Correlation of Bulk Modulus and the Constituent Element Properties of Binary Intermetallic Compounds

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The correlation between the bulk modulus B and the atomic properties of binary intermetallics (element molar volume and element valence electron density) is studied using literature data of 240 binary intermetallic compounds and alloys. It is found that the bulk modulus of binary systems may be predicted (with an average error limit of ±11%) by $B = n_{ws}^2 V$, where n_{ws} and V are estimates from elemental valence electron density and molar volume, respectively.

1. Introduction

Intermetallic compounds are of interest to scientists and engineers because of their superior structural, electrical, chemical, and mechanical stability at high temperature.[1−5] They are candidate materials not only for the next generation of efficient turbines and engines,[1,2,6] but also for new microelectronic systems.[4,5] The elastic constant (bulk modulus or shear modulus) is an important mechanical property in the design and selection of materials. The bulk modulus of intermetallics is less sensitive to thermophysical processing histories or microstructural properties. Because it is a measure of the intrinsic interatomic force, it is often used to estimate interatomic potentials used in computer simulations.

Although elastic constants for a number of binary intermetallic compounds and alloys[7−14] have been published, many have not, especially for those compounds with high melting temperature. Thus, it is important to predict or estimate the elastic constants for either theoretical study or industrial applications. Grammatickake[15−17] and Varotsos[18,19] used the thermodynamical model developed by Varotsos and Alexopoulos[20] to explain the elastic properties of substitutional alloys:

$$B = B_A[1 + x(V_B/V_A - 1)]/[1 + x(B_A V_B/B_B V_A - 1)] \quad (1)$$

where B, B_A, and B_B are the bulk moduli of alloy $A_{1-x}B_x$, consisting of metal A and metal B, respectively; V_A and V_B are the molar volumes of metal A and metal B. Normally, good agreement with experiment is reached in dilute substitutional alloy systems where the volume change after mixing is proportional linearly to the atomic fraction of the alloy. By the well-known Vegard's law, Giri obtained the following expression:[21]

$$B = [(1 - x)a_A B_A + x a_B B_B]/a \quad (2)$$

where B, B_A, and B_B have the same definitions as above; a, a_A, and a_B are lattice constants for alloy $A_{1-x}B_x$, metal A, and metal B, respectively. Reasonable agreement can be obtained when alloy $A_{1-x}B_x$ has the same crystal structure with the constituent metal A and metal B. In another study, Cohen[22] proposed a simple empirical model which can accurately predict bulk modulus for covalent solids; using this model, a new superhard material (β-C_3N_4) is predicted and synthesized. However, investigations focused on the bulk modulus of engineering materials have scarcely been performed with the empirical approach, especially for intermetallic compounds.

In this paper, starting from either Miedema's model[23] of alloys or Cho's model[24] with regards to bulk electron concentration, we derive a simple empirical model by

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Table 1. The Value of *B*, *V*, and n_{ws} of 73 Elements

atom	*B* (Gpa)	n_{ws} (e/au^3)	volume (10^{-6} m^3)	$(B/V)^{1/2}$	atom	*B* (Gpa)	n_{ws} (e/au^3)	volume (10^{-6} m^3)	$(B/V)^{1/2}$
Li	11.6	0.94	13.00	0.94	Th	54	2.10	19.80	1.65
Na	6.8	0.55	23.78	0.53	Lu	47.6	1.91	17.77	1.64
K	3.2	0.27	45.63	0.26	Tm	44.5	1.86	18.12	1.57
Rb	3.1	0.22	56.07	0.24	Er	44.4	1.86	18.45	1.55
Cs	1.57	0.17	69.23	0.15	Y	41.2	1.77	19.90	1.44
H	0.2	3.38	1.70	0.34	Dy	40.5	1.82	19.00	1.46
Be	110	4.66	4.90	4.74	Ho	40.2	1.82	18.76	1.46
Zn	69.4	2.30	9.17	2.75	Tb	38.7	1.82	19.32	1.42
Cd	51	1.91	13.00	1.98	Gd	37.9	1.77	19.90	1.38
Hg	38.2	1.91	14.08	1.65	Sm	37.8	1.77	20.01	1.37
Mg	35.6	1.60	14.00	1.59	Pm	33	1.77	20.25	1.28
Ca	17.2	0.75	26.2	0.81	Nd	31.8	1.73	20.58	1.24
Sr	12	0.59	33.93	0.59	Yb	30.5	1.86	17.97	1.30
Ba	10.2	0.53	38.1	0.52	Pr	28.8	1.73	20.79	1.18
B	178	5.36	4.70	6.15	La	27.9	1.64	22.55	1.11
Al	75.2	2.70	10.00	2.74	Ce	21.5	1.69	21.62	1.00
Ga	56.9	2.25	11.82	2.19	Eu	14.7	1.77	19.97	0.86
In	41.1	1.60	15.75	1.62	Hf	109	3.05	13.45	2.85
As	38.3	3.00	11.85	1.80	Ti	108	3.51	10.58	3.20
Sb	38.3	2.00	16.95	1.50	Zr	89.8	2.8	14.00	2.53
Bi	31.5	1.56	19.32	1.28	Au	171	3.87	10.20	4.09
P	30.4	4.49	8.60	1.88	Cu	138	3.18	7.12	4.40
Tl	28.5	1.40	17.23	1.29	Ag	104	2.52	10.25	3.18
N	1.2	4.49	4.10	0.54	Ta	196	4.33	10.81	4.26
C	443	5.55	3.25	11.68	Nb	170	4.41	10.80	3.97
Si	98	3.38	8.60	3.38	V	158	4.41	8.36	4.35
Ge	77.2	2.57	9.87	2.80	U	97.9	3.44	13.15	2.73
Sn	58.2	1.90	16.30	1.89	Pt	276	5.64	9.10	5.51
Pb	45.8	1.52	18.28	1.58	Pd	187	4.66	8.90	4.58
Pu	76	2.99	12.06	2.51	Ni	177	5.36	6.60	5.18
Sc	56.6	2.05	15.03	1.94	Ir	371	6.13	8.52	6.60
Th	54	2.10	19.8	1.65	W	311	5.93	9.55	5.71
Lu	47.6	1.91	17.77	1.64	Rh	276	5.45	8.30	5.77
Tm	44.5	1.86	18.12	1.57	Mo	261	5.55	9.40	5.27
Er	44.4	1.86	18.45	1.55	Co	182	5.36	6.70	5.20
Y	41.2	1.77	19.90	1.44	Cr	160	5.18	7.23	4.71
Dy	40.5	1.82	19.00	1.46	Os	373	6.33	8.45	6.64
Ho	40.2	1.82	18.76	1.46	Ru	286	6.13	8.20	5.91
Tb	38.7	1.82	19.32	1.42	Fe	166	5.55	7.09	4.84
Gd	37.9	1.77	19.90	1.38	Re	334	6.33	8.85	6.14
Sm	37.8	1.77	20.01	1.37	Mn	92.6	4.17	7.35	3.55
Pm	33	1.77	20.25	1.28	Tc	281	5.93	8.64	5.70
Sc	56.6	2.05	15.03	1.94					

