Correlation analysis of the dependence of the properties of steel on its composition based on the processing of reference information

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Abstract. In the article the possibility of identification of grade steel properties on the platform “structure - properties” dependence by the linear correlation analysis of information from standard reference books is considered. Clearly significant coefficients of correlation are found for a number of the alloying elements. The results can be used for forecasting of physic and mechanical properties of alloys with the alloying additives.

1. Introduction

The physic and chemical composition of steels and iron-containing compositions (alloys) on the «composition-property» platform has been thoroughly and deeply studied due to mechanical properties, research is being actively pursued for understandable materials-science and practical reasons. The amount of information in this area is simply inexhaustible. The same can be said about the influence of heat treatment regimes on the strength characteristics of materials. However, in this case, both in theory and in practice, the questions arise about the identity and reproducibility of well-known facts in this field. Some of the contradictions are fundamental and limit the ability to predict the properties of this type of materials. In particular this is due to the fact that the conclusions are based on limited experimental material obtained by specific authors often in a narrow field.

In this study, of a static nature, the authors decided to selectively test sustainable views on the composition-property relationship in this area. To do this, they carried out a comparative analysis of data from numerous reference literature on the properties of steels [1-5] (a complete list of references because of its bulkiness is not given). This data on the composition and properties of steel are tabulated. The authors note that they to a certain extent reflect integral dependencies, since they are “tied off” from subjectivity. From the tables, it can be seen that the numerical and non-numerical characteristics given in them have heterogeneity, inconsistency and uncertainty.

It turned out that according to the reference information studied, taken from State Standards, steel makers and other reference sources, including the Internet, it is impossible to clearly determine whether there is a linear correlation between the alloying components and their contribution to one or another physic-mechanical characteristic. Even more confusing is the picture when optimizing a set of final material characteristics. In connection with the bright practical side of the study, the authors note that
the use of reference data to create new materials with given integral characteristics within the framework of the question posed presents and will present an urgent problem for a long time. The authors try to understand it within the framework of the problematic of this article in more detail, somewhat limiting it to a specific method — regression-correlation analysis [6-8].

2. Methods
The analytical detection of the functional influence of individual elements contained in steel requires the study of a large array of experimental data. In many cases, these dependencies are described with varying degrees of reliability. The mutual influence of several elements on the properties is much more difficult.

The authors perform a pairwise regression-correlation analysis for standard combinations of chemical elements in the smelting of steel. Here they used a sample of 110 steels of various technical purposes: ordinary structural carbon steel of general quality, structural carbon steel of high quality, alloy structural steel, structural bearing steel, spring structural steel, tool steel, alloy steel, tool steel, steel tool high-speed, steels and alloys corrosion-resistant, heat-resistant, wear resistant steel for castings. Each of the materials of this sample has a unique physic and chemical composition.

3. Results and discussion
In this study, the authors compare each chemical element included in the steel with mechanical and physical properties: linear expansion coefficient, thermal conductivity, normal elastic modulus, torsional shear modulus, density, electrical resistivity and specific heat. All the parameters are taken to set the temperature of 20, 200, 400 and 600 °C. A small part of the sample, which characterizes the preparation of information, is shown in Table 1. Chemical elements are sorted by frequency of use in steel.

