

Quantitative Size-Factors for Metallic Solid Solutions

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Quantitative size-factors, defined in terms of the effective atomic volume of the solute, have been calculated for 469 substitutional solid solutions using precision lattice parameter data available in the literature. Values of the volume size-factor, its linear derivative and a parameter expressing the deviation from Vegard's law, are tabulated in alphabetical order of the solvents. The application of these size-factors is discussed in relation to a number of physical, chemical and mechanical properties of solid solution alloys.

1. Introduction

The physical, chemical and mechanical properties of metallic solid solutions are all affected by a difference in atomic size between the solvent and solute elements. The size-factor concept has already been applied in one form or another to the study of residual electrical resistivity [1], superconducting properties [2], electronic specific heats [2], elastic coefficients [3], solution hardening theories based on dislocation locking [4] and friction [5, 6], phase stability [7], and to the contribution of elastic strain energy to the heats of formation of solid solutions [3, 8].

The problem of defining the size of an atom has been discussed in detail in a recent review [9] in which two complementary methods of measuring atomic size are shown to be of value in the study of substitutional solid solutions. One of these makes use of the closest distance of approach of the atoms in the structure of the pure elements to provide the only reliable criterion for applying the Hume-Rothery 15% rule [10]. The alternative approach is to derive a volume size-factor from the effective volume of the solute atom in the context of the solid solution [11]. Although the latter volume size-factor is of little value for predicting new possibilities for extensive solid solutions [10], it is related directly to the strain energy introduced into the solution by the solute atoms and is therefore a suitable parameter for assessing the influence of size effects on the properties of known solid solution alloys.

Predictions of the changes in lattice spacings across a solid solution have been put forward by Pines [12], Fournet [13], Friedel [3], Eshelby [14], and by Gschneidner and Vineyard [15] on the basis of the model of a sphere inserted in a hole cut in an elastic continuum. According to these analyses, the effective volume of a solute atom in a given solution can be calculated from a knowledge of the atomic volumes and elastic coefficients of the solvent and solute. However, discrepancies have been found between the predicted effective volumes and those calculated from lattice spacing data for solutions based on copper, silver, gold, aluminium, iron and magnesium [9]. Where the solute atom is smaller than the solvent, the sign of the predicted change in atomic volume was always found to be in error. On the other hand, where the atomic volume of the solute is greater than that of the solvent, the predicted and observed values agreed to within 5% in only half of this random selection of alloy systems. This method was therefore rejected and volume size-factors have been calculated from precision lattice parameter data available in the literature. The aim of this paper is to present these size-factors in a convenient and comprehensive form and to discuss their application in various aspects of the study of the solid state.

2. Properties and Derivatives of the Volume Size-Factor

The atomic volume, Ω , of a metal or solid solu-

tion alloy is defined for the present purpose as the mean volume per atom; i.e. by taking the volume of the unit cell divided by the number of atoms in the cell. Provided the nature of the inter-atomic bonding forces remains essentially metallic, the atomic volume so defined is independent of the anisotropy or co-ordination number of the crystal structure of the material. This is confirmed, for example, by the observation [9] that the atomic volumes of two allotropic forms of a metal, measured at the transition temperature, agree to within 1%. It is also observed that the atomic volume of the bcc β -brasses fall on the extrapolation of the approximately linear trends of the volume changes with composition in the fcc primary solid solutions based on copper and silver [11, 16].

The definition of the volume size-factor, Ωsf , rests on the observation that at low values of fractional composition c the atomic volumes of solid solutions vary linearly with the atomic concentration of the solute. In many systems this linear trend continues right up to the phase boundary. In other systems it is necessary to define a limiting concentration c_{max} above which the volume changes are no longer linear. The two situations are illustrated by the systems Ag-Al and Ce-Th in fig. 1. The effective atomic volume Ω_B^* of the solute B is obtained by a linear extrapolation of the volume plot to 100% solute and, using this value, the volume size-factor is defined as

$$\Omega sf = \left(\frac{\Omega_B^* - \Omega_A}{\Omega_A} \right) \quad (1)$$

The linear plots of atomic volume against composition in fig. 1 can be expressed in the form of the following equation:

$$\Omega(c) = (1 - c) \Omega_A + c \Omega_B^* \quad (2)$$

Differentiating with respect to concentration c gives

$$\frac{\partial \Omega}{\partial c} = (\Omega_B^* - \Omega_A)$$

from which it follows that the volume size-factor may also be defined as

$$\Omega sf = \frac{1}{\Omega_A} \cdot \frac{\partial \Omega}{\partial c} \quad (3)$$