using literature data. This model may be used to predict or estimate the bulk modulus of binary intermetallic compounds and alloys.

2. Bulk Modulus for Pure Elements

Miedema[23] proposed an empirical model for the prediction of alloy formation enthalpy. In this model, two semiempirical physical parameters, the work function ϕ, and the electron density n_{ws} are used for each element. The work function ϕ has about the same meaning as the electronegativity. The second parameter, n_{ws}, is defined as the electron density at the boundary of Wigner−Seitz cell. For nontransition metals, it is obtained by summation of electron densities of free atoms, while for transition metals, it is derived from bulk modulus data. A nice linear relationship between n_{ws} and $(B/V)^{1/2}$ was presented by Miedema for Al, Cu, Fe, and five alkali metals,[23] where *B* and *V* are the bulk modulus and the molar volume of the elements, respectively. To extend this correlation beyond the above 8 elements, another 73 metal and semimetal elements are selected for testing. Their values of *B*, *V*, and n_{ws} are listed in Table 1.

Figure 1 illustrates a very good linear relationship between n_{ws} and $(B/V)^{1/2}$ for all except H, N, P, and C.

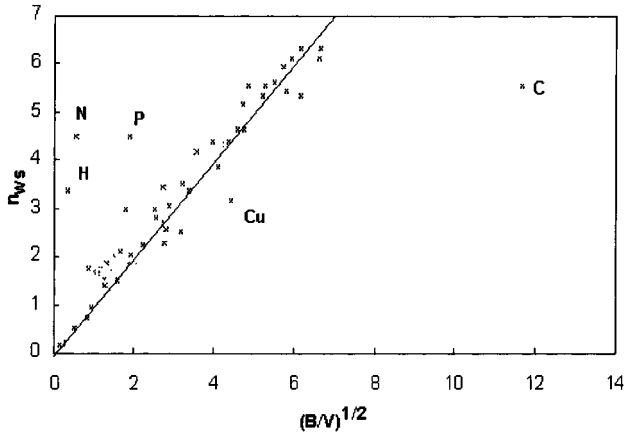

Figure 1. The linear relationship between n_{ws} and $(B/V)^{1/2}$ of 73 elements, n_{ws} in arbitrary density units [electron/(au)^3], *B* in Gpa, and *V* in 10^{-6} m^3 per mole.

This relationship can be expressed:

$$n_{ws} = (B/V)^{1/2} \tag{3}$$

The abnormity for H, N, P, and C elements may result from their typical covalent features. The elements As, Cu, Fe, P, and U also deviate to some extent from the empirical regularity. The effect of this deviation to the

bulk modulus of binary alloys containing these elements will be discussed later.

3. Bulk Modulus for Binary Systems

As mentioned above, a good linear relationship between n_{ws} and $(B/V)^{1/2}$ exists for metal or semimetal elements. Can this rule be extended to binary intermetallic compounds and alloys? If so, how are the electronic density n_{ws} and molar volume V estimated? An answer may be found by applying Miedema's semiempirical or macroscopic atom model,[23] where atoms are considered "blocks" of the elements and compounds or alloys are considered "piles" of the blocks. As an example, consider an intermetallic compound $A_{1-x}B_x$ that is formed by atom A (with the electronic density n_{wsA} and the molar volume V_A) and atom B (with the electronic density n_{wsB} and the molar volume V_B). The total valence electron numbers N contained in (1-x) mole element A and x mole element B can be obtained by Vegard's Law:

$$N = n_{wsA}V_A(1 - x) + n_{wsB}V_Bx \qquad (4)$$

The molar volume V of compound $A_{1-x}B_x$ can be predicted by Miedema's model.[23] Suppose that the total valence electron numbers N remain unchanged after compound $A_{1-x}B_x$ is formed. Then the "electron density" of compound n_{ws} can be obtained by the following equation:

$$n_{ws} = N/V = [n_{wsA}V_A(1 - x) + n_{wsB}V_Bx)]/V \qquad (5)$$

Table 2 lists the value of bulk modulus B, calculated molar volume V, total valence electron numbers N, calculated bulk modulus B_{cal}, and their prediction errors for 240 binary compounds and alloys. The values of ΔH, E, and B_{cal}' are also listed in this table; their definitions will be given later. The values of bulk modulus for these compounds and alloys are obtained from the literature.[7−14]

Figure 2 illustrates the relationship between n_{ws} and $(B/V)^{1/2}$ of these compounds and alloys. From this figure, a good linear relationship can be obtained for binary metal systems. A linear fit between n_{ws} and $(B/V)^{1/2}$ of 69 metallic or semimetallic elements is also drawn in this figure. It is astonishing that the linear relationship for binary compounds is the same as for pure elements. The relationship can be expressed in eq 3, or it can be rewritten in eq 6; bulk modulus can also be estimated using this equation:

$$B = {n_{ws}}^2V \qquad (6)$$

In Table 2 and Figure 2, the prediction using eq 6 is close to the reported value with an average error limit of ±11%.