|   | C (%) | Si (%) | Mn (%) | Cr (%) | Ni (%) | Mo (%) | W (%) | V (%) | Ti (%) |
|---|------|-------|--------|--------|--------|--------|------|------|-------|
| 1 | 0.5  | 0.27  | 0.65   | 0.25   | 0.25   |        |      |      |       |
| 2 | 0.9  | 1.4   | 0.45   | 1.1    | 0.35   | 0.2    | 0.2  | 0.15 | 0.03  |
| 3 | 0.35 | 0.22  | 0.22   | 2.45   | 0.35   | 0.5    | 8    | 0.35 |       |
| 4 | 0.9  | 0.5   | 0.5    | 4      | 0.5    | 0.35   | 0.2  | 1.9  |       |
| 5 | 0.8  | 0.5   | 0.5    | 3.1    | 0.4    | 0.35   | 0.2  | 1.9  |       |
| 6 | 0.2  | 2.5   | 1.5    | 20.5   | 1.35   | 0.2    |      |      |       |
| 7 | 0.2  | 2.5   | 1.5    | 25     | 20     | 0.3    | 0.2  | 0.2  | 1.9   |
| 8 | 0.37 | 0.65  | 8.5    | 12.5   | 8      | 1.25   | 1.4  |      |       |
| 9 | 0.45 | 0.8   | 0.7    | 14     | 14     | 0.32   | 2.4  |      |       |
| 10| 0.4  | 0.115 | 7      | 15     | 7      | 0.8    | 0.2  | 1.7  |       |
| 11| 0.1  | 0.8   | 2      | 17     | 13     | 2.5    |      | 0.7  |       |
| 12| 0.06 | 0.8   | 0.8    | 23.5   | 29     | 2.75   | 0.7  |      |       |
| 13| 0.12 | 0.6   | 0.5    | 14.5   | 65     | 3.25   | 6    | 1    | 2     |
| 14| 0.12 | 0.3   | 0.65   | 0.3    | 2      |        | 0.11 |      |       |
| 15| 0.2  | 1.05  | 1.1    | 0.75   | 1.3    | 0.125  | 0.05 |      |       |

Based on a visual review of systematic data, it is possible to detect significant data gaps and their variability. To substantiate the quantitative relationship “composition-property” by visualization is not possible. The authors apply the standard linear correlation analysis [6], associating the change in the percentage of each individual element with the change in alloy properties. In particular, they take the
The value of the correlation coefficient (Table 1) of at least 0.75. The results of the systematization and the calculated linear correlation coefficients are shown in Table 2 and Table 3. The cells with no values indicate insufficient data or non-intersection.

### Table 2. Physical and mechanical properties table

| Young’s modulus (GPa) | Modulus of torsion (GPa) | Density (kg m⁻³) |
|-----------------------|--------------------------|------------------|
| 20 200 400 600        | 20 200 400 600           | 20 200 400 600   |
| 1 216 207 180 154     | 88 84 71 61              | 7810 7830        |
| 2 190 79              |                          |                  |
| 3 224 211 196 177     | 83 8200                  | 8800 7720        |
| 5 228 219 201 181     | 83 8200                  | 8800 7720        |
| 6 171 157 140 125     | 7800 7830                |                  |
| 7 208 190 173 157     | 8000 7930 7840 7760      |                  |
| 8 150 147 147         | 7800 7720 7630 7530      |                  |
| 10 206 186 177 157    | 7900 7830 7750 7660      |                  |
| 11 - 186 171 156      | 7960                     |                  |
| 12 196 - - - - 162    |                          |                  |
| 14 211 196 181 155    | 82 76 70 59              | 7860 7880        |
| 15 209 193 176 153    | 82 76 67 58              | 7830 7850        |

### Table 2(a). Physical and mechanical properties table

| Heat conduction coefficient (W m⁻¹ K⁻¹) | Specific electrical resistivity (nOm·m⁻¹) | Specific heat capacity (J kg⁻¹ K⁻¹) |
|-----------------------------------------|------------------------------------------|-------------------------------------|
| 20 200 400 600                          | 20 200 400 600                           | 20 200 400 600                      |
| 1 48 47 41 35                            | 272 200 140                              | 487 517 559                         |
| 2 400                                     |                                          |                                     |
| 3 27 40 50                              | 200 140                                  |                                     |
| 4 28 30 36                              | 458                                      |                                     |
| 5 27 29 27                              | 419 544 718 922                          |                                     |
| 6 17 19 23                              | 946 1051 1130 1194                       |                                     |
| 7 24                                      |                                          |                                     |
| 8 18 21 25                              | 740 900 1010 1150                       |                                     |
| 9 14 17 20 22                           | 815 945 1055 1142                       | 507 523                             |
| 10 16 20 24                             |                                          |                                     |
| 11 13 15 24                             | 750                                      |                                     |
| 12 9 13 17 21                           |                                          |                                     |
| 13 37 38 37 32                         | 210 339 545 787                         | 487 517 559 617                     |
| 14 25 28 32 33                         | 433 531 705 967                         | 491 521 554 622                     |
| 15 25 28 32 33                         |                                          |                                     |
There are families of coefficients, indicating the presence of a high functional dependence "element
properties (4)."

