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Influence of Calculation Method on Value of Activation Energy in Hot Forming

Abstract: Influence of the methodology of mathematical processing of experimental data on the calculated value of the activation energy in hot forming was evaluated for three very different alloys: iron aluminide, low-alloyed steel and magnesium alloy. Application of the mean strain rates is appropriate but calculations with use of nominal strain rates of the plastometric tests do not give significantly different results. Calculations based on the processing of the simplified power dependence between strain rate and peak stress can give the results differing very substantially from those that were gained by the solution of the complex hyperbolic relationship. This has negative impacts, particularly at prediction of the maximum flow stress in the broad range of forming conditions, represented by the Zener-Hollomon parameter.

Keywords: hot forming, metal and alloys, strain rate, stress-strain curve, activation energy, regression analysis

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1 Introduction

The aim of the works was to quantify to what extent the apparent activation energy value Q [$J \cdot mol^{-1}$] in hot forming could be influenced by the methodology of mathematical processing of the relevant experimental data. The Q-value is an extraordinarily important material constant, needed e.g. for the calculation of Zener-Hollomon parameter Z [s^{-1}] (i.e. the temperature compensated strain rate). Based on its knowledge for the given material it is possible, among others, to predict effectively the maximum flow stress value or the strain value corresponding to start of the dynamic recrystallization at the given temperature T [K] and strain rate γ [s^{-1}]. The main inducement for research of these issues were literature data on various methods for determination of activation energy in hot forming and doubts about their compatibility. Moreover we took into account our own experience with detailed evaluation of plastometric data, when real parameters of individual tests often differ significantly from nominal parameters.

The apparent activation energy in the hot forming is, ideally, the material constant depending only on the chemical composition and structure of the given material. The hyperbolic law in Arrhenius type equation is conventionally used for its determination [1]:

$$\gamma = C \cdot \exp\left(\frac{-Q}{R \cdot T}\right) \cdot \left[\sinh\left(\alpha \cdot \sigma_{max}\right)\right]^n \tag{1}$$

where C [s^{-1}], n [–] and α [MPa^{-1}] are other material constants, $R = 8.314\ J \cdot mol^{-1} \cdot K^{-1}$, T [K] is the forming temperature and σ_{max} [MPa] is flow stress that corresponds to the peak stress on the certain stress-strain curve. This relationship is often solved by a simple graphic method, based on the repeatedly used linear regression. A particularity of the hyperbolic function is used in this calculation that enables to simplify the Eq. (1) for low stress values into the form of the Arrhenius power law:

$$\gamma = C_1 \cdot \exp\left[\frac{-Q}{R \cdot T}\right] \cdot {\sigma_{max}}^n \tag{2}$$

and, vice versa, for high stress values into the form of the exponential law:

$$\gamma = C_2 \cdot \exp\left[\frac{-Q}{R \cdot T}\right] \cdot \exp\left(\beta \cdot \sigma_{max}\right) \tag{3}$$

where C_1, C_2 and β are the material constants. The constant α in Eq. (1) is given by the relationship:

$$\alpha = \frac{\beta}{n} \tag{4}$$

For a chosen high-temperature level (i.e. for low stress values) the constant n is determined by the linear regression of the experimentally found points in coordinates $\ln \sigma_{max} \sim \ln \gamma$ and for a chosen low-temperature level (i.e. for high stress values) the constant β is obtained by the linear regression in coordinates $\sigma_{max} \sim \ln \gamma$. After the calculation of the quantity α according to the Eq. (4), the constants Q and C in Eq. (1) may be calculated by the final linear regression of all the data plotted in the coordinate system $T^{-1} \sim (\ln \gamma - n \cdot \sinh(\alpha \cdot \sigma_{max}))$.

Such an estimate of constants n and β is a weak point of the described method, since it can be strongly influenced by the selection of the corresponding temperature level and by the experimental data scatter. This deficiency has been eliminated by application of the specially developed software ENERGY 4.0 [2], which enables an interactive elimination of points showing the excessive deviation from the trends specified in a graphic way. The software uses the values n and β, determined by the aforementioned procedure, only as the first estimate of parameters for the final refining nonlinear regression of all the data corresponding to the Eq. (1). Such multiple regression for ensuring higher precision of results is very unreliable without the first preliminary estimate of the chosen material constants.