Of special interest are the intermetallic compounds or semiconductor compounds whose chemical constitution is near 50at. %; for example, No7 ($Al_{51}Co_{49}$), No19 (Al_2Zr), No60 (NiAl), No177 (ZnS), and No180 (CdS) in Table 2. Their prediction errors are about 30% or more. Elastic constants are determined by the derivative of free energy with respect to strain. All factors that contribute to the total energy may add on to the elastic constant. Compounds whose atomic ratio of constituent elements is close to 1 show a large enthalpy of formation (or called heat of formation). Therefore, the volume change after mixing may not be linearly proportional to the chemical constituent. To predict the bulk modulus more accurately, the enthalpy change (or short-range ordering) should be included. According to Miedema's model, cohesive enthalpies of intermetallic compounds E, consist of two parts: the average value of cohesive energy of constituent elements E_{AB} and the additional formation enthalpy ΔH. For compound $A_{1-x}B_x$, this cohesive enthalpy is defined as

$$E = \Delta H + E_{AB} = \Delta H + (1 - x)E_A + xE_B \qquad (7)$$

where E_A, E_B, and E_{AB} are cohesive energy of metal A, metal B, and their linear summation, respectively. The formation enthalpy ΔH can be predicted by Miedema's model.[23] In eq 6, the contribution of the formation enthalpy to bulk modulus is not considered; this may result in a larger prediction error for compounds whose formation enthalpy can no longer be neglected. Therefore, the contribution of formation enthalpy ΔH to bulk modulus has to be calculated.

Total bulk modulus can be expressed as

$$B = B_1 + B_2 \qquad (8)$$

where B, B_1, and B_2 are the total bulk modulus, the contribution by the linear summation energy of constituent elements, and the modification by the formation enthalpy, respectively. B_1 is obtained by eq 6, and B_2 is calculated by eq 9:

$$B_2 = B_1\Delta H/(\Delta H + E_{AB}) \qquad (9)$$

Equation 9 shows that the modification with regards to the formation enthalpy is proportional to the fraction of the formation enthalpy in the total cohesive energy. From eqs 8 and 9, the bulk modulus may be predicted by

$$B = B_1[1 + \Delta H/(E_{AB} + \Delta H)] \qquad (10)$$

Table 2 lists the value of formation enthalpy ΔH, total cohesive enthalpy E, revised calculated bulk modulus B_{cal}', and their predicted errors. It is seen from Table 2 that the new model may provide better predictions for the intermetallics of equal elemental ratio.

4. Discussion

According to Martin's one-gap model,[25] bulk moduli for tetrahedrally coordinated compounds are proportional to −3.5 power of the interatomic distance. For the diamond and the zinc blende solid, Cohen[26] found good analytic relation of the bulk modulus B=1761$d^{-3.5}$, where d is the bond length. For elemental substances, the bulk modulus B can be determined by the effective pseudopotential radius r_{ps} through an empirical relation:[27] B=$Cr_{ps}m$, where C and m are constants related to the bonding character; the powers m range from −3.1 to −3.4 (for the highly sp-bonded elemental substance).

Consider our empirical model with regards to this argument. Equation 6 can be rewritten as B=Cz^2d^{-3}

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Table 2. The Value of n_{ws} and $(B/V)^{1/2}$ for Binary Systems