Thus, not only does the volume size-factor represent the fractional difference between the effective atomic volume of the solute and the atomic volume of the solvent, but it also ex-

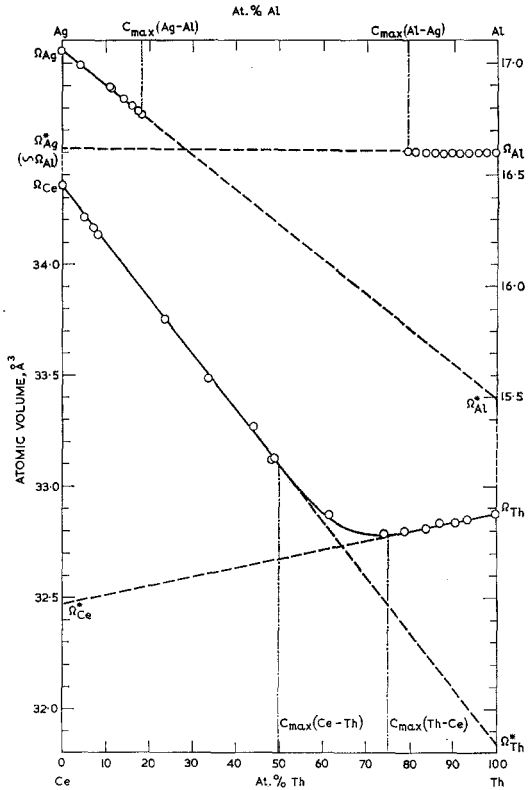


Figure 1. Atomic volume changes with composition in the systems Ag-Al and Ce-Th, showing the derivation of Ω_B^* and the significance of the limiting concentration, c_{max} .

presses the rate of change of atomic volume with composition, c .

For many applications it is more convenient to use a linear derivative of the size-factor [9]. In order that such a linear size-factor, lsf , may retain all the properties of the Ωsf , it is defined in terms of the Seitz radius $r_o = (3\Omega/4\pi)^{1/3}$, i.e.

$$lsf = \left(\frac{r_{oB}^* - r_{oA}}{r_{oA}} \right) = \frac{1}{r_{oA}} \cdot \frac{\partial r_o}{\partial c} \quad (4)$$

This size-factor is calculated from the effective atomic volume of the solute using the relationship

$$lsf = \left(\frac{\Omega_B^*}{\Omega_A} \right)^{1/3} - 1 \quad (5)$$

As may be seen in fig. 1, although the change in atomic volume with solute concentration is linear up to the limiting concentration c_{max} , this linear trend does not in general follow the straight line joining the atomic volumes of the two elements. The latter is usually referred to as

Vegard's law following his observation of a linear relationship between the molar volumes of isostructural pairs of ionic salts such as KCl-KBr, KCl-NH₄Cl and K₂SO₄-(NH₄)₂SO₄. Vegard [17] interpreted his results to mean that a characteristic volume can be associated with each particular ion; i.e. with K⁺, NH₄⁺, Br⁻, Cl⁻, etc. The linear relationship holds for the molar volumes of solid solutions of ionic salts because the electronic environment of both types of ion remains unaltered when one ion is replaced by another of identical charge – a condition imposed by the electrical neutrality of the structure as a whole. Vegard's law is only obeyed in metallic systems if once again the electronic environment of both kinds of atom is undisturbed by the formation of the solid solution. Since electrons in states just below the Fermi level can also participate in metallic bonding, this greatly reduces the number of possibilities. The tendency of a metallic solid solution to deviate from Vegard's law may be taken as a measure of the modification of the electronic environment of the *solute* atom. By the same reasoning, the breakaway of the volume plots from a linear trend at concentrations greater than c_{\max} indicates that sufficient solute element has now been added to modify the electronic environment of the *solvent* atoms. The fractional deviation from Vegard's law can be assessed by comparing the effective atomic volume of the solute with its true atomic volume, Ω_B , to give a Vegard's law factor defined as