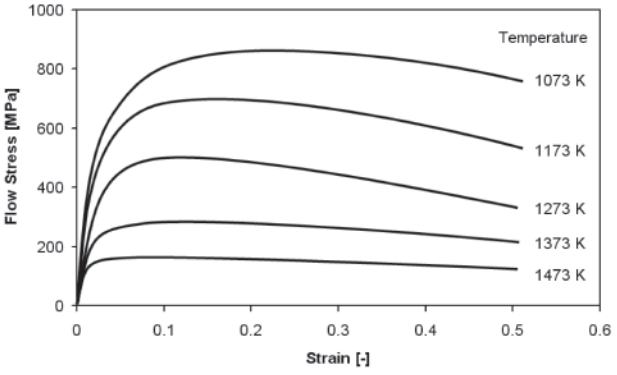
Calculation of activation energy from experimental data on the basis of the hyperbolic Eq. (1) is an established method that was successfully applied for different types of materials, recently for example for iron aluminides [3–5], various types of steel [6–9], alloys based on chromium [10], titanium [11, 12], or magnesium [13] etc.

On the other hand, numerous research workers avoid the described mathematical inconveniences and use the simplified power Eq. (2) for the activation energy calculation, which appears to be disputable for the reasons mentioned above. Such calculations were made for example for intermetallic compounds [14–17], aluminium alloys and composites [18–21], high-alloyed steels [22, 23], titanium alloy TC21 [24] or Ni-Cr-W superalloy [25].

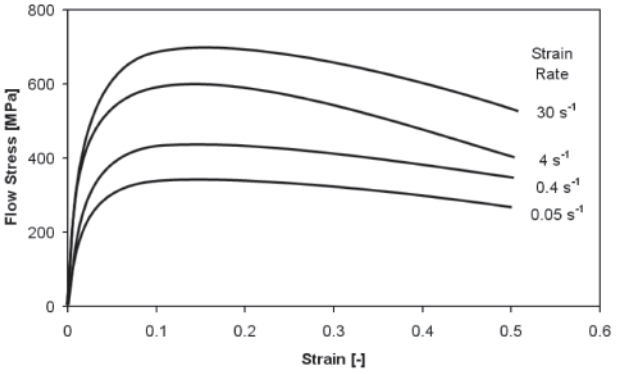
2 Experimental procedures

By means of the plastometer Gleeble 3800 three sets of the uniaxial hot compression tests were carried out on the cylindrical specimens with diameter of 10 mm and height of 12 mm. The alloys with a very different chemical composition and deformation behaviour were examined intentionally. The iron aluminide of the type Fe-40Al, hardened in the phase of laboratory melting by particles TiB_2 smaller than 10 μm [5], showed the coarse-grained cast structure and the following chemical composition: 25.0 Al – 0.04 C – 0.19 Mn – 0.16 Ti – 0.07 B (the rest is Fe; all in wt.%). After the uniform preheating to 1473 K the particular specimens were isothermally formed at temperature levels of 1073 K – 1173 K – 1273 K – 1373 K – 1473 K by nominal strain rates 0.05 s^{-1} – 0.4 s^{-1} – 4.0 s^{-1} – 30 s^{-1}. Temperature was controlled by feedback from a thermocouple spot-welded on the lateral surface of the heated specimen. Influence of forming parameters on flow stress of this material is documented by diagrams in Fig. 1.

The low-alloyed steel 42CrMo4 in the original form of a continuously cast billet with chemical composition 0.43 C – 0.77 Mn – 0.28 Si – 1.14 Cr – 0.18 Mo (rest Fe) on temperature levels of 1073 K – 1173 K – 1273 K – 1373 K by nominal strain rates of 0.02 s^{-1} – 0.09 s^{-1} – 0.47 s^{-1} – 2.3 s^{-1} – 12 s^{-1} – 60 s^{-1}. Uniform temperature of pre-heating of



