MODELING IMPACT TOUGHNESS OF INDUSTRIAL HOT ROLLED HSLA STEELS

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Abstract

A quantitative model has been developed to predict the temperature dependence of impact toughness (KCV) for hot rolled plane carbon and HSLA steels with a wide range of chemical composition (wt%): C(0.04-0.21), Mn(0.16-1.96), Si(0.01-0.93), Cr(0.01-0.97), Ni(0.01-0.51), Cu(0.02-0.45), Mo(0.001-0.50), Nb(0.001-0.056), V(0.002-0.09), Ti(0.001-0.08), N(0.003-0.009), S(0.001-0.032), P(0.005-0.025). The transition temperature at 50 % of fibrous fracture ($FATT_{50}$) is determined in terms of chemical composition and calculated final microstructure parameters. Impact energies at lower (KCV_{LS}) and upper (KCV_{US}) shelves are derived from predicted values of tensile stress and relative elongation. All physical parameters of the model are related to the industrial hot rolling conditions by means of the integral computer model STAN 2000 previously formulated for the rolling mill 2000 of PJSC Severstal. Empirical coefficients are fitted to the data base on impact toughness for 230 plates of 32 steel grades in the temperature range of -60°C to +20 °C. The modelling results comply well with experiments.

Keywords: Steels, hot rolling, impact toughness, microstructure, modelling

1. INTRODUCTION

Apart from characteristics of strength (yield stress and ultimate tensile stress) and plasticity (relative elongation), the temperature-dependent impact energy is a crucial property that determines reliability of steel constructions exploited under dynamic loads and low temperatures. Accordingly, considerable attention is paid to experimental studies of the impact toughness of high strength steels with various microstructures and chemical compositions and development of the corresponding predictive models [1-7].

Cold resistance of the high strength steels is often specified by the 50% Fibrous Fracture Appearance Transition Temperature ($FATT_{50}$). One of the first models to predict this characteristic for ferritic-pearlitic steels in terms of ferrite grain size, thickness of cementite plates at grain boundaries and other structural features was developed in [2]. Next [4, 5], the obtained dependences have been improved and empirical expressions for impact energies at lower (KCV_{LS}) and upper (KCV_{US}) shelves were proposed for several steels with more complex microstructures.

In this paper, original empirical expressions for calculating $FATT_{50}$, as well as for KCV_{LS} and KCV_{US}, are proposed depending on chemical composition, final microstructure parameters and mechanical properties of industrial hot-rolled steels with ferrite-pearlite and bainite microstructures. Using these physical parameters, a model is composed for calculating KCV as a function of temperature.

2. INVESTIGATED STEELS AND DATA USED TO CALIBRTATE THE MODEL

To develop the present model, a data base has been employed that covers 230 plates of 32 steels with a wide range of chemical composition (wt%): C(0.04-0.21), Mn(0.16-1.96), Si(0.01-0.93), Cr(0.01-0.97), Ni(0.01-0.51), Cu(0.02-0.45), Mo(0.001-0.50), Nb(0.001-0.056), V(0.002-0.09), Ti(0.001-0.08), N(0.003-0.009), S(0.001-0.032), P(0.005-0.025). Impact energies were determined at 10 temperatures in the range of -60 °C to +20 °C. The steels were hot rolled at the mill 2000 of PJSC Severstal and the plate thickness varied in the range of 2.8 to 19.5 mm.

Microstructure parameters involved in simulations, as well as mechanical properties (tensile strength and relative elongation), were calculated using previously developed computer model for hot rolling STAN 2000 [8]. All computations correspond to protocols of industrial modes of rolling and accelerated cooling. According to respective results, 158 of investigated plates had ferritic-pearlitic structures (volume fraction of pearlite up to 25 %) and 72 plates had bainitic structures (mostly granular bainite). Related mechanical properties vary in wide ranges: 250-780 MPa of yield stress, 360-880 MPa of ultimate tensile stress and 10-40 % of relative elongation.

3. DESCRIPTION OF THE MODEL, MODELING RESULTS AND DISCUSSION

The temperature dependence of impact toughness has been treated according to [3-5] with the mixture rule:

$$KCV \equiv KCV(T) = KCV_{US} X_D(T) + KCV_{LS}\left(1 - X_D(T)\right), \tag{1}$$

$X_D(T)$ - a ductile fraction of the fracture surface at temperature *T* (°C)

KCV_{US} - an upper shelf corresponding to the completely ductile fracture ($X_D(T)=1$)

KCV_{LS} - a lower shelf ($X_D(T)=0$).