$$VLF = \left(\frac{\Omega_B^* - \Omega_B}{\Omega_B} \right) \quad (6)$$

3. The Size-Factor Tables

Values of Ω_{sf} , lsf and VLF and c_{\max} are listed in table II in the Appendix and cover most alloy systems for which lattice parameter data are available in the literature up to about the end of 1964. Where two metals form a mutual solid solution across the entire phase diagram, separate size-factors are listed for the solution of *B* in *A* and for *A* in *B*. In general these two size-factors will be quite unrelated as in the system Ce-Th in fig. 1. The size-factors for solutions of the same solute in different structural forms of a solvent are found to agree quite closely with each other, provided they are calculated from lattice spacings data measured at the same temperature. This is illustrated in table I by the size-factors for solutions based on

different forms of cobalt and manganese. Hence only one size-factor is listed for each solvent-solute combination in table II.

TABLE I Volume size-factors of solutions based on different forms of cobalt and manganese

Solution	Structure	Ω_{sf}
Co-Os	FCC	21.93
	HCP	21.63
Co-Rh	FCC	30.74
	HCP	28.95
Co-Ru	FCC	20.92
	HCP	21.67
Mn-Fe	A 12	35.53
	A 13	37.17

A study of the size-factors in table II reveals that some of these combinations exhibit rather unusual properties. In a number of solutions the Ω_{sf} is less than 1% even though there may be quite a marked deviation from Vegard's law (see, for example, Al-Ag in fig. 1). Hence, although the solute atoms have to adapt their size on entering the solid solution, there is no change in the strain energy of the matrix. These systems therefore provide an ideal situation for isolating the influence of *solute valence* from size effects when studying the physical or mechanical properties of solid solutions. Conversely, in many alloy systems where the two component metals have similar, if not identical, outer electronic structures, although there may be marked changes in atomic volume, they conform quite closely to Vegard's law. These alloy systems therefore provide the ideal context for studying the effects of *atomic size* on the physical and mechanical properties of solid solutions. The Nb-Ta system is unique in showing neither lattice distortion nor a deviation from Vegard's law. In this system the substitution of one metal for another across the entire binary system does not affect the electronic structure or the elastic strain energy of the matrix, which is no doubt responsible for the complete lack of hysteresis observed in the magnetisation behaviour of Nb-Ta alloys at temperatures below the superconducting transition, T_c [18].

4. Some Applications of the Volume Size-Factors

4.1. Physical Properties

The influence of size-effects on the physical properties of solid solution alloys is usually masked by the much stronger influence of the electron-atom ratio. The *electrical resistivity* of an alloy, for example, is influenced by the square of the difference in valence between the solvent and solute atoms [19]. From a careful study of the resistivity changes with composition in alloys of copper and silver with the B-subgroup elements which follow them in the periodic table, Blatt [1] concluded that this rule should be refined to make allowances for small deviations caused by the difference in atomic size between the two kinds of atom. For the case where the solute atom is larger than the solvent, he proposed that the lattice is expanded locally causing a local reduction in the charge on the solute ion. In the approximation of an infinite isotropic elastic medium the ionic charge in the remainder of the lattice remains unchanged and so the effect is localised to a lowering of the valence of the solute. Hence Blatt defines an effective valence Z_B^* for the solute as

$$Z_B^* = Z_B - \left(\frac{\Delta V}{\Omega} \right) Z_A \quad (7)$$

where $\Delta V/\Omega$ is the *local* change in volume. Hence the effect of atomic volume and solute valence on the properties of a solid solution of composition, c , can be combined in a single parameter, the effective electron: atom ratio $(e/a)^*$ given by

$$(e/a)^* = cZ_B^* + (1 - c)Z_A \quad (8)$$

According to the empirical rule of Matthias, the *superconducting transition temperatures* of transition metals and alloys are influenced by both their atomic volume and electron: atom ratio. Supposing both these effects to be independent, Matthias, Geballe and Compton [20] have suggested the following general relationship

$$T_c \propto V^x \cdot f(e/a) \quad (9)$$

where $f(e/a)$ is an oscillatory function passing through maxima near $e/a = 4.5$ and 6.5 . DeSorbo [2], however, has demonstrated that the transition temperatures of 10 at. % solutions of Cr, Hf, Mo, Ta, Ti, W or Zr in niobium correlated better when plotted against $(e/a)^*$ rather than the electron-atom ratio, to give a distinct linear decreasing trend with increasing $(e/a)^*$.

