$

$$W_d = (1 + \mu)/(6E)[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_1 - \sigma_3)^2] \quad \text{for distortion,} \quad (10)$$

where σ_1 , σ_2 , and σ_3 are the principal stresses.

In contrast to the well-known models, we assume that the critical dilatation energy is equal to the energy required to increase the elementary volume of the material to a limiting value in rupture. This energy is the sum of the energy of thermal expansion U_{therm} from the initial temperature T to the melting point T_{melt} and the latent heat energy of melting L with the increase in volume due to first-order phase transition. Thus,

$$W_{vc} = \int_T^{T_{\text{melt}}} \alpha K dT + L, \quad (11)$$

where α is the cubic-expansion coefficient and $K = E/(3(1 - 2\mu))$ is the bulk strain modulus.

In turn, the critical distortion energy is equal to the enthalpy for heating of an elementary volume from the initial temperature to the melting point, i.e.,

$$W_{dc} = H = \int_T^{T_{\text{melt}}} C_v \rho dT, \quad (12)$$

where C_v is the specific isochoric heat and ρ is the density of the material.

In fracture, the increase in volume is accompanied by cooling of the material while its plastic deformation is accompanied by heating. According to our experimental data, the total change in temperature for steel specimens in fracture does not exceed 10–100°C. In constructional steels, it is also necessary to allow for the energy components that arise because of structural imperfections. Thus, the presence of edge dislocations in the metal structure leads to an increase in the dilatation energy in comparison to the distortion energy, and, in contrast, screw dislocations change this ratio in favor of the distortion energy.

Representing conditions (8) in generalized form, we obtain from them the *plasticity index for the material* β_e , which, with allowance for (9) and (10), is written as

$$\beta_e = \frac{CW_d W_{vc}}{W_v W_{dc}} = \frac{2C(1 + \mu)(1 - 3D)(L + U_\tau)}{(1 - 2\mu)H}, \quad (13)$$

where C is a factor that takes into account the effect of defects in the metal structure and $D = I_2/I_1^2$ is the ratio of the second invariant to the square of the first invariant. The value of the coefficient β_e predicts the type of fracture of the material. Thus, for $\beta_e > 1$, the fracture is tough and for $\beta_e < 1$, it is brittle.

Using the reference data of [11] and formulas (11) and (12), we determined the values of W_{vc} and W_{dc} for 32 metals, which are required to calculate the plasticity index. Calculation of the plasticity index involves certain difficulties due to the specification of the type of stress state at the moment of fracture of a cylindrical specimen since the ratio of the distortion energy to the dilatation energy depends on the type of stress state. Prior to fracture, a neck or a “soft interlayer,” depending on the magnitude of transverse contraction, are known to form (see, for example, [12, 13]) in cylindrical specimens. In both the neck and “soft interlayer,” a volumetric stress state arises with a varying ratio of principal stresses over the cross section of the specimen. Thus, it can be assumed that at the moment of formation of a microcrack in brittle failure, a stress similar to the stress state in the “soft interlayer” arises in a local region ahead of the crack edge even for a linear stress state of a cylindrical specimen. This assumption is rather approximate, the more so since the problem of the stress state in both the neck and “soft interlayer” which arise in extension is complex and has not been completely solved. In addition, using reference data on relative contraction for various metals, we had no data on the geometric dimensions of specimens after fracture, which are required to calculate the stress state in the neck (according to N. N. Davidenkov and P. Bridgeman) and in the “soft interlayer.” Therefore, to calculate the plasticity parameter

$$\Pi = 1 - 3D = 1 - 3(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_1\sigma_3)/(\sigma_1 + \sigma_2 + \sigma_3)^2 \quad (13')$$

we assumed equal probabilities of occurrence of all types of stress states, from linear to volumetric “hydrostatic” ($\sigma_1 = \sigma_2 = \sigma_3$) with tensile principal stresses over the cross section of the specimen at the moment of fracture. As the calculated stress state in formula (13), we took a certain intermediate state between the linear and volumetric “hydrostatic” states.

According to the solution obtained by Davidenkov and Spiridonova [12], in the plane of minimum cross section of a cylindrical specimen, the stress distribution is given by the formulas

$$\sigma_1 = \sigma_{\text{therm}}(1 + (a^2 - r^2)/(2aR)), \quad \sigma_2 = \sigma_3 = \sigma_{\text{therm}}(a^2 - r^2)/(2aR), \quad (14)$$

where a is the radius of the smallest cross section of the neck, R is the curvature radius on the neck contour, and r is the radial coordinate.

The stress distribution in the “soft interlayer” of a cylindrical specimen is given by the relations [13]

$$\sigma_1 = \sigma_{\text{therm}}(1 + 2(l - r)/(\sqrt{3}b)), \quad \sigma_2 = \sigma_3 = \sigma_{\text{therm}} \cdot 2(l - r)/(\sqrt{3}b), \quad (15)$$

where l is the radius of the round cross section of the specimen and b is the thickness of the “soft interlayer.”

