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RESEARCH ARTICLE

ASSESSMENT OF CHANGES IN VOLUME OF NICKEL COMPOUNDS INTERACTING WITH THE CHEMICAL ELEMENTS

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ABSTRACT

Based on the density reference data of substances in the condensed state the results of concentration of electrons calculations (C electron, mole/cm3) and the coefficient of consolidation (K consolidation) for initial chemical elements and their binary compounds with nickel have been presented. The purpose of the present work is to reveal the possibility of using the normalized value of the volume change as the characteristics, which allows to estimate the intensity of interaction between dissimilar atoms and the concentration of electrons as the structural characteristics of the materials. A correlation was established between the melting point, the elastic properties and the calculated characteristics for a number of Laves phases. For binary nickel compounds as example shown the possibility of using the calculations based on change the volume of compounds to predict the properties of substances.

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INTRODUCTION

Chemical interactions and phase transitions are traditionally characterized by thermodynamic parameters and state diagrams. Substance transformations are accompanied by thermal effects and volume changes. Density which is an important characteristics of substances is the result of two factors: 1) mass which is concentrated in the atomic nuclei and 2) volume which is formed by electron shells. The formation of a new substance structure is determined by the interaction of the atomic electron shells and molecules. Thermal processes are considered in sufficient detail in numerous papers on chemical thermodynamics, but there is not enough information as for the change of volume. 3 In the papers (Molchan and Fertikov, 2011, 2015, 2016) the normalized value of the volume change during chemical reactions (coefficient of consolidation) which is correlated to the thermodynamic characteristics is presented. Since the volume is formed by electrons, such value as "concentration of electrons" is introduced which can be used as the structural characteristics of the material. The purpose of the present work is to reveal the possibility of using the normalized value of the volume change as the characteristics, which allows toestimate the intensity of interaction between dissimilar atoms and the concentration of electrons defined in terms of mole / cm3 as a value that allows to estimate the structure of the material.

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MATERIALS AND METHODS

In the papers (Molchan and Fertikov, 2015, 2016) the formula for determining the concentration of elemental substances electrons on the basis of reference data (JCPDS PCPDFWIN, 2002; NPO «Professional», 2007; Babichev *et al*., 1991) according to their density in the condensed state is presented:

$$C_{electron} = \frac{d}{M} Z \qquad (1)$$

Where
$C_{electron}$ is for the concentration of electrons in a unit of volume, mole/cm^3;
D is for substance density in the condensed state, g/cm^3;
M is for molecular weight, g/mole;
Z is for the ordinal number of the element in the Periodic table.

For chemical compounds the electron density is determined through the following expression:

$$\boldsymbol{C_{electron} = \frac{number\ of\ electrons\ in\ compound\ (in\ one\ mole)}{volume\ of\ mole\ of\ compound\ (condenced\ state)}} \qquad (2)$$

A_aB_b type compound has a concentration of electrons

$$C_{electron} \approx \frac{a Z_A + e Z_B}{M/d} \qquad (2a),$$

Where
a is for the subscript of element A,
ZA is for the ordinal number of element A,
B is for the subscript of element B,
ZB is for the ordinal number of the element B,

Metal alloys are not simple mixture of various components, but represent different chemical compounds of the elements forming the alloy. To estimate the depth of interaction between atoms it is convenient to compare the volumes of substances before the reaction (*Vcomponent*) and the volumes of substances after the reaction (*Vproduct*). The value obtained is then standardized to the finished product volume. The result (in %) characterizes the change in the volume of the substances in the course of reaction. This value can be designated as a coefficient of consolidation:

$$K_{consolidation.} = \left(\frac{\Sigma V_{компон.} - V_{прод.}}{V_{прод.}} \right) \times 100\% \quad (3)$$

The coefficient of consolidation be positive or negative. It means that the reaction product may have a volume which is smaller than the sum of volumes of the initial elements, and can be greater than the sum of the initial volumes (loosening of the electron shells).

RESULTS

In the paper (Martin, 2007) a table for a number of the Laves phases with the indication of elastic characteristics is presented. In the presented Table 1 columns 1 - 5 are filled by Thoma (unpublished data from F. Chu and D.J. Thoma), and columns 6 and 7 are filled with data by the formulas (2a) and (3) given above in the present work. Having performed the correlation analysis of the presented data, we see that for 15 pairs the critical correlation coefficient at a confidence level of 0.95 is equal to 0.51 (Muller *et al*., 1979).

