Prediction of the Martensite Start Temperature in High-Carbon Steels

Jerome Ingber* and Maik Kunert

A new model for estimating the martensite start temperature ($M_s$) as a function of chemical composition is presented. It is developed and optimized for high-carbon steels with a $M_s$ range between 0 and 50 °C. It is based on the mean value of the best 8 of 21 considered models from the literature. A comprehensive evaluation is made by comparing the calculated $M_s$ with experimental $M_s$ data. Within the targeted $M_s$ range, the average absolute deviation of the calculated $M_s$ is as low as 13 °C. The investigations further show that the new model also makes accurate predictions outside the targeted $M_s$ range. The average absolute deviation in the $M_s$ range from 0 to 400 °C is found to be 21 °C, the lowest of all compared models. Furthermore, 75% of all calculations are within a deviation of 25 °C and 93% are within 50 °C. In general, the new model outperforms the models from which it is built.

1. Introduction

The knowledge of the martensite start temperature ($M_s$) is very important for the targeted heat treatment of steels. Therefore, many models have been developed to predict $M_s$ without having to perform time-consuming experiments. These models are usually based on thermodynamic equations, equations derived from artificial neural networks or by regression.

Early models\cite{1-6} rely on empirical equations and are generally built according to Equation (1), where $k_0$ is the $M_s$ of pure iron, $k_i$ represents an element-specific coefficient in degrees Celsius per wt%, and $x_i$ is the content of the corresponding element $i$ in wt%.

$$M_s = k_0 - \sum_i k_i \cdot x_i$$  

These linear regression models are based on the assumptions that 1) the various alloying elements are completely dissolved in the austenite and 2) the influence of the alloying elements on $M_s$ can be considered independent of each other.

Figure 1 shows the influence of different alloying elements on $M_s$ in binary Fe–X alloys.\cite{7} Additionally, in this figure also the influence of Al, Si, Cr, and Mn on $M_s$ of ternary Fe–C–X alloys is presented.\cite{8} Comparing the curves, it is evident that the influence of a given element X on $M_s$ of a binary Fe–X alloy is significantly different from its influence on $M_s$ of a ternary Fe–C–X alloy. For example, aluminum strongly increases $M_s$ in binary Fe–Al alloys. In the case of a Fe–0.76C–Al alloy, aluminum still increases $M_s$, but the increase per wt% is much smaller. Similarly, the effect of manganese on $M_s$ depends on the carbon content: for steels with carbon contents up to about 0.9 wt %, Mn leads to a significant reduction of $M_s$. For higher carbon contents, however, this effect is substantially reduced. In even more complex systems, such as quaternary Fe–C–Mn–Al steels, the mutual influence is even more pronounced. Simple linear models cannot reflect the interactions among the different alloying elements. Therefore, further models have attempted to account for the interactions of at least two elements by adding product terms,\cite{9,10} square rooted product terms,\cite{11,12} or exponential functions.\cite{13} Artificial intelligence methods were also used.\cite{11,14,15}

A collection of equations for estimating $M_s$ from a known alloy composition is summarized in Table 1. (More models are available on the following website: https://www.eah-jena.de/scitec/personen/maik-kunert/martensite-start-temperature.) All equations shown in Table 1 provide more or less good approximations for $M_s$ in a certain range of alloy compositions, but none of these equations is equally suitable for all compositions. Rather, different models are needed for specific composition ranges or steel grades.

Figure 2 shows the relative frequency of measured $M_s$ values in the publicly available $M_s$ database,\cite{16} which contains 1099 steels, their $M_s$, and the corresponding compositions. Obviously, $M_s$ data have been collected mainly for low and medium carbon steels and tool steels. Some data are available for austenitic steels. However, few data are available for alloys whose $M_s$ values are in the range of 0–50 °C. As a result, the accuracy of the available models for estimating $M_s$ is—if applicable at all—expected to be much lower for alloys with $M_s$ values in this temperature range.

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J. Ingber, M. Kunert
SciTec
Ernst-Abbe-Hochschule Jena
Carl-Zeiss-Promenade 2, Jena 07745, Germany
E-mail: Jerome.Ingber@eah-jena.de

The ORCID identification number(s) for the author(s) of this article can be found under https://doi.org/10.1002/srin.202100576.