The stresses averaged over the cross section of the cylindrical specimen are $\bar{\sigma}_i = \frac{1}{\pi l^2} \int_0^{2\pi} \int_0^l \sigma_i r dr d\varphi$.

Using the last expression, we obtain the average stresses in the minimum cross section of the neck

$$\sigma_1 = \sigma_{\text{therm}}(1 + a/(4R)), \quad \sigma_2 = \sigma_3 = \sigma_{\text{therm}} a/(4R) \quad (16)$$

and in the “soft interlayer”

$$\sigma_1 = \sigma_{\text{therm}}(1 + 2l/(3\sqrt{3}b)), \quad \sigma_2 = \sigma_3 = \sigma_{\text{therm}} \cdot 2l/(3\sqrt{3}b). \quad (17)$$

If we assume that $a = l$ and the radius of the neck is approximately equal to half the thickness of the “soft interlayer” or larger than it, i.e., $R \geq b/2$, formulas (16) and (17) give close results. A simple comparison of formulas (14) and (16) and (15) and (17) shows that in the neck, the average stresses are 50% lower than the maximum stresses, and in the “soft interlayer,” they are 30% lower.

We transform expression (13') by introducing the relative stresses $n = \sigma_2/\sigma_1$, and $m = \sigma_3/\sigma_1$:

$$\Pi = 1 - 3(n + m + nm)/(1 + n + m)^2. \quad (18)$$

For cylindrical specimens in which $n = m$, relation (18) becomes $\Pi = ((1 - n)/(1 + 2n))^2$.

If we assume the stress distribution (14) or (15), the average values of Π_{av} over the cross section of a cylindrical specimen are, respectively,

$$\Pi_{\text{av}} = 2R/(2R + 3a) \quad \text{or} \quad \Pi_{\text{av}} = b\sqrt{3}/(3l) - b^2/(6l^2) \ln((b + 2\sqrt{3}l)/b). \quad (19)$$

Since determination of the values of b and R involves difficulties, we assume that at the moment of fracture of a cylindrical specimen at its center due to plastic strains, the stress σ_1 reaches the limiting value $(2.57-3.0)\sigma_{\text{therm}}$. For this, in relations (14) or (15), it is necessary to set $R = (0.25-0.32)a$ and $b = (0.58-0.74)l$. Substituting these relations into relations (19), we obtain $\Pi_{\text{av}} = 0.14-0.18$ for the first case and $\Pi_{\text{av}} = 0.23-0.27$ for the second case.

In calculations of the plasticity index for all metals tested for rupture, we use the plane stress state with stresses $\sigma_1 = \sigma_2$ and $\sigma_3 = 0$. For this stress state, the value of Π given by expression (18), is 0.25. The same value of Π is obtained for the volumetric stress state $\sigma_2 = \sigma_3 = 0.25\sigma_1$.

Calculating β_e from formula (13), we assume that the coefficient C_1 is 1, and the specific isochoric heat is approximately equal to the specific isobaric heat: $C_v = C_p$. Figure 1 shows the relative contraction ψ (from the reference data of [11]) versus the plasticity index β_e for a group of metals.

For a mathematical description of this relation, we use the following theoretical equation with empirical coefficients [14]: $\psi = 1/(1 + \exp(C_1(1/\beta_e - 1/C_2)))$. The numerical values of the coefficients C_1 and C_2 are

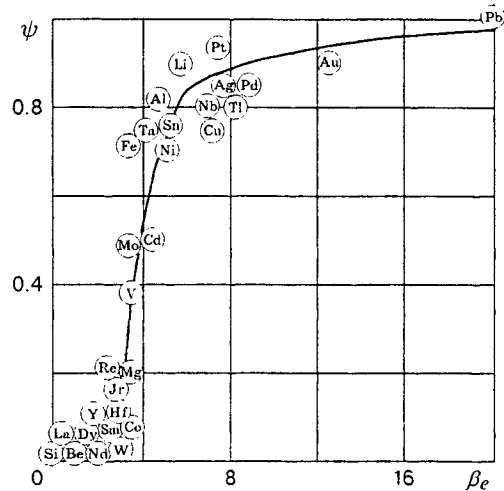


Fig. 1

determined by the least squares method using the standard programs. Thus, the general relation takes the form

$$\psi = \frac{1}{1 + \exp [16.68(1/\beta_e - 1/3.81)]}, \quad (20)$$

and is graphically displayed in Fig. 1.

The regression ratio (the index of accuracy of regression of the random quantity ψ with respect to the random quantity β_e) is 0.91, which indicates that the relationship between β_e and ψ is similar to a functional dependence. Substituting the value $\beta_e = 1$ into Eq. (20), we obtain $\psi \cong 0$, which confirms the adopted assumption of the brittleness of the material when the plasticity index $\beta_e \leq 1$.

The main conclusion on the effect of the plasticity index on the brittle fracture of structural steel is that it depends markedly on the temperature and decreases as the latter decreases. This is most pronounced in second-order phase transitions with sharp peak-like changes in the bulk elastic modulus or the temperature coefficient of linear expansion.

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