no	compound	B (GPa)	N (M e)[a]	V (10^{-6}m^3)	ΔH (KJ)	E (KJ)	B_{cal} (GPa)	error (%)	B_{cal}' (GPa)	error (%)
1	Al42.5Co57.5	136.0	31.88	7.81	43.1	425.9	130.1	4.3	143.2	5.3
2	Al51Co49	138.0	31.16	8.10	42.4	416.9	119.8	13.2	132.0	4.3
3	Al52.5Co47.5	153.0	31.03	8.16	41.9	414.9	118.0	22.8	129.9	15.0
4	Aal48Co52	156.0	31.41	8.00	43.1	420.6	123.3	20.9	136.0	12.8
5	Al49Co51	158.0	31.33	8.03	42.9	419.4	122.2	22.6	134.7	14.7
6	AlCo	162.0	31.24	8.07	42.7	418.2	121.0	25.3	133.3	17.7
7	Al51Co49	173.0	31.16	8.10	42.4	416.9	119.8	30.7	132.0	23.7
8	Al46Co54	180.0	31.58	7.93	43.3	422.7	125.8	30.1	138.7	22.9
9	Al38Co62	189.0	32.26	7.67	41.8	428.9	135.7	28.1	148.9	21.1
10	Al2Gd	78.0	29.74	12.94	65.2	416.5	68.3	12.3	79.0	1.3
11	Al52Ru48	199.0	37.99	8.71	48.0	530.0	165.8	16.6	180.8	9.1
12	Al48Ru52	206.0	38.91	8.63	48.6	543.5	175.5	14.8	191.2	7.1
13	Al50Ru50	208.0	38.45	8.66	48.4	536.9	170.6	17.9	186.0	10.5
14	Al40Ru60	222.0	40.74	8.49	46.7	567.5	195.4	11.9	211.5	4.7
15	Al42Ru58	222.0	40.28	8.52	47.6	561.9	190.4	14.2	206.5	6.9
16	Al2U	83.0	29.39	10.85	55.7	452.3	79.6	4.1	89.4	7.6
17	Al2Y	89.2	29.74	12.94	65.2	423.9	68.3	23.3	78.9	11.6
18	Al3Zr	95.4	30.06	11.02	58.5	454.5	82.0	14.0	92.6	2.9
19	Al2Zr	117.0	31.09	11.36	73.2	492.2	85.1	27.2	97.7	16.4
20	AuCd	85.0	32.13	11.03	19.8	259.8	93.6	10.0	100.7	18.4
21	B6La	90.0	24.79	6.65	28.2	364.1	92.4	2.6	99.6	10.6
22	Be17Nb2	141.0	25.38	5.50	14.0	377.2	117.1	16.9	121.4	13.8
23	Be12Nb	177.0	24.67	5.33	10.2	361.8	114.1	35.5	117.3	33.7
24	Be12Ti	117.0	23.84	5.28	12.1	343.5	107.6	8.0	111.4	4.8
25	Be13Zr	122.0	23.92	5.44	17.4	357.6	105.1	13.8	110.2	9.6
26	CaAl2	49.0	24.47	12.54	13.7	291.0	47.7	2.6	50.0	1.9
27	Co2Hf	167.0	37.29	8.55	48.8	538.5	162.6	2.6	177.4	6.2
28	Co2Zr	153.0	36.74	8.64	56.9	540.6	156.3	2.1	172.8	12.9
29	Cr2Nb	200.0	40.90	8.40	9.7	516.3	199.1	0.4	202.8	1.4
30	CoSi2	201.1	39.00	10.19	37.6	476.3	149.2	25.7	161.0	19.9
31	CrSi2	172.0	39.66	10.46	38.0	467.0	150.4	12.5	162.6	5.4
32	TiSi2	148.9	39.52	11.57	81.4	534.8	135.0	9.3	155.5	4.4
33	Cu2Mg	88.0	28.25	8.76	−25.6	246.7	91.2	3.5	81.7	7.1
34	CuZn	116.0	26.14	8.02	−11.1	221.9	85.2	26.5	81.0	30.1
35	ErFe2	103.0	34.31	9.94	33.1	414.1	118.4	14.9	127.9	24.1
36	GdAl2	80.0	29.74	12.95	65.2	416.5	68.3	14.6	79.0	1.2
37	IrNb	301.0	50.17	9.53	78.5	778.5	264.0	12.2	290.7	3.4
38	LaAl2	71.0	30.35	13.73	66.0	427.7	67.1	5.5	77.4	9.0
39	MgAg	66.0	24.12	11.76	15.8	230.3	49.5	25.0	52.9	19.9
40	Mg2Si	55.0	28.50	12.73	12.2	257.6	63.8	16.0	66.8	21.5
41	Mg2Sn	41.0	25.20	14.61	11.1	208.8	43.5	5.9	45.8	11.6
42	!MnS2	64.0	27.92	13.74	104.6	381.9	56.7	11.3	72.2	12.8
43	Mo48.7Nb	215.5	50.02	10.04	8.4	701.4	249.0	15.5	252.0	16.9
44	Mo0.25Nb0.75	188.8	48.88	10.45	5.1	717.1	228.7	21.1	230.4	22.0
45	Mo0.31Nb0.69	194.5	49.14	10.35	6.3	714.0	233.3	19.9	235.3	21.0
46	Mo24.8Nb	243.5	51.05	9.72	5.6	681.4	268.2	10.1	270.4	11.0
47	Mo0.37Nb0.63	194.5	49.40	10.26	7.3	710.6	237.9	22.3	240.3	23.5
48	Mo0.44Nb0.56	206.6	49.70	10.15	8.1	706.4	243.3	17.7	246.1	19.1
49	Mo0.53Nb0.47	217.1	50.09	10.02	8.4	700.2	250.4	15.3	253.4	16.7
50	Mo0.72Nb0.28	235.8	50.91	9.76	6.2	684.4	265.6	12.6	268.0	13.6
51	Mo16.1Re	282.0	52.75	9.30	4.1	680.9	299.4	6.1	301.2	6.8
52	Mo27Re	292.5	53.19	9.23	6.9	696.5	306.4	4.7	309.4	5.7
53	Mo35Re	293.0	53.50	9.19	8.6	707.6	311.6	6.3	315.4	7.6
54	MoSi2	209.7	44.55	11.18	39.9	556.5	177.5	15.3	190.2	9.2
55	Nb33Cr77	192.7	40.56	8.29	9.0	504.5	198.5	3.0	202.1	4.8
56	NbCr2	200.0	40.90	8.40	9.7	516.3	199.1	0.4	202.8	1.4
57	Nb23.3Mo	187.7	48.81	10.47	4.8	718.0	227.5	21.2	229.0	22.0
58	Nb33.9Mo	197.4	49.27	10.31	6.8	712.4	235.5	19.2	237.8	20.4
59	NbSi2	191.5	43.11	11.73	69.2	609.8	158.5	17.2	176.5	7.8
60	NiAl	166.0	31.16	8.01	48.0	425.5	121.3	26.9	134.9	18.7
61	Ni3Al	170.9	33.24	7.23	35.5	438.3	152.8	10.5	165.2	3.3
62	Ni3Fe	180.6	35.07	6.71	0.9	425.1	183.3	1.4	183.7	1.7
63	Ni3Ga	146.2	33.13	7.53	28.8	417.5	145.9	0.2	156.0	6.6
64	Ni3Ge	182.6	35.26	8.16	28.8	442.8	152.3	16.6	162.2	11.1
65	Ni3Mn	193.1	34.19	6.75	8.1	399.6	173.1	10.3	176.6	8.5
66	NiTi	140.3	36.18	8.35	50.2	498.2	156.6	11.6	172.4	22.9
67	PdTi	143.7	39.14	9.50	95.4	517.4	161.2	12.2	191.0	32.9
68	ReSi2	165.0	45.87	10.89	33.3	589.0	193.2	17.1	204.2	23.7
69	RuSc	148.0	40.37	10.31	62.9	575.9	158.1	6.8	175.4	18.4
70	Ru53Ta47	251.0	48.57	9.26	58.5	770.6	254.7	1.4	274.0	9.1
71	Ra11Ta9	255.0	48.62	9.21	58.4	767.8	256.8	0.6	276.3	8.3
72	Ru49Ta51	255.0	48.45	9.37	57.8	775.1	250.5	1.7	269.2	5.5
73	Ru11Ta9	255.0	48.62	9.21	58.4	767.8	256.8	0.6	276.3	8.3
74	Ru51Ta49	259.0	48.51	9.32	58.3	773.0	252.6	2.4	271.6	4.8
75	SbY	66.0	35.80	18.86	65.8	409.3	67.9	2.9	78.9	19.5
76	Si2V	166.0	39.44	10.86	53.4	521.4	143.2	13.7	157.9	4.8