Following [4,5], the ductile fraction is expressed by:

$$X_D(T) = 1 - exp\left(-k\left(\frac{FATT - T}{100} - \left(\frac{0.69}{k}\right)^{1/m}\right)^m\right), \tag{2}$$

$FATT \equiv FATT_{50}$ - the ductile-to-brittle transition temperature

$k = 4,\ m = 2$.

Apparently, the employed phenomenological model cannot explicitly follow numerous concurrent effects of microstructure and chemical composition on the sought parameters (*FATT*, KCV_{US}, KCV_{LS}). Instead, to allow for such effects, we will make use of *FATT* as a characteristic most sensitive to them. To further facilitate the modeling, specific approximations will be applied to the upper and lower shelves of *KCV*.

To determine *FATT* (°C) at various chemical compositions and microstructures, contributions of different physical mechanisms [1,2,4,5] are allowed for:

$$FATT = FATT_0 + \Delta FATT_{ss} + \Delta FATT_P + \Delta FATT_S + \Delta FATT_{ppt} + \Delta FATT_{cem} + \\ \Delta FATT_{PF} + \Delta FATT_{PE} + \Delta FATT_B, \tag{3}$$

where successive terms respectively correspond to the contributions of:

$FATT_0$ - constant base contribution

$\Delta FATT_{ss}$ - solid solution

$\Delta FATT_P$, $\Delta FATT_S$ - phosphorus and sulphur impurities

$\Delta FATT_{ppt}$ - different types of precipitate particles

$\Delta FATT_{cem}$ - cementite particles formed along the boundaries of ferrite grains (tertiary cementite)

$\Delta FATT_{PF}$, $\Delta FATT_{PE}$, $\Delta FATT_B$ - polygonal ferrite, pearlite and bainite in the final structure.

Depending on quantities of alloying elements and free nitrogen in the solid solution (wt%), the second term of Eq. (3) is expressed by:

$$\Delta FATT_{ss} = -7w_{Mn} + 48w_{Si} - 26w_{Cr} - 22w_{Ni} + 4400w_{N_{free}}, \tag{4}$$

$w_{N_{free}}$ - the content of free nitrogen calculated as:

$$w_{N_{free}} = w_N - w_N^{TiN} - w_N^{Nb(C,N)} - w_N^{V(C,N)}, \tag{5}$$

w_N - is total content of nitrogen in steel

w_N^{TiN} , $w_N^{Nb(C,N)}$, $w_N^{V(C,N)}$ - quantify of nitrogen captured by respective particles formed both before (TiN) and after (Nb(C,N), V(C,N)) hot rolling. In the latter case the precipitation is located at dislocations of deformed austenite.

Parameter w_N^{TiN} is expressed in terms of titanium content (w_{Ti}) in steel:

$$\begin{cases} w_N^{TiN} = w_N\,, \; if \quad w_{Ti}/3.4 > w_N \\ w_N^{TiN} = w_{Ti}\,, \quad if \quad w_{Ti}/3.4 \le w_N \end{cases} . \tag{6}$$

Contributions of various elements in $\Delta FATT_{ss}$ according to Eq. (4) are close to respective estimates in [1]. Although the physical meaning of such terms still is not rigorously established, the effect of Si and free N may be attributed to diminishing the stacking fault energy in ferrite whereas growth of this energy because of Mn, Cr and Ni results in decreasing $\Delta FATT_{ss}$.

Contributions of P and S are approximated by expressions:

$$\Delta FATT_P = 880{w_P}^{0.9},\; \Delta FATT_S = 1260{w_S}^{0.6}. \tag{7}$$

Note that the effect of S is much stronger than that of P. Probably, this is due to an implicit allowance of MnS inclusions also reducing the cold resistance. Contributions of various precipitates are expressed as follows:

$$\Delta FATT_{ppt} = \Delta FATT_{Nb(C,N)} + \Delta FATT_{V(C,N)} + \Delta FATT_{TiN}, \tag{8}$$

$$\Delta FATT_{Nb(C,N)} = \alpha_{Nb(C,N)} \bar{R}_{Nb(C,N)}^{0.5} f_{Nb(C,N)}^{0.5}, \tag{9}$$

$$\Delta FATT_{V(C,N)} = \alpha_{V(C,N)} \bar{R}_{V(C,N)}^{0.5} f_{V(C,N)}^{0.5}, \tag{10}$$

$\bar{R}_{Nb(C,N)}$, $\bar{R}_{V(C,N)}$; $f_{Nb(C,N)}$, $f_{Nb(C,N)}$ - respectively correspond to the average radii and volume fractions of the related particles

$\alpha_{Nb(C,N)}$, $\alpha_{V(C,N)}$ - empirical parameters of the model

Model calibration has resulted in $\alpha_{Nb(C,N)} = 7.2\times10^7$, $\alpha_{V(C,N)} = 2.3\times10^7$ (°C/nm$^{-0.5}$).