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of metastable austenite in the quenched state. In two-body wear tests, mechanically induced martensite formation was observed on the wear surface, which exhibited a hardness of up to 1100 HV after the wear test.\textsuperscript{[17,18]}

2. Experimental Section

2.1. Materials

Several high-carbon low-alloy steels were used to develop and to evaluate the model for the estimation of $M_s$. Designations and chemical compositions of these steels can be found in Table 2.

The steel R1 was used as the reference steel in the development of the model. The steels labeled E1--E6 have specially been produced for this project. Those and further steels from the literature were used to evaluate the new model. E1--E6 were melted and cast into blocks. After casting, the slabs were hot-forged to improve homogeneity, followed by hot-rolling to a thickness of 14 mm. After cooling, 2 mm were milled off from each side of the strip to remove the decarburized layer. The strips were then cut to specimens of $10 \times 10 \times 100$ mm. These specimens were austenitized in a furnace with argon atmosphere at 950 °C or 1000 °C for 4–15 min and then quenched in 20 °C cold water.

Table 1. Overview of considered equations for estimating $M_s$, sorted by year of publication. For a larger number of models, please have a look at https://www.eah-jena.de/scitec/personen/maik-kunert/martensite-start-temperature.

| Year | Model | Equation for estimating $M_s$, in °C |
|------|-------|-------------------------------------|
| 1944 | Payson & Savage\textsuperscript{(1)} | $M_s = (930 - 570C - 60Si_{24} - 20Mn_{22} - 50Cr_{22} - 20Mo_{09} - 20Cu_{09} - 30Nb_{12}) - 32 \cdot 5/9$ |
| 1944 | Carapella\textsuperscript{(9)} | $M_s = (925 \cdot \{1 - 50/\{1 - 0.62x_C\} \cdot \{1 - 0.092x_Mn\} \cdot \{1 - 0.033x_Cr\} \cdot \{1 - 0.045x_Si\} \cdot \{1 - 0.07x_Mn\} \cdot \{1 - 0.029x_Cr\} \cdot \{1 - 0.018x_Cu\} \}^{1/10} - 1)\{1 + 0.12x_Co\} - 32 \cdot 5/9$ |
| 1946 | Rowland & Lyle\textsuperscript{(2)} | $M_s = (930 - 600C - 60Si_{22} - 20Mn_{22} - 20Mo_{09} - 20Cu_{09} - 30Nb_{12}) - 32 \cdot 5/9$ |
| 1946 | Grange & Stewart\textsuperscript{(7)} | $M_s = (1000 - 650C - 70Si_{22} - 50Cr_{22} - 50Mo_{09} - 35Nb_{12}) - 32 \cdot 5/9$ |
| 1946 | Nehrenberg\textsuperscript{(4)} | $M_s = (930 - 540C - 60Si_{22} - 20Mn_{22} - 20Mo_{09} - 30Nb_{12}) - 32 \cdot 5/9$ |
| 1956 | Steven & Haynes\textsuperscript{(6)} | $M_s = 561 - 474x_C - 33x_{Mn} - 17x_{Cr} - 21x_{Mo} - 17x_{Nb}$ |
| 1965 | Andrews\textsuperscript{(10)} | $M_s = 539 - 423x_C - 30.4x_{Mn} - 12.1x_{Cr} - 7.5x_{Mo} - 17.7x_{Nb}$ |