a) nominal strain rate 30 s^{-1}



b) temperature 1173 K

Fig. 1: Selected stress-strain curves at forming of the alloy Fe-40Al+TiB_2

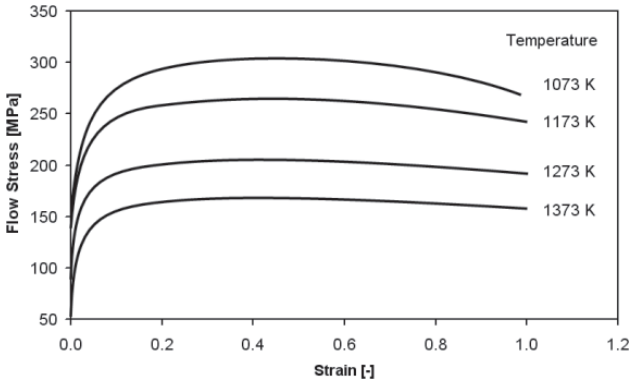


Fig. 2: Stress-strain curves of the steel 42CrMo4 obtained at the nominal strain rate 60 s^{-1}

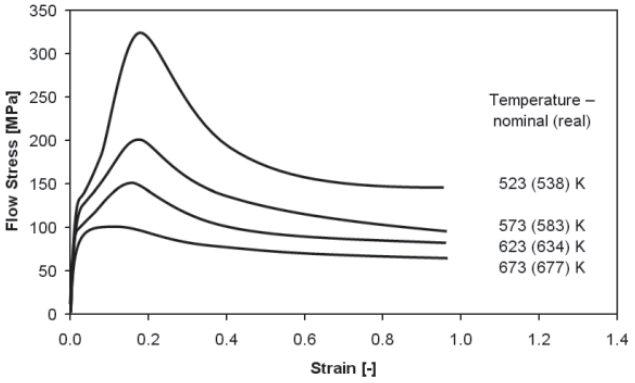


Fig. 3: Influence of temperature on the shape of the stress-strain curves of the alloy AZ80 at nominal strain rate 1 s^{-1}

samples was 1373 K. Figure 2 shows an example of the obtained results.

The magnesium alloy AZ80 in the originally deformed state had the chemical composition 8.2 Al – 0.34 Zn – 0.13 Mn (rest Mg). After preheating to 673 K, the specimens were tested at the temperature levels of 523 K – 573 K – 623 K – 673 K by nominal strain rates 0.01 s^{-1} – 0.1 s^{-1} – 1.0 s^{-1} – 10 s^{-1} – see Fig. 3 for some results. In case of this material more important differences between nominal deformation temperatures and real temperatures, corresponding to the stress peak, were recorded (see the values in parentheses in the diagram in Fig. 3) That's why at calculations of activation energy of the alloy AZ80 this influence of deformation heat generation was taken into account and only real and not nominal forming temperatures were used.

The peak stress value σ_{max} [MPa] and the corresponding value of mean strain rate were determined for each stress-strain curve. This mean strain rate value often differs significantly from the nominal strain rate value, especially at higher forming speeds – see Fig. 4 for example.

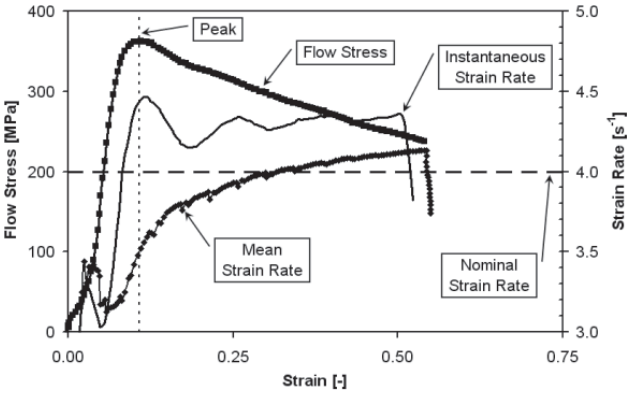


Fig. 4: Example of deviations between true and nominal strain rates – alloy Fe-40Al+TiB_2 formed at the temperature of 1273 K by nominal strain rate 4 s^{-1}

3 Mathematical processing and discussion of the experimental data

The most complex procedure of solution the hyperbolic Eq. (1) with the final refining multiple regression was chosen as the most accurate and representative way of determining the activation energy of the examined alloys. Using the interactive ENERGY 4.0 software, this method was applied for each material for two sets of data, differing by the nominal and mean strain rate values. Table 1 illustrates deviations of the incorporated variables in case of one analyzed data set.