This correlation gives physical significance to the volume effect, since it can now be regarded that the locally expanded regions in the vicinity of solute atoms act as sinks for extra electrons and so reduce the electron concentration of the matrix.

In order to apply the concept of effective electron: atom ratio to the physical properties of solid solutions it is necessary to know the local distortion in the volume surrounding a solute atom. The studies of Blatt [1] and DeSorbo [2] (and a recent discussion of T_c by Claiborne [21]) refer to cubic materials and the local volume change (equation 7) is derived from the change in lattice parameter using the following expression due to Eshelby [22]

$$\frac{\Delta V}{\Omega} = \frac{3}{\gamma} \left(\frac{\Delta a}{a} \right) \quad (10)$$

where $\gamma = 3(1 - \sigma)(1 + \sigma)$, σ being Poisson's ratio and $\Delta a/a$ the relative change in lattice parameter per at. % solute. This equation can also be written in terms of the observed changes in atomic volume, i.e.

$$\frac{\Delta V}{\Omega} = \frac{1}{\gamma} \left(\frac{1}{\Omega} \cdot \frac{\partial \Omega}{\partial c} \right) = \frac{1}{\gamma} (\Omega_{sf}) \quad (11)$$

Hence the use of the volume size-factors listed in table II enables the effective electron: atom ratio concept to be applied to all superconducting solid solutions even if the crystal structures are anisotropic. Studies of the influence of size-effects on the T_c of solutions based on indium and tin, for example, are at present in progress in the author's laboratory.

4.2. Chemical Properties

The effect of a difference in size between the solvent and solute atoms in a solid solution is to cause an increase in the elastic strain energy. As discussed by Friedel [3], this increase affects the *free energy of formation* of the solid solution causing it to have a negative curvature when plotted against composition, c . Although both the solvent matrix and the solute atom undergo a distortion the major part of the strain energy is stored in the matrix [3] and hence the elastic strain energy, E_s , can be computed as a function of solute concentration, using the shear modulus of the matrix, from the following equation [8, 14]

$$E_s(c) = \frac{2}{3} \mu \frac{1}{\Omega} \left(\frac{\partial \Omega}{\partial c} \right)^2 \cdot f(c) \quad (12)$$

where μ is the shear modulus of the solvent and $f(c)$ is linear for dilute solutions. The elastic strain energy for concentrations up to the limiting value of c_{\max} can be readily calculated from the volume size-factors and a knowledge of the atomic volume of the solvent, since equation (12) can be re-written as

$$E_s(c) = \frac{2}{3} \mu \Omega (\Omega_{sf})^2 \cdot f(c) \quad (13)$$

To facilitate these calculations the atomic volumes and Seitz radii of the elements are listed in table III in the Appendix

A more direct correlation between size effects and *phase stability* has been reported recently by Warlimont [7]. As mentioned above, in alloys based on copper, the atomic volumes of the β -phases lie on extrapolations of the trends established in the primary solid solutions, and hence the solid solution volume size-factors can also be applied to the β -phases [11]. Warlimont reports that, when the Ω_{sf} is large ($\sim 80\%$), the β -phases form stable ordered $L2_1$ superlattices, whereas for small size-factors ($\sim 20\%$), the superlattices become unstable at low temperatures and decompose martensitically.

4.3. Mechanical Properties

The direct interaction between solute atoms and dislocations is one of the factors which contribute to *solid solution hardening*. The presence of a solute atom, different in size from that of the matrix, results in a localised strain field, which interacts with the strain field of the dislocation causing it to become locked. An additional stress is thus required to release the dislocation before it can move in the solid solution. As discussed by Haasen [4], this additional stress is proportional to a misfit parameter, δ , defined as

$$\delta = \frac{1}{a} \cdot \frac{\partial a}{\partial c} \quad (14)$$

where a is the lattice constant of a cubic material.