| 1955 | Andrews E.\textsuperscript{(11)} | $M_s = 512 - 453x_C - 16.9x_{Si} + 15x_{Mn} - 9.5x_{Nb} + 217x_{Cr} - 71.5x_{Cr} - 67.6x_{Cr}$ |
| 1970 | Kunitake & Ohtani\textsuperscript{[24]} | $M_s = 521 - 353x_C - 24.3x_{Mn} - 17.7x_{Cr} - 22x_{Si} - 17.3x_{Nb} - 7.7x_{Mo} - 25.8x_{Mn}$ |
| 1970 | Tamura\textsuperscript{[24]} | $M_s = 550 - 361x_C - 39x_{Mn} - 20x_{Cr} - 5x_{Mo} - 30x_{Si} - 15x_{Cr} - 10x_{Mo} - 17x_{Nb} - 35x_{Nb}$ |
| 1970 | Stein\textsuperscript{[24]} | $M_s = 550 - 350x_C - 40x_{Mn} - 20x_{Cr} - 10x_{Mo} - 17x_{Nb} - 15x_{Cr} - 10x_{Mo} - 17x_{Nb}$ |
| 1972 | Momma\textsuperscript{[24]} | $M_s = 531 - 391.2x_C - 43.3x_{Mn} - 16.2x_{Cr} - 21.8x_{Nb}$ |
| 1977 | Eldis\textsuperscript{(11)} | $M_s = 492 - 125x_C - 65.5x_{Mn} - 10x_{Cr} - 29x_{Nb}$ |
| 1979 | Kulmburg\textsuperscript{[22]} | $M_s = 514 - 470.4x_{Mn} - 37.7x_{Cr} - 3.96x_{Mo} - 21.5x_{Mo} - 38.6x_{Mo}$ |
| 1995 | Ishida\textsuperscript{[13]} | $M_s = 545 - 330x_C - 23.4x_{Mn} - 7x_{Si} - 14x_{Nb} - 13x_{Cr} - 5x_{Mo} - 2x_{Si} - 7x_{Cr} - 4x_{Mn} - 3x_{Mn} + 4x_{V}$ |
| 2000 | Wang\textsuperscript{[11]} | $M_s = 545 - 470.4x_{Mn} - 37.7x_{Cr} - 3.96x_{Mo} - 21.5x_{Mo} - 38.6x_{Mo}$ |
| 2000 | Wang\textsuperscript{[11]} | $M_s = 540 - 584x_{Mn} - 23.4x_{Cr} - 117.7x_{Cr} - 42.5x_{Cr} + 49.9x_{Mo} - 62.5(x_{Cr} \cdot x_{Mo})^{1/2} + 178.3(x_{Cr} \cdot x_{Mo})^{1/2} - 10x_{Cr} \cdot x_{Mo})^{1/2}$ |
| 2001 | Kunitake\textsuperscript{[24]} | $M_s = 560.5 - 407.3x_{Mn} - 37.8x_{Cr} - 7.3x_{Si} - 14.8x_{Cr} - 19.5x_{Mo} - 20.5x_{Mo}$ |
| 2002 | Capdevila\textsuperscript{[16]} | $M_s = 491.05 - 302.6x_{Cr} - 30.6x_{Mo} - 14.5x_{Cr} - 8.3x_{Mo} - 16.6x_{Mo} + 8.5x_{Mo} + 2.4x_{Mo} + 7.4x_{Mo} - 11.3x_{Mo}$ |
| 2004 | Dai\textsuperscript{[12]} | $M_s = 501 - 199.8(x_{Cr} \cdot 1.4x_{Mo}) - 17.9x_{Mo} + 21.7x_{Mo} - 6.8x_{Mo} - 45x_{Mn} - 55.9x_{Mo} - 1.9x_{Cr}(x_{Cr} \cdot x_{Cr}) + 1.9x_{Cr}(x_{Cr} \cdot x_{Mo}) - 14.4[(x_{Cr} \cdot x_{Mo})]/10x_{Cr} - 12x_{Mo}$ |
| 2012 | van Bohemen\textsuperscript{[21]} | $M_s = 565 - 600[1 - \exp(-0.96x_{Cr}) - 31x_{Mo} - 13x_{Si} - 18x_{Mo} - 10x_{Cr} - 12x_{Mo}$ |
After that, a 10 mm piece has been cut off, embedded, and prepared. Details on sample preparation routine can be found elsewhere.[18,19]

2.2. Determination of $M_s$

$M_s$ of the steels was calculated using the Koistinen–Marburger equation (Equation (2)).[20] This equation relates $M_s$ to the martensite content $f_M$ formed at a given quenching temperature $T_q$. $B$ is a composition-dependent constant ($B = -0.011 \, °C^{-1}$).