In case of steel 42CrMo4 the real mean strain rates ranged between 0.02 s^{-1} and 72 s^{-1} (while nominal strain rate varied from 0.02 s^{-1} to 60 s^{-1}), in case of alloy AZ80 they ranged between 0.009 s^{-1} and 12 s^{-1} (while nominal strain rate varied from 0.01 s^{-1} to 10 s^{-1}). The calculation based on the mean strain rate is the optimal one because it reflects the entire history of forming up to the moment of reaching the peak stress. The material constants obtained by this most precise method are given in Table 2.

Strain rate [s^{-1}]	
nominal	**mean**
0.05	0.036–0.046
0.4	0.30–0.38
4.0	2.6–3.5
30	20–32

Table 1: Ranges of mean strain rates corresponding to peak stress values for alloy Fe-40Al+TiB_2, in relation to nominal strain rates

Material	Strain rate	Q [kJ · mol^{-1}]	n [–]	α [MPa^{-1}]	C [s^{-1}]
Fe-40Al+TiB_2	nominal	448	2.00	0.0091	5.88E+16
	mean	455	2.01	0.0092	8.91E+16
42CrMo4	nominal	335	4.83	0.0106	2.57E+12
	mean	342	4.91	0.0105	5.38E+12
AZ80	nominal	145	3.93	0.0080	2.22E+11
	mean	150	4.06	0.0079	5.32E+11

Table 2: Material constants in Eq. (1) determined for the tested materials and considered types of strain rate

Temperature level		Q [kJ · mol^{-1}]	n [–]	α [MPa^{-1}]	C [s^{-1}]
High	Low				
1473 K	1073 K	570	3.24	0.0071	3.53E+21
1473 K	1173 K	461	3.24	0.0052	1.02E+18
1373 K	1073 K	566	3.14	0.0073	2.14E+21
1373 K	1173 K	456	3.14	0.0054	5.57E+17

Table 3: Influence of selection of temperature levels on calculation of material constants in the Eq. (1), using the system of linear regressions only (alloy Fe-40Al+TiB_2, calculation with the mean strain rates)

It is evident that Q-value is influenced by inclusion of different types of strain rate in the calculation only slightly – the deviations amount max. to 3%. Selection of the temperature levels in the regression solution of Eqs. (2) and (3) can influence the results much more, unless it is not followed by the final refining multiple nonlinear regression – see Table 3.

It is obvious that the activation energy value is affected substantially by the previous estimate of constants n and α (in that particular case with deviation of the quantity Q up to 25%). The activation energy thus loses the meaning of the material constant and becomes a purely mathematical quantity, which arose as a result of the combination of parameters in the Eq. (1). Many such combinations are potential; without the final refining nonlinear regression it is impossible to determine the very one that gives the true representative results, substantiated from the point of view of physical metallurgy. In case of other two investigated materials the maximum deviations of Q-values determined in this way were a bit more favourable, i.e. up to 22% for steel 42CrMo4, or up to 15% for magnesium alloy AZ80.

Significantly different results can be obtained also by application of the simplified methodology, based exclusively on the solution of the power law Eq. (2). The following material constants were gained in this case from the data sets including the mean strain rates: $Q = 540$ kJ · mol^{-1} and $n = 10.1$ for aluminide Fe-40Al+TiB_2, $Q = 331$ kJ · mol^{-1} and $n = 10.4$ for steel 42CrMo4, or $Q = 157$ kJ · mol^{-1} and $n = 7.8$ for alloy AZ80. As it follows from the comparison with the data presented in Table 2, the values of thus calculated activation energy values differed by –3% to +19% from the calculations based on the solution of the hyperbolic law Eq. (1). As far as the order of magnitude of the Zener-Hollomon parameter is concerned, the highest deviation is connected with the greatest difference of Z-parameter in case of testing the given iron aluminide (i.e. 10^{14} s^{-1} to 10^{23} s^{-1}, whereas for the investigated steel the range was 10^{11} s^{-1} to 10^{18} s^{-1} and for the magnesium alloy only 10^{9} s^{-1} to 10^{15} s^{-1}). This deviation also yields in a markedly lower accuracy of the prediction of σ_{max}-values for particular experimental conditions in relation to the Zener-Hollomon parameter [26]:

$$Z = \gamma \cdot \exp\left(\frac{Q}{R \cdot T}\right) \tag{5}$$

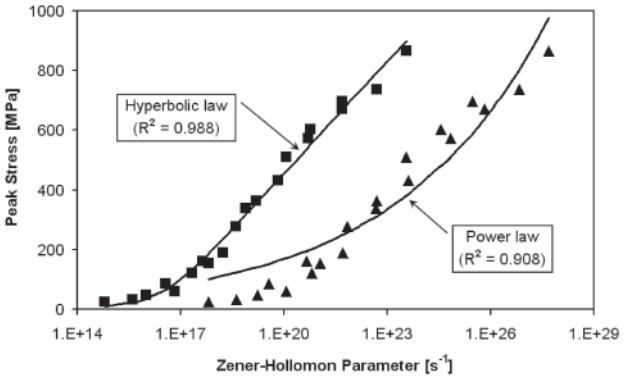
It is possible to obtain the following relation by transformation of the Eq. (2):

$$\sigma_{max} = \sqrt[n]{\frac{Z}{C_1}} \tag{6}$$

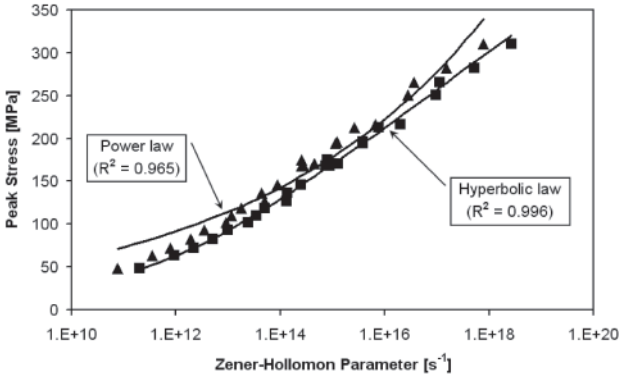
while modification of the Eq. (1) leads to the relationship:

$$\sigma_{max} = \frac{1}{\alpha} \cdot \operatorname{arc\,sin\,h} \sqrt[n]{\frac{Z}{C}} \tag{7}$$

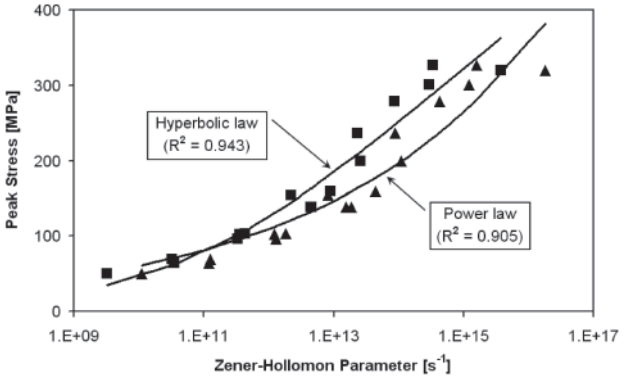
Comparison of accuracy of prediction of the peak stress with use of equations of the type (6) and (7) is illustrated by the diagrams in Fig. 5 for all the tested materials. The shift of data against the horizontal axis is for each