The presence of solute atoms also results in an internal stress field which imposes a friction on the movement of dislocations through the lattice. According to Cottrell [5], the effect of this interaction on the yield strength, σ , of the

material is given by

$$\sigma = 2.5\mu (\delta)^{\frac{2}{3}} c \quad (15)$$

where μ is again the shear modulus. In a refinement of the theory to take account of the influence of the solute atom on the shear modulus, Fleischer [6] has proposed an equation for the critical resolved shear stress in a crystal which may be written in the form [4, 23]

$$\tau_c \simeq \mu |\eta' - \alpha \delta|^{\frac{2}{3}} \cdot c^{\frac{2}{3}} / 700 \quad (16)$$

where $\eta' = \eta / (1 + \frac{1}{2} |\eta|)$, $\eta = 1/\mu (\partial \mu / \partial c)$, α is equal to 10 for edge dislocations and 3 for screw dislocations and δ is the misfit parameter.

The misfit parameter δ , which has been defined for cubic materials, is mathematically equivalent to the linear size-factor in equation 4. Hence yet again the size-factors supply a ready means for computing yield strengths or critical resolved shear stresses which may be used for testing the validity of the theories of solid hardening as shown by Haasen [23] in a recent discussion of the subject.

5. Appendix

Values of Ω_{sf} , lsf and VLF and c_{\max} are listed in table II in alphabetical order of solvents and solutes. The same order is preserved in table III which contains the room temperature atomic volumes and Seitz radii of the elements. While every attempt has been made to cover the literature thoroughly, no doubt some alloy systems have been inadvertently overlooked. Perhaps in future those who consider that a solid solution is of sufficient importance to warrant a study, or remeasurement, of its lattice parameter changes with composition will make the additional effort to calculate the size-factors according to equations 1, 5 and 6, so that the present coverage can be extended or the accuracy of the values improved. The importance of keeping the tables up to date is illustrated by the values in table II for Ag-Hg, Ag-Mn, Al-Cu, Al-Mg, Al-Mn, Au-Co, Au-Cu, Cu-Cd, Fe-Mo, Fe-Ti, Fe-W, Mg-Al, and Mg-In, which differ significantly from earlier calculations [9, 11] based on less accurate lattice parameter data.

TABLE II Volume size-factors (Ωsf), linear size factors (lsf), Vegard's law factors (VLF) and limiting concentrations (c_{max}) for metallic solid solutions

† Lattice parameters have been measured across these mutual solid solutions from 0 to 100% solute.