$$M_s = \frac{B}{1} \ln(1 - f_M) + T_q$$

(2)

The martensite content $f_M$ of the quenched steels E1–E6 was determined using quantitative Rietveld analyses of X-ray diffraction (XRD) measurements of polished specimens. XRD measurements were conducted using a D8 Discover diffractometer (Bruker) in Bragg–Brentano geometry with copper radiation ($\lambda = 0.154 \, nm$). Diffractograms were measured from 42 to 98° 2θ with a step size of 0.03° per step and 3 s measuring time per step. A 2.5° soller slit was mounted on the primary track. On the secondary track, a 2.5° soller slit and a nickel filter were used. TOPAS 5 (Bruker) was utilized for full-pattern Rietveld refinement.

3. Results and Discussion

3.1. Determination of $M_s$

The martensite content of the reference steel R1 after quenching was $f_M = 0.06$ (6 vol%).[17] According to Equation (2), this corresponds to $M_s = 26 \, °C$.

The XRD patterns of the quenched evaluation steels E1–E6 are shown in Figure 3. Along with the measured curves (green), the calculated curves from the Rietveld refinement are shown (red). Note that the calculated curves and the measured diffraction patterns are in fairly good agreement. The weighted profile $R$ factors ($R_{wp}$) of the refinements are between 5% and 8% with expected $R$ factor ($R_{exp}$) of approximately 3%. The martensite content of these steels as calculated using Equation (2) is shown in Table 3.

![Figure 2. Relative distribution of measured $M_s$ values; data taken from publicly available $M_s$ database.[16] To plot the distribution curve, the 1099 values in the $M_s$ database were divided into 41 classes with ±10 K around the classification mean value.](image)

![Figure 3. Measured (green) and calculated (red) diffraction patterns of the evaluation steels E1–E6 after quenching.](image)

| Steel | $f_M$ [vol%] | Exp. $M_s$ [°C] | Calc. $M_s$ [°C] | $|\Delta M_s|$ [K] |
|-------|-------------|----------------|-----------------|----------------|
| R1    | 6           | 26             | 26              | 0              |
| E1    | 5           | 33             | 26              | 5              |
| E2    | 5           | 31             | 26              | 5              |
| E3    | 11          | 29             | 29              | 9              |
| E4    | 5           | 31             | 25              | 6              |
| E5    | 4           | 26             | 13              | 13             |
| E6    | 16          | 50             | 25              | 20             |

Table 2. Chemical composition of the high-carbon low-alloy steels (wt%) used for developing (R1) and evaluating the model (E1–E6).

| Steel | C  | Si  | Mn  | Al  | Cr  | S   | P   | References |
|-------|----|-----|-----|-----|-----|-----|-----|------------|
| R1    | 1.21 | 1.59 | 2.56 |     |     |     |     | [17]       |
| E1    | 1.01 | 1.56 | 4.04 | 0.02 | 0.52 | 0.003 | 0.01 | [18]       |
| E2    | 0.99 | 1.52 | 4.06 | 1.49 | 0.51 | 0.002 | 0.01 | [18]       |
| E3    | 1.09 | 1.51 | 3.24 | 0.02 | 0.50 | 0.001 | 0.01 | [18]       |
| E4    | 1.09 | 1.53 | 3.22 | 1.43 | 0.50 | 0.001 | 0.01 | [18]       |
| E5    | 1.23 | 1.51 | 2.46 | 0.02 | 0.51 | 0.001 | 0.01 | [18]       |
| E6    | 1.23 | 1.50 | 2.41 | 1.43 | 0.50 | 0.001 | 0.01 | [18]       |

After that, a 10 × 10 × 10 mm piece has been cut off, embedded, and prepared. Details on sample preparation routine can be found elsewhere.[18,19]

Table 3. Martensite content ($f_M$) and measured $M_s$ (exp. $M_s$) as well as calculated (calc. $M_s$) and absolute deviation $|\Delta M_s|$ of the steels defined in Table 2 derived using Equation (4) and (5).
As mentioned in Section 2.2, the constant B in Equation (2) depends on the chemical composition of the steel. According to van Bohemen,[13] the composition dependence can be described using Equation (3).