a) iron aluminide Fe-40Al+TiB_2

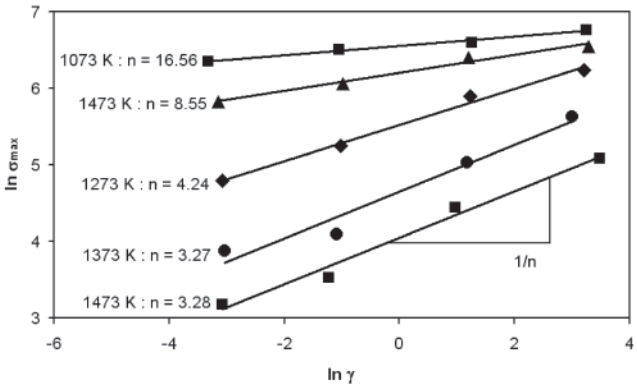


b) steel 42CrMo4

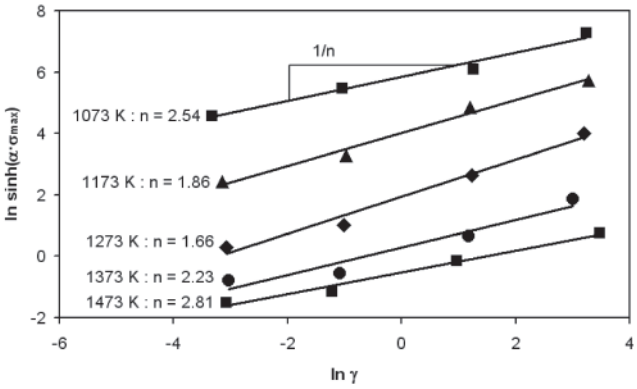


c) magnesium alloy AZ80

Fig. 5: Comparison of accuracy of type (6) equation – power law, and type (7) equation – hyperbolic law evaluated for all three tested materials (points – experimental data; lines – calculations made by relevant equations)



a) power law



b) hyperbolic law

Fig. 6: Values of the constant *n* calculated for various temperature levels in case of the Eq. (2) – a), or Eq. (1) – b); alloy Fe-40Al+TiB_2, mean strain rate

diagram given by various values of the activation energy in the Zener-Hollomon parameter.

Accuracy of equations based on the hyperbolic law is in all cases higher than accuracy of simpler relations based on the power law. Even if in all cases the coefficients of determination $R^2 > 0.9$, the applicability of the simplified Eqs. (2) or (6) is unreliable for a wide range of deformation conditions. Hence the mutual comparability of the activation energy values calculated by means of the Eqs. (1) and (2) is also questioned; this fact often complicates the comparative analysis of results, published by different authors.

The basic issue consists in the fact that at application of the simplified Eq. (2) the value of the constant *n* does not come out as temperature independent. As it is evident from Fig. 6a, this quantity significantly rises with the falling deformation temperature. This unfavourable phenomenon manifested itself in greater or smaller extent in all three sets of experimental data. On the other hand, the deviations of *n*-values calculated for various temperature levels are given only by scattering of the experimental data in case of the hyperbolic Eq. (1) (see Fig. 6b).

The Eq. (2) is a simplified form of the Eq. (1), and it is valid only for the low stress values (and/or for low values of the parameter *Z*) [27]. Application of the Eq. (2) to a wide range of deformation conditions leads to the results that differ more or less from the results obtained by the complex hyperbolic Eq. (1). Use of this simplified procedure cannot eliminate the unacceptable temperature dependence of

the constant n. This conclusion is in agreement for example with the diagram published in the work [25]. Variation of flow stress with strain rate at different temperatures for as-cast Ni–Cr–W superalloy confirms the temperature dependence of the quantity n in the Eq. (2), although authors of that work prefer themselves the simple Arrhenius power law. Researchers using hyperbolic equation for calculation of activation energy often state that the hyperbolic law in Arrhenius type equation gives better approximation between the Zener-Hollomon parameter and stress [10] or that the universal constitutive Eq. (1) correlates well the Z-parameter in a wide range of stresses [7]. It is, however, interesting that even the authors preferring in this case the power law, recognize higher precision of the hyperbolic function [21], as well as the fact that it is a more general formula suitable for description of stresses over a wide range. The main reason for application of the power law function remains then the fact that it is easier to obtain the n-value by linear regression through the Eq. (2) [19].

4 Summary

It is most trustworthy to use the established hyperbolic relationship with the application of mean strain rate values for the calculation of activation energy in hot forming from the plastometric data set. Simplified application of nominal strain rates has only an insignificant influence on the results. Much more important is the elimination of errors associated with the scatter of input data on various temperature levels and the selection of these levels in the partial linear regressions. For this reason the final nonlinear regression of the hyperbolic law Eq. (1) is necessary; it uses the preliminarily determined material constants only as the initial estimate of parameters for the final refining calculation, based on multiple nonlinear regression. The calculations based on the application of the Arrhenius power dependence between the strain rate and peak stress can give the results differing by tens of per cent from those that were gained by the solution of the complex hyperbolic relationship. This is valid particularly for a wide range of the experimental conditions defined by the temperature compensated strain rate.

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