The contribution of TiN particles is represented by:

$$\Delta FATT_{TiN} = 0.32\,exp\left(1000w_N^{TiN}\right). \tag{11}$$

To express the effect of tertiary cementite, we use expression:

$$\Delta FATT_{cem} = 0.22\,exp\left(140w_C^{cem}\right)d_{PF}^{-0.5}X_{PF}, \tag{12}$$

w_C^{cem} - involved carbon content

d_{PF} (μm) - polygonal ferrite grain size

X_{PF} - polygonal ferrite volume fraction.

As to w_C^{cem}, it is determined as follows:

$$\begin{cases} w_C^{cem} = w_C^*, \ if \ \ w_C^* > 0 \\ w_C^{eff} = 0, \ \ if \ \ w_C^* \le 0 \end{cases} \tag{13}$$

$$w_C^* = w_C^{\Sigma} - 0.17\left(w_{Nb}^{free} + w_{Ti}^{free} + w_V^{free}\right) - 0.011 w_{Mn}, \tag{14}$$

$w_C^{\Sigma} \equiv w_{C_{eq}}^{PF}\left(\tilde{T}_{PF}\right)$ - carbon content in ferrite at the complete transformation of austenite in continuous cooling

$\tilde{T}_{PF}$ - average temperature of ferritic transformation

$w_{Nb}^{free} = w_{Nb} - w_{Nb}^{Nb(C,N)}$, $w_{Ti}^{free} = w_{Ti} - w_{Ti}^{TiN} - w_{Ti}^{TiC}$, $w_V^{free} = w_V - w_V^{V(C,N)}$ - contents of free microalloying elements, calculated with allowance for their interaction with carbide or carbonitride particles

w_{Nb}, w_{Ti}, w_V - total quantities of the considered elements and $w_{Nb}^{Nb(C,N)}$, $w_{Ti}^{TiN} + w_{Ti}^{TiC}$, $w_V^{V(C,N)}$ are their immobilized parts.

Contributions of polygonal ferrite, pearlite and granular bainite, respectively, are expressed as follows:

$$\Delta FATT_{PF} = 0.6 d_{PF}^{-0.5} X_{PF}, \tag{15}$$

$$\Delta FATT_{PE} = 300 X_{PE}, \tag{16}$$

$$\Delta FATT_{GB} = \left(40 + 4w_C\left(1 + \frac{1 - X_{PE}}{1 - X_{PF}}\right)\right) X_{GB}, \tag{17}$$

w_C - total content of carbon

X_{GB} - volume fraction of granular bainite

Contributions of lath bainite (LB) and acicular ferrite (AF) (sometimes called as deformation bainite) are represented by:

$$\Delta FATT_{LB} = 80 X_{LB}, \ \Delta FATT_{AF} = 40 X_{AF}, \tag{18}$$

X_{LB}, X_{AF} - volume fractions

It is worth noting that the second term in Eq. (17) is proportional to the carbon quantity in the retained austenite before the bainitic transformation. This factor allows for the effect of cementite particles appearing in the transformed structure. However, since the LB and AF fractions were rather low in the considered steels, the corresponding contribution has been quantified only for the granular bainite predominating in the investigated structures.

To evaluate the upper shelf level, we use expression:

$$KCV_{US} = 27 + 0.01\sigma_{TS}\delta\left(J / cm^2\right), \tag{19}$$

σ_{TS} (MPa), δ (%) - ultimate stress and relative elongation at room temperature

Here, the product of ultimate stress and relative elongation at room temperature reflects the virtual plastic work. As to the lower shelf, its invariant impact energy is employed:

$$KCV_{LS} = 58\left(J/cm^2\right). \tag{20}$$

Although Eq. (20) ignores actual KCV_{LS} variations, the latter do not notably affect predicted $FATT_{50}$. Besides, from the practical viewpoint, these variations as such do not matter insofar as the considered ductile-to-brittle transition temperature commonly limits admitted working conditions. At the same time the employed KCV_{LS} seemingly overestimate the true (least) impact toughness of the lower shelf; to determine it when necessary, tests should be performed at lower temperatures (say, T < 80 °C).