Table 2 (Continued)

no	compound	B (GPa)	N (M e)[a]	V (10^{-6}m^3)	ΔH (KJ)	E (KJ)	B_{cal} (GPa)	error (%)	B_{cal}' (GPa)	error (%)
77	SiV3	175.0	37.78	9.31	50.9	546.4	153.3	12.3	167.6	4.2
78	Si3V5	187.0	38.27	9.79	67.6	554.9	149.7	19.9	167.9	10.1
79	Sn3Ce	55.0	30.32	16.34	56.6	388.1	56.3	2.2	64.5	17.2
80	TaSi2	192.5	42.86	11.73	69.8	627.8	156.6	18.6	174.0	9.5
81	TaV2	218.0	40.21	9.18	1.3	603.3	176.1	19.2	176.5	19.0
82	TbFe2	93.0	34.59	10.18	31.9	437.6	117.6	26.4	126.1	35.6
83	TiAl3	106.0	29.51	10.18	39.4	401.6	85.6	19.2	93.9	11.3
84	Ti3Al	118.0	34.52	10.45	38.1	470.8	114.0	3.3	123.3	4.4
85	Ti28.4Cr	115.7	37.15	9.53	7.1	454.4	144.9	25.2	147.1	27.1
86	Ti50Cr50	147.0	37.24	8.77	10.9	442.4	158.2	7.5	162.1	10.2
87	Ti46Cr54	147.0	37.26	8.63	11.0	439.6	160.8	9.3	164.8	12.1
88	Ti44Cr56	150.0	37.27	8.57	11.0	438.1	162.1	8.0	166.2	10.7
89	Ti42Cr58	153.0	37.27	8.50	10.9	436.6	163.4	6.8	167.5	9.4
90	Ti40Cr60	154.0	37.28	8.44	10.8	435.0	164.7	6.9	168.8	9.6
91	Ti48Cr52	155.0	37.25	8.70	11.0	441.0	159.5	2.8	163.4	5.4
92	TiCr2	159.0	37.31	8.23	9.9	429.2	169.2	6.4	173.1	8.8
93	Ti13.8Cr	108.6	37.09	10.05	3.5	461.4	136.8	25.9	137.9	26.9
94	Ti9.4Cr	107.8	37.07	10.21	2.4	463.5	134.6	24.8	135.3	25.4
95	Ti7Cr	108.5	37.06	10.30	1.8	464.7	133.4	22.9	133.9	23.3
96	Ti5Ge3	82.0	36.29	11.86	11.5	443.5	111.1	35.4	113.9	38.9
97	Ti94Ge6	116.0	36.91	10.76	14.3	476.5	126.6	9.1	130.4	12.4
98	Ti20Re80	309.0	52.27	9.03	20.4	734.0	302.6	2.0	311.0	0.6
99	Ti5Re24	322.0	52.80	9.01	17.6	739.7	309.5	3.8	316.9	1.5
100	Ti64Ru36	173.0	41.66	9.40	52.9	586.4	184.6	6.7	201.2	16.3
101	TiRu	247.0	43.46	9.01	63.5	622.5	209.7	15.1	231.1	6.4
102	Ti87Sn13	97.0	36.23	11.36	19.9	466.5	115.5	19.1	120.5	24.1
103	Ti3Sn	97.5	35.49	12.10	37.6	464.3	104.0	6.7	112.5	15.3
104	Ufe2	134.0	34.26	8.66	7.9	461.9	135.5	1.1	137.8	2.8
105	Uni2	126.0	34.94	8.23	16.9	480.9	148.3	17.7	153.5	21.8
106	Uni5	182.0	35.13	7.38	9.7	455.7	167.1	8.1	170.7	6.2
107	Upd3	167.0	39.47	9.47	46.6	462.6	164.5	1.4	181.1	8.4
108	Urh3	261.0	42.43	9.00	28.2	577.7	200.0	23.3	209.8	19.6
109	Uru3	264.0	45.96	8.85	13.6	635.1	238.7	9.5	243.8	7.6
110	V3Ge	168.0	36.35	9.73	37.0	514.0	135.7	19.2	145.5	13.3
111	Vsi2	167.2	39.44	10.86	53.4	521.4	143.2	14.3	157.8	5.6
112	V0.294Ti0.706	113.0	36.96	9.87	1.7	482.7	138.4	22.4	138.9	22.9
113	V0.385Ti0.615	116.7	36.93	9.66	2.2	487.1	141.2	21.0	141.8	21.5
114	V0.53Ti0.47	125.9	36.90	9.33	2.5	493.8	145.8	15.8	146.6	16.3
115	V0.73Ti0.27	138.1	36.85	8.90	1.8	501.9	152.5	10.3	153.0	10.7
116	Wsi2	222.4	46.01	11.20	34.7	618.4	189.1	14.9	199.7	10.2
117	W0.096Ta0.904	205.1	47.97	10.72	2.6	792.0	214.7	4.6	215.4	4.9
118	W0.785Ta0.215	216.7	49.10	10.54	5.8	804.4	228.8	5.5	230.4	6.3
119	W0.60Ta0.40	237.9	50.85	10.25	10.0	822.8	252.1	5.9	255.2	7.2
120	W0.36Ta0.64	266.1	53.11	9.93	9.8	841.1	283.9	6.7	287.3	7.9
121	W0.10Ta0.90	297.7	55.57	9.64	2.9	854.2	320.3	7.5	321.4	7.9
122	Yal2	82.0	29.74	12.94	65.2	423.9	68.3	16.6	78.8	3.8
123	Yfe2	97.0	34.61	10.32	29.6	445.6	116.1	19.7	123.9	27.6
124	Yzn	62.0	28.15	14.32	51.3	327.3	55.3	10.7	64.0	3.2
125	ZrCo2	156.0	36.74	8.65	56.9	540.6	156.1	0.0	172.5	10.6
126	ZrCr2	142.0	38.05	9.19	16.8	481.1	157.6	11.0	163.1	14.8
127	TiAl	110.0	32.02	10.33	60.4	457.9	99.2	9.8	112.3	2.0
128	Al−Li alloy	72.0	26.26	9.93	0.7	319.3	69.4	3.5	69.6	3.3
129	Al−Li alloy	68.5	25.52	9.87	1.4	311.5	66.0	3.6	66.3	3.2
130	Al−Li alloy	69.0	25.15	9.83	1.8	307.7	64.3	6.7	64.7	6.2
131	Al−Li alloy	67.0	24.78	9.80	2.1	303.8	62.7	6.4	63.1	5.8
132	Al−Li alloy	65.5	24.41	9.77	2.5	299.9	61.0	6.8	61.5	6.0
133	AlNi	156.0	31.16	8.03	48.0	425.5	121.0	22.4	134.6	13.7
134	Co68Ni32	183.1	35.43	6.61	0.3	425.5	189.9	3.7	190.0	3.7
135	NbCr2	229.4	40.90	8.40	9.7	516.3	199.1	13.2	202.8	11.5
136	HfV2	104.0	38.15	9.93	3.0	551.3	146.7	41.0	147.5	41.7
137	Mo7.0Re	270.8	52.39	9.35	1.8	668.0	293.6	8.4	294.4	8.7
138	Mo16.6Re	278.5	52.77	9.29	4.2	681.7	299.7	7.6	301.6	8.2
139	Mo26.9Re	284.1	54.25	9.08	10.1	731.0	324.0	14.0	328.5	15.6
140	Nb16.8Mo	179.3	48.53	10.57	3.4	721.3	222.7	24.2	223.8	24.8
141	Nb23.3Mo	183.4	48.81	10.47	4.8	718.0	227.5	24.0	229.0	24.8
142	Nb33.9Mo	196.4	49.27	10.31	6.8	712.4	235.5	19.8	237.8	21.0
143	Nb51.6Mo	216.8	50.03	10.04	8.4	701.2	249.3	14.9	252.3	16.3
144	Nb75.2Mo	242.8	51.05	9.71	5.6	681.4	268.2	10.4	270.4	11.3
145	Nb92.1Mo	257.7	51.77	9.49	1.8	665.5	282.4	9.5	283.1	9.8
146	Cr67Zr33	147.0	38.05	9.15	16.7	480.3	158.2	7.6	163.7	11.3
147	Cr64Cr36	147.0	38.10	9.34	17.3	487.2	155.4	5.7	160.9	9.4
148	Cr69Zr31	152.0	38.01	9.03	16.1	475.6	160.1	5.3	165.5	8.8
149	Mo5Si3	264.7	47.86	10.40	48.1	626.6	220.2	16.8	237.1	10.4
150	Nb83.2Mo16.8	179.3	48.53	10.57	3.4	721.3	222.7	24.2	223.8	24.8
151	Nb76.7Mo23.3	185.2	48.81	10.47	4.8	718.0	227.5	22.8	229.0	23.6
152	Nb66.1Mo35.9	196.4	49.27	10.31	6.8	712.4	235.5	19.8	237.8	21.0

