J. KLIMEŠ

ISSN 0543-5846
METABK 49(2) 95-98 (2010)
UDC – UDK 669.14-418:539.37:620.17=111

FORMAL CONCEPT ANALYSIS APPLIED TO THE PREDICTION OF ADDITIVES FOR GALVANIZING PROCESS

Received – Prispjelo: 2008-10-24
Accepted – Prihvaćeno: 2009-08-10
Original Scientific Paper – Izvorni znanstveni rad

Formal concept analysis is a new mathematical approach to data analysis, data mining and to discavering patterns in data. The result of the application of the formal concept analysis method to the behaviour of the galvanizing of rimmed steel is presented. Effects of additives in the galvanizing process have been correlated to the chemical element properties of the additives. This model may also help to design new alloys as additives in the galvanizing process.

Key words: galvanizing process, steel weight loss, formal concept analysis, implications in conceptual lattice

Formal concept analize za procjenu dodataka na proces galvanizacije. Formal concept analiza je novi matematički pristup analizi podataka, pretraživanjem podataka i otkrivanja. Rezultati primjene metodologije formal concept analize na ponašanje galvaniziranih čeličnih naplatake su dani. Efekti dodataka u procesu galvanizacije su u korelaciji sa svojstvima kemijskih elementa aditiva. Taj model može također pomoći u dizajniranju novih legura kao aditiva u procesu galvanizacije.

Ključne riječi: proces galvanizacije, gubitak mase čelika, formal concept analize, implikacije u konceptu rešetke

INTRODUCTION

The crystal structure of acompound is fully defind by the following data: (1) chemical formula, (2) pace group and unit-cell dimension, and (3) coordinates of the point sets-atomic position. Because of the larger number of different structure, it is impossible to find connection within crystal stuctures, which makes it difficult to predict bulk properties of materials. To reduce the number of distinctly different crystal structures, in [1] is applied the atomic-environment approach, with the following six groups of its constituent chemical element properties: (1) size factor, (2) atomic-number factor, (3) electrochemical factor, (4) valence-electron factor, (5) cohesive-energy factor, and (6) angular valence-orbital factor. Hot dip galvanizing is one of the principal technologies to protect against atmospheric corrosion of steel. The quality of zinc coating on steel depends on the physical and chemical nature of zinc-ironintermetalic layers formed. Other elements, which exist in the bath either as alloy additions or remnants of galvanizing operations, have a strong effect on the formation kinetics and thermodynamic stability of all intermetallics. Sebisty [2] measured the effects of additives like Ag, Co, Mg, Th, U, Si, Ti, V, Ni, Cr, Zr, and Mn on the steel weight loss at 460 °C. When no additive, the original steel weight loss was 27,8 g/m^2. By adding 0,5 % Zr, 0,5 % Mn, 0,2 % Ni, 0,1 % V, 0,05 % Ti, 0,2 % Cr, or 0,05 % Si the correspondig steel weight loss was rapidly reduced to 23,4; 22,8; 22,3; 23,8; 25,8; 21,2; and 26,8 g/m^2, respectively. His results showed that Zr, Mn, Ni, V, Ti, Cr, and Si were effective in reducing iron weight loss, and others either increased (like Ag, Co, and Mg) or had minor effects (like U and Th) on iron weight loss. The aim of this paper is to analyze a relation between chemical element properties and their effects on the steel weight loss by using the theory of formal concept analysis.

FORMAL CONCEPT ANALYSIS

Formal concept analysis mathematically is founded on the assumption that with every object of the universe of discourse we associete some information (data, knowledge). Given a data set which characterizes various materials, arrange the data into objects (rows) that consist of a material and a set of attributes. Next, create a table whose columns contain the attributes and whose rows contain the objects. The table is the universe in which the analysis is conducted. Note that as in statistics, the larger and more representative the data set, the more profound the analysis that results. Various attributes can be considered as outputs and others as inputs, which, when changed, affect the outputs.

Formal concept analysis is a new mathematical approach to data analysis and data mining and has found many interesting applications. The main advantage of this theory is that it does not require any preliminary or additional information about the data to be analyzed, un-

J. Klimeš, Faculty of Applied Informatics, Tomas Bata University in Zlin, Czech Republic

like probability in statistics and grade of membership or the value of possibility in fuzzy set theory. This theory has been successfully applied in many real-life problem in medicine, pharmacology, engineering, financial and market analysis and others. There are many applications in medicine and pharmacology where the analysis of relationships between the chemical structure and the antimicrobial activity has been investigated.