- The coefficient of correlation between thes hear modulus and Young's modulusis 0.99.
- The coefficient of correlation between the shear modulus and bulk modulus is 0.57.
- The coefficient of correlation between the shear modulus and the melting point is 0.89.
- The coefficient of correlation between the Young's modulus and bulkmodulus is 0.64.
- The coefficient of correlation between the Young's modulus and coefficient of consolidation is 0.86.
- The correlation coefficient between the bulk modulus and the melting point is 0.53.
- The correlation coefficient between the bulk modulus and the concentration of electrons is 0.52.
- The correlation coefficient between the melting point and the concentration of electrons is 0.56.
- From presented data on a number of Laves phase, it can be claimed that interrelation between the properties, coefficient of consolidation and presented structural characteristics i.e. "concentration of electrons" exists and should be taken into account.

The value of coefficient of consolidation with the plus sign "+" indicates that the formation of compounds took place with the compression of the electron shells of the initial components, and the value with minus sign "-" indicates a reverse process - the loosening of the electron shells. Table 2 presents the characteristics of the chemical elements interacting with nickel, and the compounds formed as a result.

DISCUSSION

The lack of correlation dependence between the coefficients of consolidation and the thermodynamic characteristics for the nickel halides gives reason to doubt the correctness of existing reference data on the density of these chemical compounds, since the data series for the thermodynamic parameters (Lidin *et al*., 2006) is logical. According to calculated data from Table 2 it is evident that iron, chromium and vanadium do not dissolve in nickel. Silicon strongly interacts with nickel. Such harmful impurity elements in nickel alloys as bismuth, calcium, sulfur, phosphorus, selenium and tin strongly interact with nickel. Molybdenum alloying element weakly interacts with nickel.

Table 1. Elastic properties and melting points of a number of Laves phase

1	2	3	4	5	6	7
substance	G (GPa) shear modulus	E (GPa) Young's modulus (of elasticity)	B (GPa) bulk modulus of elasticity	$T_{melt.}$ (ºC) melting points	$K_{consolidation.}$ % coefficient of consolidation	$C_{electron.}$ mole/cm^3 concentration of electrons
HfV_2	32	79	110	1550	-1.3	3.87
$NbCr_2$	80	215	229	1730	-2.0	3.44
$HfCo_2$	78	209	229	1670	7.3	5.06
$TaCr_2$	88	232	220	2020	0.2	4.77
$ZrCr_2$	65	204	157	1677	2.2	3.15
$HfCr_2$	73	188	153	1825	-2.7	4.36
$TiCr_2$	79	204	165	(1370)*	-0.4	2.78
TiAl	74	181	110	(1453)	6.6	1.82
Ti_3Al	57	146	106	(1164)	3.8	1.97
Ni_3Al	92	238	190	(1360)	5.6	3.44
NiAl	70	183	156	1638	14.3	2.82
$NbSi_2$	153	363	192	1940	28.0	2.59
$TaSi_2$	151	359	192	2040	30.6	3.87
$MoSi_2$	186	431	213	2020	34.2	2.88
Mo_5Si_3	127	325	243	2180	14.6	3.53

*Within the brackets you can find the limit of stability.