Table 2 (Continued)

no	compound	B (GPa)	N (M e)[a]	V (10^{-6}m^3)	ΔH (KJ)	E (KJ)	B_{cal} (GPa)	error (%)	B_{cal}' (GPa)	error (%)
153	Nb48.4Mo51.6	216.8	50.03	10.04	8.4	701.2	249.3	14.9	252.3	16.3
154	Nb24.8Mo75.2	242.8	51.05	9.71	5.6	681.4	268.2	10.4	270.4	11.3
155	Nb7.2Mo92.8	257.1	51.80	9.48	1.6	664.8	283.0	10.0	283.7	10.3
156	Ta90W10	201.7	48.02	10.72	2.7	792.4	215.2	6.7	215.9	7.0
157	Ta70W30	220.7	49.94	10.41	8.0	813.1	239.6	8.5	242.0	9.6
158	TaW	243.7	51.85	10.12	11.0	831.5	265.7	9.0	269.2	10.4
159	Ta33W67	268.9	53.48	9.91	9.3	842.9	288.6	7.3	291.8	8.4
160	Ta17W83	288.9	55.01	9.73	5.0	850.9	310.9	7.6	312.7	8.2
161	Cu92.7Ni7.3	181.2	31.50	7.05	2.6	345.3	140.8	22.2	141.9	21.6
162	Cu82.2Ni17.8	175.5	31.93	6.98	6.4	358.8	146.0	16.7	148.6	15.3
163	Cu80Ni20	176.2	32.02	6.97	7.2	361.6	147.2	16.4	150.1	14.8
164	Ci77.2Ni22.8	174.2	32.14	6.95	8.2	365.2	148.6	14.7	151.9	12.8
165	Cu64.5Ni35.5	169.7	32.66	6.88	12.3	380.9	155.2	8.5	160.1	5.6
166	Cu53.8Ni46.2	164.7	33.10	6.82	14.2	392.7	160.8	2.4	166.6	1.1
167	Cu31.1Ni68.9	151.0	34.04	6.71	11.4	410.8	172.7	14.3	177.5	17.5
168	AlP	86.0	27.22	9.17	44.1	373.1	80.8	6.0	90.3	5.0
169	AlAs	77.0	27.72	10.98	8.8	315.0	70.0	9.0	72.0	6.5
170	AlSb	58.2	29.43	14.18	−8.1	287.9	61.1	4.9	59.3	1.9
171	GaP	88.7	27.00	9.88	47.1	348.1	73.8	16.8	83.8	5.5
172	GaAs	74.8	27.51	11.79	13.2	291.3	64.2	14.2	67.1	10.3
173	GaSb	57.0	29.21	15.09	−0.4	267.6	56.6	0.7	56.5	0.9
174	InP	71.0	26.29	11.28	47.3	334.3	61.2	13.7	69.9	1.5
175	InAs	60.0	26.79	13.41	15.2	279.3	53.5	10.8	56.4	5.9
176	InSb	47.4	28.49	16.89	7.4	261.4	48.1	1.3	49.4	4.2
177	ZnS	77.1	25.62	13.34	139.1	341.6	49.2	36.1	69.3	10.1
178	ZnSe	62.4	24.74	13.82	58.9	242.4	44.3	29.0	55.0	11.7
179	ZnTe	51.0	24.65	15.91	10.6	181.1	38.2	25.1	40.4	20.7
180	CdS	62.0	25.66	14.57	169.1	362.6	45.2	27.0	66.3	6.9
181	CdSe	53.0	24.78	15.28	83.7	258.2	40.2	24.2	53.2	0.3
182	CdTe	42.4	24.69	17.58	36.0	197.5	34.7	18.2	41.0	3.3
183	HgSe	50.0	25.81	15.79	71.7	222.7	42.2	15.6	55.7	11.4
184	HgTe	42.3	25.72	18.05	26.9	164.9	36.6	13.3	42.6	0.7
185	Cu alloy	133.9	30.73	7.17	−1.4	325.1	131.7	1.6	131.1	2.0
186	Cu alloy	136.3	30.99	7.22	0.3	335.8	133.0	2.4	133.1	2.3
187	Cu alloy	131.6	30.78	7.36	0.5	335.6	128.6	2.2	128.8	2.1
188	Cu alloy	134.5	31.12	7.16	−0.5	334.5	135.3	0.6	135.1	0.4
189	Cu alloy	135.7	31.00	7.27	−1.2	332.0	132.1	2.6	131.6	2.9
190	Cu alloy	138.7	31.59	7.30	2.1	342.7	136.7	1.4	137.6	0.8