Solution	c_{max} (at. %)	Ωsf (%)	lsf (%)	VLF (%)	Solution	c_{max} (at. %)	Ωsf (%)	lsf (%)	VLF (%)
Ag-Al	18	-9.18	-3.16	-8.89	-Ge	3.0	+5.54	+1.81	-20.94
-As	8.5	+10.35	+3.33	-12.61	-Hf	5.0	-3.30	-1.11	-26.01
-Au†	34	-1.78	-0.60	-1.22	-Hg	18	+18.90	+5.94	-13.95
-Bi	2.6	+70.92	+19.56	-17.59	-In	12	+20.57	+6.43	-21.86
-Cd	12	+14.84	+4.71	-9.10	-Li	15	-19.24	-6.88	-36.62
-Cu	12	-27.75	-10.27	+43.09	-Mn	7.0	-5.35	-1.82	+31.46
-Ga	18	-5.09	-1.73	-17.38	-Mo	1.2	-14.86	-5.22	-7.30
-Ge	7.5	+1.66	+0.53	-23.42	-Ni†	10	-21.92	-7.92	+21.03
-Hg	23	+14.00	+4.46	-17.06	-Pd†	40	-14.20	-4.98	-1.07
-In	12	+23.50	+7.28	-51.84	-Pt†	30	-12.62	-4.40	-1.87
-Mg	25	+7.13	+2.32	-21.38	-Sb	1.0	+34.62	+10.41	-24.44
-Mn	15	+0.09	+0.02	-86.02	-Sn	5.0	+28.78	+8.80	-19.27
-Pb	2.2	+54.52	+15.60	-13.09	-Ta	6.5	+3.40	+1.11	-2.68
-Pd†	21	-17.21	-6.10	-4.15	-Ti	12	-7.76	-2.66	-11.46
-Pt	10	-20.05	-7.19	-9.40	-Tl	0.8	+23.82	-7.43	-26.45
-Sb	6	+44.93	+13.16	+18.21	-V	8.0	-8.94	-3.08	+11.42
-Sn	10	+32.40	+9.81	-16.53	-Zn	18	-13.82	-4.84	-3.93
-Tl	6.5	+39.42	+11.71	-16.85	-Zr	7.0	+13.19	+4.21	-17.48
-Zn	35	-13.74	-4.80	-3.27	Ba-Ca	11	-10.03	-3.46	+31.38
Al-Ag	20	+0.12	+0.03	-2.55	-Sr	20	-9.32	-3.21	+3.11
-Ca	1.1	+177.10	+40.46	+6.12	Be-Al	0.6	+74.81	+20.46	-15.11
-Cr	0.8	-57.23	-24.66	-40.82	-Ni	1.5	+45.65	+13.36	+7.33
-Cu	2.2	-37.77	-14.62	-12.52	Bi-Sb†	100	+14.12	+4.95	Nil
-Ga	0.5	+4.94	+1.62	-11.06	Ca-Ba	30	+49.84	+14.44	+2.61
-Ge	2.0	+13.13	+4.19	-17.03	-Sr†	100	+30.51	+9.28	Nil
-Li	12	-2.10	-0.70	-24.82	Cd-Ag	6.0	-34.45	-13.13	-16.98
-Mg	15	+40.82	+12.08	+0.58	-Hg	25	+4.43	+1.45	-3.98
-Mn	3.5	-46.81	-18.98	-27.70	-Mg†	45	-1.60	-0.54	-8.32
-Pb	0.2	-53.63	-22.66	-84.67	Ce-Eu	5.0	+9.32	+3.01	-23.16
-Si	1.0	-15.78	-5.56	-30.17	-La†	25	+10.05	+3.24	+1.28
-Sn	0.1	+24.09	+7.45	-23.84	-Pu	30	-28.49	-10.58	-1.42
-Th	0.4	+156.61	+36.91	+29.65	-Th†	50	-7.29	-2.49	-3.12
-Ti	1.0	-15.06	-5.22	-20.17	Co-Al	17	+16.98	+5.36	-21.50
-V	0.6	-41.42	-16.37	-30.04	-Au	30	+59.12	+16.74	+4.43
-Zn	25	-5.74	-1.95	+2.89	-Cu	24	+6.99	+2.28	+1.09
As-Ge	16	-6.89	-2.35	-11.44	-Fe	20	+5.24	+1.71	-0.44
-Sb†	10	+6.49	+2.12	-24.20	-Ga	13	+17.42	+5.49	-33.22
-Sn	22	+14.19	+4.51	-8.89	-Ge	17	+15.08	+4.79	-43.36
Au-Ag†	32	-0.64	-0.21	-1.20	-Ir	50	+25.85	+7.96	-0.16
-Al	14	-10.17	-3.51	-8.26	-Mn	40	+7.33	+2.39	-2.14
-As	0.2	+17.69	+5.57	-7.31	-Mo	18	+29.44	+8.98	-7.54
-Cd	24	+13.14	+4.20	-10.94	-Ni†	100	-1.73	-0.61	Nil
-Co	8.5	-25.22	-9.23	-11.68	-Os†	25	+21.93	+6.82	-3.21
-Cr	20	-16.45	-5.82	+18.08					
-Cu†	46	-27.81	-10.29	+3.66					
-Fe	16	-19.87	-7.12	+10.16					
-Ga	11	-4.32	-1.46	-17.17					