Formal concept analysis applications to materials reseaarch provides a new algorithmic method for autonomous discovery of relations between material properties and/or proccessing conditions, which can be useful in designing new materials and/or their associated processing conditions (cf. [3]). Application of this theory requires suitable software. Assume we have a group of compounds comprised of elements from the periodic table. The compounds can be organized in many ways using the periodic table as a reference, e.g. by group number and by period number. Formal concept analysis (FCA) was invented by Rudolf Wille in the early 80s.

The basic notions of FCA are described in this section but without their mathematical details, which can be found in [4]. A central notion of FCA is a duality called a Galois connection. This duality can often be observed between two types of items that relate to each other in a application, such as objects and attributes. The elements of one type are called formal objects, the elements of the other type are called formal attributes. The adjective formal is used to emphasize that these are formal notions. The sets of formal objects and formal attributes together with their relation to each other form a formal context, which can be represented by a cross table. Starting with any set of formal objects one can identify all formal attributes which they have in common.

This pair of a set of formal objects an a set of formal attributes that is closed in this manner and called aformal concept. An important advantage of FCA is that the Galois connections and the set of formal concepts can be visualized by a so-called line diaagram of a concept lattice. A concept lattice consists of the set of concepts of a formal context and the subconcept-superconcept relation between the concepts (cf. [4] for the mathematical details). This relation is represented by edges in the line diagram. The top (the least element) and bottom (the greatest element) concepts in a concept lattice are special. The top concept has all formal objects in its extension. Its intension is often empty but does not need to be empty. The bottom concept has all formal attributes in its intension. The top concept can be thought of as representing the universal concept and the bottom concept the null or contradictory concept of a formal context.

Visualisation of concept lattices are only of interest if they are not too messy to be comprehensible for a human user. A single concept lattice of large sets of objects and attributes can become fairly large and complex. The set of formal objects of a formal concept is called its extension; the set of formal attributes its intension. For a given formal context, the formal concepts, their extensions and intensions are uniquely defined and fixed.

ACHIEVED RESULTS AND THEIR ANALYSIS

In [2] is measured the effect of additives like Zr, Mn, Cr, Ni, Ag, Co, Mg, Th, and U on the steel weight loss in the galvanizing rimmed steel. For a given chemical elements to develop the relation data were obtained for the following three factors:

(i) Atomic number
(ii) Entropy of solid /kJ(kg·K)
(iii) Melting point /K

as shown in Table 1.

We now have the chemical elements, atomic numbers-A, entropy-E, and melting points-M. To keep the complexity of the example to a reasonable level, we will consider the scaling of the above three factors (i)-(iii) by the following attributes: **a-l.** This choice of attribute results is a rather poor classification. The problem one has with such methods is determing the type of the transformation of the numeric data into meaningful symbols. According to Wille [4], we can now use conceptual scaling process for this attributes. Typical conceptual scales are nominal scales, ordinal scales and interval scales. The results of scaling are shown in Table 2.

Table 1. **Additivess on the steel weigt loss in the galvanizing process**

Chemical elements	Ag	Co	Mg	Th	U	Zr	Mn	Cr	Ni
A-Atomic number	47	27	12	90	92	40	25	24	28
E-Entropy of solid	42,71	30,06	32,7	53,42	50,36	38,89	32,09	23,86	29,89
M-Melting point	1234	1768	922	2028	1405	2125	1517	2130	1725

Table 2. **Scaling of attributes of chemical elements**

Attributes of elements	a	b	c	d	e	f
Belongs into the interval	A 1-19	A 20-39	A 40-59	A 80-99	M 500-999	M 1000- 1499
Attributes of elements	**g**	**h**	**i**	**j**	**k**	**l**
Belongs into the interval	M 1500	M 2000-	E 20-29	E 30-39	E 40-	E 50-59

An interval scale as shown in Table 2 is suitable for formal attribute which have a range of possible values. Now that we have created these various data sets, we must use them to generate some useful output that tells us something about the dependency we are seeking to explore. As illustrated in Table 2 for a given set of formal objects G = {Ag, Co, Mg, Th, U, Zr, Mn, Cr, Ni} we have obtained the set of formal attributes M = {**a, b, c, d, e, f, g, h, i, j, k, l**}. If we gather together these two sets, we can create a cross table with rows- the set of formal objects, columns- the set of formal attributes, and the incidence relation between them. The resulting model for the using of formal concept analysis is presented in Table 3, where the incidence relation betwen objects and attributes is denoted by R.