191	Cu alloy	132.8	31.69	7.35	2.6	344.3	136.6	2.8	137.6	3.6
192	Cu alloy	139.5	31.93	7.48	3.8	348.3	136.3	2.2	137.8	1.1
193	Cu alloy	136.2	31.24	7.16	0.0	336.3	136.3	0.0	136.3	0.0
194	Cu alloy	133.2	31.26	7.20	−0.1	336.5	135.7	1.8	135.6	1.8
195	Cu−Ni alloy	137.7	31.29	7.08	0.9	339.0	138.4	0.5	138.7	0.7
196	Cu−Ni alloy	137.7	31.32	7.07	1.1	339.9	138.7	0.7	139.2	1.0
197	Cu−Ni alloy	138.0	31.38	7.06	1.6	341.8	139.4	1.0	140.1	1.5
198	Cu−Ni alloy	138.6	31.45	7.05	2.2	343.7	140.2	1.1	141.1	1.7
199	Cu−Ni alloy	139.2	31.60	7.03	3.5	348.4	142.0	2.0	143.4	3.0
200	Cu−Au alloy	138.8	31.21	7.10	0.1	336.2	137.3	1.0	137.3	1.0
201	Cu−Au alloy	139.0	31.43	7.18	1.3	338.2	137.6	1.0	138.1	0.6
202	Cu−Au alloy	145.5	32.02	7.41	4.5	343.7	138.3	4.9	140.2	3.6
203	Cu−Al alloy	136.9	31.07	7.18	0.2	335.9	134.5	1.7	134.6	1.7
204	Cu−Al alloy	135.5	30.89	7.29	0.4	335.7	130.8	3.4	130.9	3.3
205	Cu−Al alloy	134.3	30.74	7.39	0.6	335.6	127.9	4.7	128.2	4.5
206	Cu−Al alloy	137.6	31.16	7.11	0.0	336.0	136.6	0.7	136.6	0.7
207	Cu−Al alloy	136.9	31.05	7.18	0.2	335.9	134.2	1.9	134.3	1.8
208	Cu−Al alloy	136.6	30.99	7.22	0.3	335.8	133.0	2.6	133.1	2.5
209	Cu−Al alloy	135.8	30.91	7.28	0.4	335.7	131.2	3.3	131.4	3.2
210	Cu−Al alloy	135.4	30.88	7.30	0.4	335.7	130.7	3.4	130.9	3.3
211	Cu−Al alloy	135.2	30.84	7.32	0.4	335.7	129.9	3.8	130.1	3.7
212	Cu−Al alloy	134.4	30.76	7.37	0.5	335.6	128.4	4.4	128.6	4.3
213	Cu−Al alloy	133.0	30.64	7.45	0.7	335.5	125.9	5.3	126.2	5.1
214	Pb−Tl alloy	44.8	27.78	18.28	0.0	196.0	42.2	5.6	42.2	5.6
215	Pb−Tl alloy	45.0	27.75	18.27	0.0	195.9	42.1	6.3	42.1	6.3
216	Pb−Tl alloy	44.5	27.72	18.26	0.0	195.8	42.1	5.4	42.1	5.4
217	Pb−Tl alloy	44.7	27.70	18.25	0.1	195.7	42.0	5.9	42.0	5.9
218	Pb−Tl alloy	44.3	27.66	18.24	0.1	195.6	41.9	5.3	42.0	5.2
219	Pb−Tl alloy	43.9	27.56	18.21	0.1	195.3	41.7	4.9	41.7	4.8
220	Pb−Tl alloy	42.8	27.24	18.11	0.4	194.3	41.0	4.2	41.0	4.0
221	Pb−Tl alloy	42.6	27.14	18.08	0.4	194.0	40.7	4.4	40.8	4.2
222	Zn−Cu alloy	133.9	29.97	7.45	−0.4	296.5	120.7	9.8	120.5	10.0
223	Zn−Cu alloy	126.6	29.33	7.63	−0.6	275.7	112.7	11.0	112.4	11.1
224	Fe−Ni alloy	173.1	36.42	6.73	1.6	425.6	197.1	13.8	197.9	14.3
225	Au−Ni alloy	172.6	39.31	10.08	−0.7	369.1	153.3	11.1	153.0	11.3
226	Au−Ni alloy	171.4	39.04	9.84	−2.3	371.5	154.9	9.6	153.9	10.2
227	Au−Ni alloy	170.7	38.44	9.32	−5.8	376.7	158.6	7.0	156.2	8.5
228	Au−Ni alloy	170.5	37.69	8.66	−9.6	383.8	164.1	3.7	160.0	6.1