Table 2. Binary compounds of Nickel

Elements and compounds	$C_{electron,}$ mole/cm^3	$K_{consolidation,}$ %	Elements and compounds	$C_{electron,}$ mole/cm^3	$K_{consolidation,}$ %
Ni	4.25		Mo	4.47	
H	0.075		Mo Ni_4	4.39	+1.8
Ni_2H	3.81	+67.6	NiMo	4.42	+0.8
$NiH_{1.11}$	3.68	+171	Ni_3Mo	4.40	+1.8
Be	0.82		Cd	3.69	
$Be_{21}Ni_5$	1.84	+1.3	Cd_5Ni	3.80	+1.4
BeNi	2.91	+4.5	In	3.12	
B	1.08		$InNi_2$	4.30	+18.2
Ni_3B	3.89	+6.6	Ni_4In	4.25	+11.2
Ni_2B	3.83	+10.3	Sn	2.46	
NiB	3.42	+13.7	Ni_3Sn	4.31	+29.1
Ni_4B_3	3.56	+10.9	NiSn	3.98	+37.4
C	1.80		Ni_4Sn	4.21	+21.3
Ni_3C	3.87	-0.7	Sb	2.80	
N	0.71		NiSb	3.93	+23.4
Ni_4N	3.76	+14.6	Te	2.81	
Ni_3N	3.80	+23.7	NiTe	3.70	+16.2
O	1.27		Ni_3Te_2	3.27	+5.3
NiO_2	3.59	-4.1	I	2.06	
NiO	3.28	+17.7	NiI_2	2.49	+9.5
F	0.93		La	2.52	
NiF_2	2.30	+29.7	La_2Ni_3	3.34	+9.7
Mg	0.86		$LaNi_5$	3.77	+6.4
$MgNi_2$	2.84	+13.5	LaNi	3.04	+4.4
Mg_2Ni	1.67	+11.0	$LaNi_3$	3.76	+13.0
Al	1.30		Ce	2.80	
Al_4Ni_3	2.43	+6.9	$CeNi_2$	4.05	+7.0
AlNi	2.82	+14.3	$CeNi_3$	3.98	+2.9
$AlNi_3$	3.44	+5.4	CeNi	3.27	-10.7
Ni_5Al_3	3.17	+11.4	Pr	2.84	
Al_3Ni_2	2.25	+2.1	NiPr	3.31	+4.3
Al_3Ni	1.91	+4.3	Ni_5Pr	3.91	+5.8
Si	1.19		Nd	2.91	
NiSi	2.86	+25.0	Nd_2Ni_7	3.62	+0.2
Ni_2Si	3.79	+35.3	NdNi	3.39	+4.7
P	1.40		$NdNi_5$	3.94	+5.6
Ni_2P	3.52	+18.3	Sm	3.12	
Ni_3P	3.74	+15.1	NiSm	3.56	+4.9
NiP	2.81	+12.8	Eu	2.17	
S	1.06		$EuNi_5$	4.05	+23.8
Ni_3S_2	2.83	+21.7	Gd	3.20	
NiS	2.68	+31.1	Gd_3Ni	3.41	+3.4
Cl	1.01		Gd_2Ni_7	4.13	+9.9
$NiCl_2$	1.68	+9.1	$GdNi_3$	4.18	+12.4
Ca	0.77		GdNi	3.71	+7.2
$CaNi_5$	3.18	+16.9	Tb	3.37	
Ca_2Ni_7	3.00	+24.5	Tb_3Ni	3.57	+3.2
$CaNi_3$	2.61	+26.9	$TbNi_2$	4.35	+16.7
Ca_2Ni_5	2.64	+24.5	NiTb	3.83	+6.7
Sc	1.41		Dy	3.47	
NiSc	2.75	+20.4	Dy_3Ni_2	3.83	+5.7
$ScNi_5$	3.69	+9.7	DyNi	3.91	+6.4
Sc_2Ni_7	3.57	+14.1	$DyNi_5$	4.22	+6.5
Sc_2Ni	2.09	+8.6	Ho	3.58	
Ni_2Sc	3.08	+12.4	$HoNi_3$	4.36	+11.1
Ti	2.07		HoNi	3.99	+6.3
TiNi	3.04	+4.8	Ni_5Ho	4.22	+5.4
Ni_3Ti	3.77	+8.1	Er	3.68	
$NiTi_2$	2.64	+2.1	Er_3Ni_2	3.99	+5.3
V	2.75		$ErNi_3$	4.41	+11.2
NiV_3	3.08	+0.5	ErNi	4.09	+7.0
Ni_2V	3.18	-13.2	$ErNi_5$	4.26	+5.6
Cr	3.31		Tm	3.81	
Cr_3Ni_2	3.58	-2.2	Ni_3Tm	4.47	+10.9
Fe	3.66		NiTm	4.18	+6.7
$FeNi_3$	4.10	+0.1	Yb	2.82	
Cu	4.07		Ni_7Yb_2	4.37	+24.7
$Cu_{3.8}Ni$	4.11	+2.0	$NiYb_3$	3.79	+29.1
$Cu_{0.81}Ni_{0.19}$	4.12	+0.5	Lu	3.99	
Zn	3.28		LuNi	4.35	+7.3
$NiZn_3$	3.66	+5.7	Hf	5.34	
NiZn	3.93	+6.8	Hf_3Ni_7	5.10	+7.2
Ga	2.62		$HfNi_3$	5.01	+6.8
Ga_3Ni_5	4.06	+19.2	HfNi	5.10	+2.3
$NiGa_4$	3.37	+19.5	Ta	6.70	
Ga_4Ni_3	3.72	+20.0	NiTa	4.76	+2.0

Continue……..