\[
B = 27.2 - 0.14x_{\text{Mn}} - 0.21x_{\text{Si}} - 0.11x_{\text{Cr}} - 0.08x_{\text{Ni}} - 0.05x_{\text{Mo}} - 19.8 \cdot [1 - \exp(-1.56x_{\text{C}})]
\] (3)

This equation does not take aluminum into account. Therefore, no unambiguous statement can be made for the steels E2, E4, and E6. Nevertheless, for the steels R1, E1, E3, and E5, the difference of \( M_s \) is found to be only 0.8 °C at max when B is corrected using Equation (3). Therefore, in this article, the constant B is assumed to be independent of the steel composition and for the calculation of \( M_s \) the value \( B = -0.011 \text{ °C}^{-1} \) is used as proposed by Koistinen and Marburger.[20]

3.2. Development of Model

All the models stated in Table 1 were used to estimate \( M_s \) of the reference steel (R1). The results of these estimations are shown in Figure 4. It can be seen that the \( M_s \) values determined this way vary greatly; from approximately –125 to 275 °C. The solid line represents the experimentally determined \( M_s \) of R1 (26 °C). Some models calculate the \( M_s \) of R1 with an only minor deviation to the experimental \( M_s \). A new model is developed by calculating the mean value of these models. A similar approach was used by Peet.[21] To find the best set of models from which to calculate the mean, an interval \( x \) around the experimental \( M_s \) is introduced (26 °C ± \( x \)). Models within the interval are included in the mean; models outside the interval are not. By calculating the mean value with varying intervals from \( x = 100 \text{ °C} \) (dashed line in Figure 4) to \( x = 5 \text{ °C} \) at 1 °C step size and calculating the deviation to the experimental \( M_s \), the best interval value is found to be 28 °C (dotted line in Figure 4). The following eight models are within this best interval: 1) Payson & Savage[11]; 2) Grange & Stewart[11]; 3) Nehrenberg[4]; 4) Tamura[22]; 5) Steim[21]; 6) Monna[24]; 7) Capdevila[14]; and 8) van Bohemen.[11]

By averaging the above named models, Equation (4) is obtained.

\[
M_s = \frac{1}{8} \left\{ 4241.9 - 2322.27x_{\text{C}} - 284x_{\text{Mn}} - 54.4x_{\text{Si}} - 166.4x_{\text{Cr}} - 137.4x_{\text{Ni}} - 83.5x_{\text{Mo}} - 30x_{\text{Al}} + 38.58x_{\text{Co}} 
- 600[1 - \exp(-0.96x_{\text{C}})] \right\}
\] (4)

This equation estimates \( M_s \) of the reference steel R1 to \( M_s = 26 \text{ °C} \), which equals the experimentally determined value.

Applying Equation (4) to determine \( M_s \) of the steels E1–E6, a good agreement with the experimentally determined values is obtained (cf., Table 3). However, the coefficient for aluminum is negative in Equation (4). This is in contrast to Figure 1, which implies that an addition of aluminum leads to an increase in \( M_s \). To account for this, the aluminum coefficient was refined as follows: The \( M_s \) of the 16 aluminum containing alloys from Table 4 were calculated using Equation (4) for different aluminum coefficients. Then the differences of the calculated \( M_s \) and the experimental \( M_s \) were determined, and the squares of these differences were summed up. A minimum deviation (the lowest value of the sum of the squares of the differences of calculated and experimental \( M_s \)) was found at 7.1 °C/wt% aluminum. Equation (5) emerges from this. The \( M_s \) values calculated using Equation (5) are also given in Table 3.

\[
M_s = 530.2 - 290.3x_{\text{C}} - 35.5x_{\text{Mn}} - 6.8x_{\text{Si}} - 20.8x_{\text{Cr}} - 17.2x_{\text{Ni}} - 10.4x_{\text{Mo}} - 7.1x_{\text{Al}} + 4.8x_{\text{Co}} 
- 75[1 - \exp(-0.96x_{\text{C}})]
\] (5)