QUANTITATIVE SIZE-FACTORS FOR METALLIC SOLID SOLUTIONS

Solution	c_{\max} (at. %)	Ω_{sf} (%)	lsf (%)	VLF (%)	Solution	c_{\max} (at. %)	Ω_{sf} (%)	lsf (%)	VLF (%)
-Pd†	20	+40.08	+11.89	+6.74	Er -Gd†	25	+10.14	+3.27	+1.91
-Pt†	25	+40.01	+11.87	+4.19	Fe -Al	25	+12.79	+4.08	-19.67
-Re	25	+30.50	+9.28	-1.61	-Au	0.6	+44.16	+12.96	+0.11
-Rh	40	+30.74	+9.34	+5.59	-Be	20	-26.23	-9.64	+6.90
-Ru	50	+21.67	+6.75	-0.73	-Co	20	+1.54	+0.50	+7.37
-Si	13	-6.39	-2.18	-47.87	-Cr†	9.0	+4.36	+1.43	+2.52
-Sn	3.0	+69.12	+19.13	-30.35	-Cu	0.7	+17.53	+5.52	+17.19
-W	7.0	+22.52	+6.99	-14.20	-Ge	10	+16.48	+5.21	-39.41
-Zn	10	+17.40	+5.48	-13.58	-Mn	10	+4.89	+1.60	+1.16
Cr -Al	38	+25.95	+7.99	-8.97	-Mo	2.0	+27.51	+8.43	-3.62
-Be	5.0	-18.17	-6.43	+21.18	-Nb	3.0	+17.58	+6.10	-23.08
-Co	25	-5.15	-1.75	+1.52	-Ni	5.0	+4.65	+1.52	+12.62
-Fe†	30	-2.07	-0.70	-0.41	-P	3.5	-13.16	-4.59	-46.56
-Ir	2.5	+53.34	+15.31	+30.08	-Pd	5.5	+62.19	+17.49	+29.67
-Mn	10	+0.65	+0.20	-0.83	-Ru	1.8	+19.92	+6.24	+4.21
-Mo†	40	+33.66	+10.14	+2.98	-Sb	2.5	+36.40	+10.90	-46.17
-Ni	11	-4.80	-1.63	+4.41	-Si	10	-7.88	-2.70	-45.82
-Rh	15	+17.57	+5.53	+2.47	-Sn	10	+67.70	+18.81	-26.64
-Si	7.5	-15.05	-5.29	-49.07	-Te	0.6	+8.66	+2.80	-62.34
-Ta	2.5	+43.98	+12.91	-3.71	-Ti	1.8	+14.44	+4.39	-23.72
-V†	18	+8.79	+2.86	-5.95	-V†	30	+10.51	+3.38	-6.27
-W†	20	+37.35	+11.15	+3.76	-W	7.0	+32.99	+9.97	-1.24
Cs -K†	25	-40.94	-16.10	-9.95	-Zn	24	+21.07	+6.58	-6.50
-Rb†	80	-20.80	-7.58	-0.44	Gd -Er†	55	-6.94	-2.37	+0.57
Cu -Ag	4.2	+43.52	+12.79	-0.60	-Lu†	20	-12.03	-4.18	-1.24
-Al	20	+19.99	+6.26	-14.66	-Y†	10	+0.21	+0.06	+11.86
-As	4.2	+38.77	+11.53	-23.87	Ge -Ga	1.0	+2.21	+0.72	+18.11
-Au†	40	+47.59	+13.85	+2.79	-Si†	25	-20.65	-7.42	-11.55
-Be	13	-26.45	-9.73	+7.10	-Sn	1.0	+49.53	+14.35	+25.12
-Cd	2.5	+67.40	+18.74	-8.22	In -Bi	4.0	+31.09	+9.44	-3.06
-Co	15	-3.78	-1.28	+1.84	-Cd	4.0	-15.24	-5.36	+2.86
-Cr	1.6	+19.72	+6.18	+17.85	-Hg	6.0	-11.55	-4.01	-3.53
-Fe	2.6	+4.57	+1.50	+4.87	-Li	14	-13.61	-4.76	+19.55
-Ga	20	+24.11	+7.46	-25.18	-Mg	35	-1.16	-0.39	+12.25
-Ge	11	+27.77	+8.51	-33.34	-Pb	12	+21.52	+6.70	+4.72
-Hg	3.0	+5.44	+1.78	-47.10	-Sn	7.5	+5.22	+1.70	+1.73
-In	10	+79.03	+21.42	-19.21	-Tl	20	+10.97	+3.52	+1.58
-Mg	3.2	+50.80	+14.67	-23.37	Ir -Cr	16	-16.12	-5.69	-1.11
-Mn	15	+34.19	+10.30	+28.69	-Mn	40	+6.04	-2.06	+8.84
-Ni†	32	-8.45	-2.90	-1.22	-Mo	18	+6.48	+2.11	-3.33
-P	2.0	+16.51	+5.22	-28.12	-Pd†	26	+2.83	+0.93	-1.21
-Pd†	31	+27.96	+8.56	+2.59	-Pt†	25	+8.09	+2.90	+1.24
-Pt†	40	+31.19	+9.47	+2.58	-Rh†	100	-2.64	-0.88	Nil
-Sb	6.0	+91.87	+24.25	-24.99	-Ru	25	-4.43	-1.50	-0.27
-Si	12	+5.08	+1.68	-38.02	-Ta	10	-14.14	+4.50	-10.38
-Sn	9.0	+83.40	+22.41	-19.92	-Ti	10	+8.62	+2.79	-13.03
-Th	1.5	+49.12	+14.25	-46.44	-W	20	+6.93	+2.26	-4.59
-Ti	0.25	+25.74	+7.93	-15.95	K -Cs†	25	+41.53	+12.27	-7.17
-Tl	2.5	+129.16	+31.84	-5.33					
-Zn	15	+17.10	+5.40	-9.09					