The formal context, which is represented by this cross table (Table 3) is a triple (G, M, R), where G and M are sets of objects and attributes, respectively, and R is a relation between G and M. This is indicated by crosses. It was the idea of Wille [4] to combine in a first step objects, attributes and the relation R via the cross tables.

For defining the formal concepts, we need the following derivation operators defined for arbitrary set X of objects G and arbitrary set Y of attributes M, respectively, by the following way: X′ = {y in M: xRy for all x in X}, and Y′ = { x in G: xRy for all y in Y}. Then X′ gives us all the common attributes of the chemical elements contained in X, and Y′ gives us the common chemical elements of the attributes contained in Y.

A concept is a pair (X, Y) - a set of objects (the extent) and a set of attributes (the intent) such that X = Y′ and Y = X′. In other words, a concept is a maximal collection of objects sharing common attributes.

Table 3. **Cross table of a formal context**

R	**a**	**b**	**c**	**d**	**e**	**f**	**g**	**h**	**i**	**j**	**k**	**l**
Ag			x			x					x	
Co		x					x			x		
Mg	x				x					x		
Th				x				x				x
U				x		x						x
Zr			x					x		x		
Mn		x					x			x		
Cr		x						x	x			
Ni		x					x		x			

If one starts with Cr and Ni one obtains **b** and **i** and then no further objects or attributes because no other formal objects have both these formal attribute. Thus ({Cr, Ni}, {**b**, **i**}) form a formal concept and ({Th, U}, {**d**, **l**}) form a different formal concept. In Table 3, the formal concepts are the maximal rectangles. By this way we can obtained all formal concepts of a given context.

Application of formal concept analysis requires suitable software. The inhouse FCA software was applied to compute all the expected concepts. The data in Table 3 was input into the Toscana software. The purpose of the Toscana software is to facilitate interactive exploration of such concepts and their line diagrams. The results are shown in Table 4.

Table 4. **Formal concepts of a formal context**

top	({all elements}, Ø)
C1	({Ag}, {c, f, k})
C2	({Co}, {b, g, j})
C3	({Mg}, {a, e, j})
C4	({Th}, {d, h, l})
C5	({U}, {d, f, l})
C6	({Zr}, {c, h, j})
C7	({Mn}, {b, g, j})
C8	({Cr}, {b, h, i})
C9	({Ni}, {b, g, i})
C10	({Ag, U}, {f})
C11	({Ag, Zr}, {c})
C12	({Co, Mn}, {b, j})
C13	({Th, U}, {d,l})
C14	({Cr, Ni}, {b, i})
C15	({Co, Mn, Ni}, {b, g})
C16	({Co, Zr, Cr}, {h})
C17	({Co, Mg, Zr, Mn}, {j})
C18	({Co, Mn, Cr, Ni}, {b})
bottom	(Ø , {all attributes})

Table 4 proposed two groups of elements which may help to reduce the steel weight loss {Co, Mg, Zr, Mn} and {Co, Mn, Cr, Ni}. Co was the only element that was included in these groups but was observed increasing the steel weight loss. Melting temperatures of chemical elements reported in [5] were used in this study. Since the element melting temperature, which is strongly related to its self-diffusion parameter, has been identified as one of the most important factors on the steel weight loss, it is suggested that the formation of iron-zinc intermetallics in galvanizing may be a diffusion controlled process.

CONCLUSIONS

By using an artificial intelligent software for formal concept analysis, the additive efect on steel weight loss in galvanizing was investigated to three additive chemical properties. It is suggested that diffusion of additives may be a key control factor in the formation of iron-zinc intermetallics. The developed correlation was in good agreement with available experiments (cf. [2]) and results in [6], except the case of Co. This formal concept analysis approach may also help to design new alloys as additives in the galvanizing process (cf. [3]).

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Note: The responsible translator for English language is Ing. Anežka Lengálová, Ph.D., Institute of Languages, Thomas Bata University in Zlin, Czech republic