3.3. Evaluation of Model

In order to assess the new model (Equation (5)) a set of steels found in the literature and their experimentally determined \( M_s \) are used for evaluation (cf., Table 4). The evaluation is done by comparing the performance of the new model with the eight models it is developed of. Figure 5a–i show the calculated \( M_s \) as a function of the experimental \( M_s \) of those models. The prediction accuracy of a model is better, the closer the calculated \( M_s \) points are to the solid line. If a data point lies on the solid line, there is no deviation between calculated and experimental \( M_s \). As displayed, the \( M_s \) are reasonably good estimated by all models. However, larger deviations are found in some cases. The Payson & Savage model[11] tends to underestimate the \( M_s \), which is why the majority of points are mapped below the solid line in Figure 5a. Monma’s model,[24] Figure 5e, on the other hand, tends to overestimate the \( M_s \). As all models are different and each has been built using different fundamental data, performance may be better for some temperature ranges or specific compositions than for others. For example, almost all models show the lowest scatter for \( M_s \) between 200 and 300 °C. Exceptions are the models of Nehrenberg,[4] Capdevila,[14] van Bohemen,[11] and the new model. Apart from a few outliers, these show a rather homogeneous distribution.
Table 4. Overview on compositions and experimental $M_s$ values of the steels used for evaluation.