As it can be seen from the data of Table 3, the correlation coefficients are significantly scattered. There are families of coefficients, indicating the presence of a high functional dependence "element in the composition of steel - property." The authors clarify their possible meaning. To do this, it is necessary to join the analysis table with the values of physical parameters for individual chemical elements (table 4). Some contextual conclusions from the values of the correlation coefficients linking the sample properties are made.

1) **Density.** The activity of tungsten, nickel and molybdenum is obvious. Due to the high density of tungsten and molybdenum, their low concentrations lead to an increase in the density of the alloy. Large values of the correlation coefficients for nickel are associated with the use of this element in significant concentrations in the alloy.

2) **Thermal conductivity.** The effect of chromium on our calculations is negative, but most likely it is controversial. Tungsten also attracts attention.

3) **Specific electrical resistance.** Titanium and chromium have a significant resistivity compared to iron. Therefore, the introduction of these elements has a clear direct effect on this characteristic of the alloy, and the effect of chromium is more pronounced due to the greater difference in the resistance value of the net resistivity.
4) Modulus of torsion is clearly dependent on the molybdenum content.

Table 4. Summary Information

| Element | Density (kg m⁻³) | Specific electrical resistance (mΩ·m) | Thermal conductivity of chemical elements (W m⁻¹ K⁻¹) | Specific heat capacity (J kg⁻¹ K⁻¹) |
|---------|-----------------|-------------------------------------|---------------------------------------------|-----------------------------------|
| Fe      | 7870            | 98                                  | 200  400  600                                  | 100  200  400  600               |
| C       | 3510            | 1.2                                 | 596  260                                      | 596  260                         |
| Si      | 2330            | 1400                                | 1294 1400                                    | 1294 1400                        |
| Mn      | 7450            | 6.87                                | 529  529                                      | 529  529                         |
| Cr      | 7140            | 1400                                | 1294 1400                                    | 1294 1400                        |
| Ni      | 8910            | 87                                  | 1294 1400                                    | 1294 1400                        |
| Mo      | 10280           | 59                                  | 1294 1400                                    | 1294 1400                        |
| W       | 19260           | 55                                  | 1294 1400                                    | 1294 1400                        |
| V       | 6090            | 202                                 | 1294 1400                                    | 1294 1400                        |
| Ti      | 4510            | 600                                 | 1294 1400                                    | 1294 1400                        |

4. Conclusion

Thus, in this work, using the linear correlation analysis on the “composition - property” platform, the explicit correlation dependences obtained during the processing of reference information on the properties of steels are refined containing besides iron sets of various elements of the periodic table.

In this regard it is possible to point out that the non-obviousness and non-linearity of the “chemical composition - properties” correlations for steels, using standard statistical approaches, makes it impossible to identify the characteristics of the alloys by the mass fractions of the alloying elements contained in them. This is most likely based on deep physicochemical and structural patterns linking chemical elements in the metal compositions inside the crystal lattice.

Another reason may be an incomplete series of mechanical and physical parameters for steel in the reference literature. Due to this, for example, it is extremely difficult to identify the relationship of the specific heat capacity with the composition. The same can be said about other interdependencies, which, in principle, enable analytic methods to control the properties of steel. The authors point out that the next step may be multiple correlation and regression analysis, followed by the use of methods of fuzzy mathematics and neural networks.

References

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