Figure 1 allows one to compare experimental and calculated temperature dependences of impact toughness for (a) ferritic-pearlitic steel **S1** (0.2C, 1.24Mn, 0.42Si, 0.026Ti) and (b) steel **S2** with the mostly bainitic structure (0.07C, 0.6Mn, 0.34Si, 0.53Cr, 0.3Ni, 0.21Cu, 0.026Nb, 0.074V, 0.018Ti). According to **Figure 2** summarizing such results, the proposed model satisfactorily complies with experiments over the whole range of the considered steels.

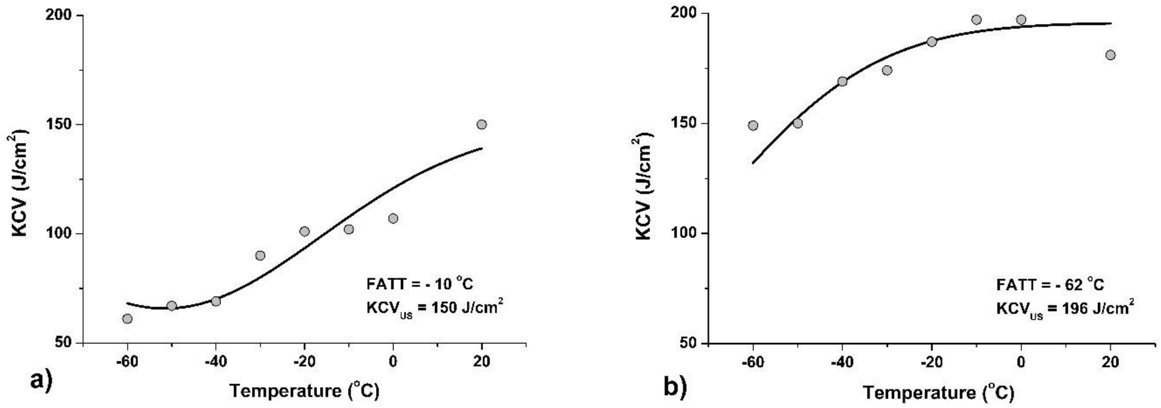

Figure 1 Calculated (lines) and experimental (dots) temperature dependences of impact toughness for steels (a) **S1** and (b) **S2** with ferritic-pearlitic (0.77PF + 0.23P) and mostly bainitic (0.97GB + 0.03LB) microstructures, respectively.

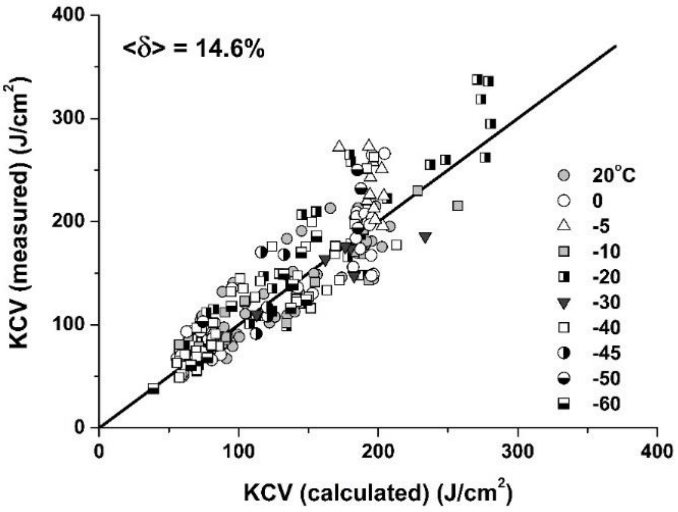

Figure 2 Comparison of the calculated and measured KCV values for the investigated steels. <δ> is an average magnitude of the relative error.

4. CONCLUSION

The model has been developed for evaluating impact toughness of industrial hot rolled steels with ferritic-pearlitic and bainitic microstructures in dependence of chemical composition, combination of microstructural parameters and mechanical properties. All these characteristics were derived from the hot rolling conditions by means of previously developed integral computer model of hot rolling STAN 2000. The present modelling results are in good agreement with the experimental data. Average value of the relative error of calculations over the entire set of considered steel strips is 14.6 %.

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