| No. | C   | Mn  | Si  | Cr  | Ni  | Mo  | Al  | Exp. $M_s$ [K] | References |
|-----|-----|-----|-----|-----|-----|-----|-----|----------------|------------|
| 1   | 0.1 | 2.7 | 17  | 4   | 0   | 0   | 0   | 290.15        | [35]       |
| 2   | 1.09| 3.24| 1.51| 0.5 | 0   | 0   | 0   | 293.16        | E3         |
| 3   | 1.21| 2.56| 1.59| 0   | 0   | 0   | 0   | 296.15        | R1         |
| 4   | 1.23| 2.46| 1.51| 0.51| 0   | 0   | 0   | 299.16        | E5         |
| 5   | 0.99| 4.06| 1.52| 0.51| 0   | 0   | 0   | 304.16        | E2         |
| 6   | 1.01| 4.04| 1.56| 0.52| 0   | 0   | 0   | 304.16        | E1         |
| 7   | 1.09| 3.22| 1.53| 0.5 | 0   | 0   | 0   | 304.16        | E4         |
| 8   | 1.22| 2.58| 2.03| 0   | 0   | 0   | 0   | 306.16        | [36]       |
| 9   | 1.23| 2.41| 1.5 | 0.5 | 0   | 0   | 0   | 318.16        | E6         |
| 10  | 0.1 | 2   | 17  | 4   | 0   | 0   | 0   | 320.15        | [35]       |
| 11  | 0.4 | 8   | 2   | 3   | 0   | 0   | 0   | 355.15        | [35]       |
| 12  | 0.2 | 7.73| 2.15| 3.02| 1.23| 0   | 0   | 2.27          | [35]       |
| 13  | 0.98| 1.9 | 1.5 | 1.4 | 0   | 0   | 0   | 363.16        | [37]       |
| 14  | 0.93| 0.5 | 0.3 | 1.13| 4.25| 0.16| 0   | 0   | 388           | [38]       |
| 15  | 0.96| 1.18| 0.6 | 1.48| 0.03| 0   | 0   | 0   | 401.15        | [39]       |
| 16  | 0.95| 0.4  |2.66| 0.36| 2.95| 0.08| 0   | 0   | 403           | [38]       |
| 17  | 0.8 | 2.03| 1.41| 0.22| 1.05| 0.38| 0   | 0   | 403.15        | [40]       |
| 18  | 0.99| 0.76| 1.5 | 0.46| 0   | 0   | 0   | 0   | 403.16        | [41]       |
| 19  | 0.99| 0.74| 2.47| 0.17| 0.12| 0.03| 0   | 0   | 407.15        | [42]       |
| 20  | 0.96| 0.74| 0.26| 0.84| 1.19| 0.09| 0   | 0   | 408           | [38]       |
| 21  | 0.95| 0.56| 0.29| 0.32| 1.61| 0.29| 0   | 0   | 413           | [35]       |
| 22  | 0.25| 8.1 | 2.66| 0   | 0   | 0   | 0   | 2.38          | [35]       |
| 23  | 0.9 | 0.79| 1.65| 0.48| 0   | 0   | 0   | 0   | 433.16        | [41]       |
| 24  | 0.98| 0.77| 2.9 | 0.45| 0   | 0   | 0   | 0   | 433.16        | [41]       |
| 25  | 0.58| 2.21| 1.76| 0.54| 0.76| 0.33| 0.45| 0   | 446.15        | [40]       |
| 26  | 0.99| 0.74| 2.47| 0.98| 0.12| 0   | 0   | 0   | 446.15        | [43]       |
| 27  | 0.99| 0.35 |0.01| 1.48| 0   | 0   | 0   | 0   | 447           | [38]       |
| 28  | 0.93| 0.71| 0.38| 1.7 | 2.1 | 0.2 | 0   | 0   | 448           | [38]       |
| 29  | 0.68| 1.32| 1.67| 1.73| 0.2 | 0.15| 0   | 0   | 451.15        | [42]       |
| 30  | 0.18| 7.9 | 3.09| 0   | 0   | 0   | 0.65| 0   | 457.15        | [35]       |
| 31  | 0.79| 0.5 | 0.02| 0.22| 1.76| 0.23| 0   | 0   | 458           | [38]       |
| 32  | 0.78| 2 | 1.6 | 1   | 0   | 0.24| 3.96| 1.65| 461.15        | [44]       |
| 33  | 0.7 | 0.35| 0.16| 0.96| 3.24| 0.06| 0   | 0   | 462           | [38]       |
| 34  | 0.96| 0.55| 0.32| 0.11| 0.08| 0   | 0   | 0   | 463           | [38]       |
| 35  | 0.7 | 1.18| 2.47| 0 | 0 | 0 | 0 | 0.87 | 463.15 | [45] |
| 36  | 0.96| 0.6 | 0 | 0 | 0 | 0 | 0 | 0 | 469 | [38] |
| 37  | 0.865| 0.75 |0.01| 0   | 0   | 0   | 0   | 0   | 473           | [38]       |
| 38  | 0.078| 7.87| 2.16| 0.039| 1.29| 0   | 0   | 2.44| 473.15 | [35] |
| 39  | 0.78 | 0.33 |0.02| 1.42| 0.27| 0   | 0   | 0   | 481           | [38]       |
| 40  | 0.64| 0.7 | 0.23 |0.8 | 1.83| 0.25| 0   | 0   | 483           | [38]       |
| 41  | 0.75| 0.7 | 0.33 |0.17| 0.2 | 0   | 0   | 0   | 483           | [38]       |
| 42  | 0.965| 0.4 |0.01| 0   | 0   | 0   | 0   | 0   | 483           | [38]       |
| 43  | 0.78| 0.86 |0.01| 0.49| 0.59| 0.21| 0   | 0   | 485           | [38]       |
| 44  | 0.86 |0.01| 0.6 | 0   | 0   | 0   | 0   | 0   | 488           | [38]       |
| 45  | 0.865| 0.4 |0.01| 0   | 0   | 0   | 0   | 0   | 488           | [38]       |
| 46  | 0.54| 1.89| 1.7 | 0   | 1.63| 0.24| 0   | 0   | 488.15        | [46]       |

When looking at the results, it should be remembered that the $M_s$ data and these compositions are also subject to measurement errors. Depending on the publication, different $M_s$ temperatures...
are found for the same compositions, even from the same authorship. These fluctuations can be attributed to factors influencing the M_s, such as the prior austenite grain size,\textsuperscript{25,26} the stress state,\textsuperscript{27} the cooling rate,\textsuperscript{28} and even the measurement method itself.\textsuperscript{29}

In order to quantify the qualitative graphs, four parameters have been determined (Table 5): the coefficient of determination $R^2$ to assess the quality of a linear fit of the plotted data, $\overline{\Delta M_s}$ is the average absolute deviation between experimental and calculated $M_s$, and $F_{25}$ and $F_{50}$ represent the percentage of calculations

![Graphs](image-url)