Ge	2.35		Hg	5.41	
Ni_3Ge	4.22	+21.7	NiHg	6.41	+27.1
$GeNi_2$	4.11	+25.5	Hg_4Ni	5.31	+0.4
As	2.52		Bi	3.90	
NiAs	3.55	+14.5	β-BiNi	4.77	+19.8
$NiAs_2$	3.28	+14.5	Th	4.15	
Se	2.06		Ni_2Th	4.64	+11.0
Ni_3Se_2	3.32	+15.3	NiTh	4.48	+7.6
NiSe	3.33	+23.9	$Ni_{17}Th_2$	4.40	+4.4
$NiSe_2$	2.97	+22.3	U	7.36	
Br	1.36		Ni_5U	4.94	-3.2
$NiBr_2$	2.28	+35.2	Ni_2U	5.59	-2.9
Y	1.96		Np	8.02	
Ni_2Y_3	2.40	+14.3	$NpNi_2$	5.53	-7.9
NiY_3	2.17	+3.3	Pu	7.64	
Ni_3Y	3.50	+13.0	NiPu	5.24	-18.8
Ni_5Y	3.22	+7.3	$PuNi_2$	5.50	-6.5
Zr	2.85		$PuNi_5$	4.75	-8.1
Zr_2Ni_7	3.91	+5.0	Am	5.34	
$NiZr_2$	3.11	-0.4	$AmNi_2$	5.87	+20.6
NiZr	3.39	+2.7			
Nb	3.78				
NbNi	4.03	+2.2			
Ni_3Nb	4.63	+13.7			
Ni_8Nb	4.23	+1.6			

Conclusion

1. The results of the normalized characteristics of volume change in binary compounds of nickel have been presented.
2. It has been suggested to use density, as one of the values that can characterize the interaction of atoms in the condensed system to estimate the properties of substances.
3. Coefficients of consolidation may be used as the relative chemical potentials for the constituents of the chemical compounds.
4. It has been suggested to use the value of the concentration of electrons for element or compound, defined in terms of mole/cm^3, as the structural characteristics of the material.
5. It has been suggested to use coefficient of consolidation to estimate the degree of interaction of initial components during the compound formation.

REFERENCES

Babichev A., Babushkina N., Bratkovsky A. *et al*. 1991. Fizicheskie velichini. Spravochnik [Physical quantities. Reference book], Energoatomizdat, Russia. International Centre for Diffraction Data. *JCPDS PCPDFWIN*. 2002. V.2.03.

Lidin R., Andreeva L. and Molochko L. 2006. Konstanti neorganicheskikh veshchestv. Spravochnik [The constants of inorganic substances. Reference book], Drofa, Russia.

Martin J.W. 2007. Concise Encyclopedia of the Structure of Materials, Elsevier Ltd., Netherlands, p. 245.

Molchan N.V. and Fertikov V.I. 2011. Compressibility of Substances and Dimensions of Atoms. *Material Science*, 6: 2-6.

Molchan N.V. and Fertikov V.I. 2015. Determination of Concentration of Electrons for Description of the Structure of Materials, with Sulfides as an Example. *Journal of Materials Sciences and Applications*, 2(1): 38-44.

Molchan N.V. and Fertikov V.I. 2016. Interrelation of Thermodynamic Parameters and Structural Characteristics, with Halides of Groups 1 and 2 Elements as an Example. *American Journal of Chemistry and Application*, 5(3): 28-32.

Muller P., Neumann P. and Storm R. 1979. Tafeln der mathematischen Statistik, VEB Fachbuchverlag, Germany. 10

Noviy spravochnik khimika i tekhnologa. Osnovnie svoistva neorganicheskikh, organicheskikh i elementorganicheskich soedinenii [The new reference chemist and technologist. Key properties of inorganic, organic and element organic compounds], NPO «Professional», Russia, 2007

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