Table 2 (Continued)

no	compound	B (GPa)	N (M e)[a]	V (10^{-6}m^3)	ΔH (KJ)	E (KJ)	B_{cal} (GPa)	error (%)	B_{cal}' (GPa)	error (%)
229	Cu−Ni alloy	181.1	35.02	6.62	2.8	424.0	185.3	2.3	186.5	3.0
230	Cu−Ni alloy	175.9	34.59	6.66	6.7	418.4	179.7	2.1	182.6	3.7
231	Cu−Ni alloy	174.9	34.38	6.68	8.6	415.6	177.0	1.2	180.7	3.3
232	Zn−Cu alloy	133.9	30.87	7.18	−0.1	325.6	132.7	0.9	132.6	0.9
233	Mg−Li alloy	37.1	22.21	13.95	0.0	145.2	35.4	4.5	35.4	4.5
234	Mg−Li alloy	36.9	22.06	13.92	0.0	145.4	35.0	5.1	35.0	5.1
235	Mg−Li alloy	36.7	21.85	13.87	0.1	145.7	34.4	6.1	34.4	6.0
236	Mg−Li alloy	36.2	21.66	13.83	0.1	146.0	33.9	6.4	33.9	6.3
237	Mg−Li alloy	35.8	21.35	13.77	0.1	146.4	33.1	7.5	33.1	7.4
238	Mg−Li alloy	35.4	21.15	13.73	0.1	146.7	32.6	8.0	32.6	7.9
239	Mg−Li alloy	35.2	20.93	13.68	0.2	147.0	32.0	8.9	32.1	8.8
240	Mg−Li alloy	34.7	20.75	13.64	0.2	147.3	31.6	9.0	31.6	8.9
	average							11.0		10.3

[a] M is a constant and equals 6.748×10^{24}.

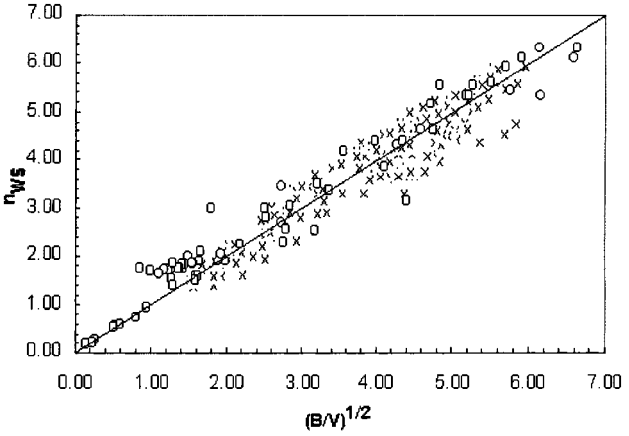

Figure 2. The linear relationship between n_{ws} and $(B/V)^{1/2}$ of pure elements and binary compounds, n_{ws} in arbitrary density units [electron/(au)^3], B in Gpa, and V in 10^{-6} m^3 per mole. ○, Pure elements; ×, binary intermetallics.

because n_{ws} is proportional to z/V, where V is roughly proportional to d^3, C is a constant, z is the number of valence electrons contained in the unit cell, V is the unit cell volume, and d is the equilibrium interatomic distance. In our model, bulk modulus B is also proportional to d^m, and the power m is equal to -3 which is very close to the previous results.

For a terminal solid solution, the formation enthalpy (or heat of formation) ΔH is close to zero; eq 10 will reduce to eq 9, which means our model can also be applied to a terminal solid solution. As to more complicated intermetallic compounds and alloys, because their formation enthalpies can no longer be neglected, the additional term $\Delta H/(E + \Delta H)$ must be considered to predict their bulk modulus. That is, our model can predict the bulk modulus for intermetallic compounds, alloys, and ideal dilute solid solutions.

The trends in the elastic constant of the simple and transition elemental cubic metals is investigated by Rose and Shore[28] in terms of a uniform electron-gas theory. The elastic properties of metals depend primarily on two parameters: the average electron density at the cell boundary and less importantly the bonding valence. This conclusion is very similar to ours which may be rearranged as $B = n_{ws}^2 V = n_{ws}(n_{ws}V) = n_{ws}Z$. But unlike the model by Rose and Shore, eq 6 may cover binary alloys.

As noted above, carbon does not obey this linear relationship, so carbides (e.g., TiC and SiC) are not included in Figure 2, which means that the carbides may not obey this empirical rule. Attention is also needed for copper alloys because copper also shows some abnormality (see Figure 1). If we still use the original value of $n_{ws} = 3.18$ in Figure 2, all alloys containing Cu will obviously deviate from the ideal line in this figure. Therefore, it is reasonable to use the curve fit best estimate, $n_{ws} = 4.40$, for copper alloys. The same correction is also applied to element As(2.4), P(3.19), Fe-(4.84), and U(2.72). The value of n_{ws} for elements S(1.71), Se(1.5), and Te(1.2) is not given in Miedema's model; the value of n_{ws} is supposed to equal the value of $(B/V)^{1/2}$ to estimate the bulk modulus of compounds containing these elements.

5. Conclusions

The correlation between the bulk modulus and the constituent element properties of binary intermetallic compounds and alloys has been constructed on the basis of literature data of 240 compounds and alloys. Using this model, the following results have been obtained:

(1) A relationship among bulk modulus B, molar volume V, and valence electron density n_{ws} for 69 metal or semimetal elements (except H, N, P, and C elements) exists and can be expressed by eq 6.

(2) A relationship among bulk modulus B, molar volume V, and valence electron density n_{ws} for binary compounds and alloys exists and can also be expressed by eq 6, with average predicted error limits of ±11%.

(3) For compounds whose atomic ratio is near to 1 and which have a large formation enthalpy, the contribution of formation enthalpy must be considered to predict their bulk modulus; the bulk modulus may be predicted by eq 10.

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