**Figure 5.** a) Experimental $M_s$ and calculated $M_s$ with the model proposed by Payson & Savage.\textsuperscript{[1]} b) Experimental $M_s$ and calculated $M_s$ with the model proposed by Grange & Stewart.\textsuperscript{[3]} c) Experimental $M_s$ and calculated $M_s$ with the model proposed by Nehrenberg.\textsuperscript{[4]} d) Experimental $M_s$ and calculated $M_s$ with the model proposed by Tamura.\textsuperscript{[5]} e) Experimental $M_s$ and calculated $M_s$ with the model proposed by Monma.\textsuperscript{[6]} f) Experimental $M_s$ and calculated $M_s$ with the model proposed by Steim.\textsuperscript{[7]} g) Experimental $M_s$ and calculated $M_s$ with the model proposed by Capdevila.\textsuperscript{[8]} h) Experimental $M_s$ and calculated $M_s$ with the model proposed by van Bohemen.\textsuperscript{[9]} i) Experimental $M_s$ and calculated $M_s$ with the developed model.
within a 25 or 50 °C interval, respectively. $R^2$ indicates how well the model fits the observation. The new model shows the highest $R^2$ of all models and the lowest average absolute deviation $|\Delta M_s|$.

If only the experimental $M_s$ range up to 50 °C is considered, the new model makes the most accurately $M_s$ prediction. The average absolute deviation in the range up to 50 °C is just 13 °C in case of the new model, which is the lowest value achieved by any model. Considering the $M_s$ temperature range from 0 to 400 °C, the average absolute deviation is found to be 21 °C, which is also the lowest of all compared models. For the given experimental data, 75% of all calculations of the new model are within a 25 °C deviation. This is only exceeded by van Bohemen’s\textsuperscript{[13]} model (77%). Within a 50 °C deviation range are 93% of all calculations, which also applies for Nehrenberg\textsuperscript{[4]} and van Bohemen.\textsuperscript{[13]}

### 4. Conclusion

This article presents a model for the $M_s$ calculation of steels in relation to their chemical compositions. It was created by averaging eight other $M_s$ calculation models and shows improved accuracy, especially in the $M_s$ range from 0 to 50 °C, compared to the other models considered. It has been demonstrated that the new model best reflects the relationship between chemical composition and $M_s$, and shows the lowest average deviation of all models. The models described by Nehrenberg.\textsuperscript{[4]}

### Table 5. Correlation coefficient $R^2$, average absolute deviation of experimental and calculated $M_s$ $|\Delta M_s|$, average absolute deviation of experimental and calculated $M_s$ (exp. $M_s < 50$ °C) $|\Delta M_s|_{50}$, confidence intervals $F_{25}$ and $F_{50}$ of the presented calculation model and the models used for development.

| Model             | $R^2$  | $|\Delta M_s|$ | $|\Delta M_s|_{50}$ | $F_{25}$ | $F_{50}$ |
|-------------------|--------|----------------|-------------------|---------|---------|
| Payson & Savage   | 0.884  | 29.8           | 42.9              | 0.60    | 0.84    |
| Grange & Stewart  | 0.827  | 35.6           | 64.5              | 0.58    | 0.84    |
| Nehrenberg        | 0.894  | 24.5           | 17.4              | 0.68    | 0.93    |
| Tamura            | 0.834  | 32.5           | 41.6              | 0.50    | 0.77    |
| Monna             | 0.876  | 28.6           | 22.9              | 0.55    | 0.83    |
| Steim             | 0.881  | 27.8           | 24.4              | 0.51    | 0.85    |
| Capdevila         | 0.814  | 23.1           | 44.5              | 0.70    | 0.90    |
| van Bohemen       | 0.799  | 21.9           | 55.3              | 0.77    | 0.93    |
| Equation (4)      | 0.901  | 21             | 17.3              | 0.72    | 0.92    |
| Equation (5)      | 0.914  | 20.9           | 13                | 0.75    | 0.93    |
Capdevila,[14] and van Bohemen[13] also predict decent results in the $M_s$ calculation, but have greater deviations than the proposed model, particularly at lower $M_s$. This may be due to the data sets from which the models are derived. The data usually contain more $M_s$ (and the associated compositions) above 200 °C.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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