Solution	c_{\max} (at. %)	Ω_{sf} (%)	lsf (%)	VLF (%)	Solution	c_{\max} (at. %)	Ω_{sf} (%)	lsf (%)	VLF (%)
La -Ce†	25	-7.04	-2.40	+1.00	-V†	50	-10.64	-3.69	-0.83
-Y†	15	-8.97	-3.08	+3.34	-W†	34	+1.74	+0.57	-0.02
Li -Mg	50	-4.16	-1.41	-10.85	Nb-Fe	1.0	-38.37	-14.92	-5.87
Lu -Gd†	20	+14.03	+4.46	+1.57	-Hf	50	+18.58	+5.84	-4.32
-Tb†	23	+10.09	+3.25	+1.46	-Mo†	30	-16.45	-5.81	-3.04
Mg-Ag	3.0	-63.42	-28.48	+60.15	-Re	20	-25.37	-9.29	-8.70
-Al	9.3	-35.80	-13.73	-10.11	-Ru	25	-32.48	-12.27	-10.48
-Bi	1.0	+23.41	+7.25	-18.94	-Si	2.0	+4.96	+1.62	+23.49
-Cd†	16	-21.08	-7.59	-14.85	-Ta†	100	-0.26	-0.09	-0.26
-Cu	0.4	-6.59	-2.25	+83.73	-Ti	45	-3.00	-1.01	+5.02
-Ga	2.5	-35.58	-13.63	-18.44	-U†	20	+5.03	+1.65	-10.16
-Ge	0.1	+9.47	+3.06	+12.36	-V†	30	-17.81	-6.33	+6.68
-Hg	1.2	-41.78	-16.50	-42.24	-W†	30	-98.22	-6.49	-7.47
-In	10	-7.12	-2.43	-17.50	-Zr†	50	+27.11	+8.32	-1.65
-La	0.5	+80.80	+21.82	+12.54	Ni -Al	10	+14.70	+4.67	-24.41
-Li	5.8	-12.53	-4.38	-6.00	-Au†	15	+63.60	+17.83	+5.54
-Mn	2.5	-17.43	-6.18	+57.71	-Co†	100	+1.76	+0.58	Nil
-Pb	7.0	+14.11	+4.49	-12.54	-Cr	40	+10.34	+3.33	+0.86
-Sn	2.5	-1.25	-0.42	-15.15	-Cu†	68	+7.18	+2.33	-0.66
-Tl	9.1	-4.82	-1.63	-22.61	-Fe	58	+10.57	+3.40	+2.80
-Yb	1.2	+23.11	+7.17	-13.38	-Ga	20	+17.16	+5.41	-34.40
-Zn	3.0	-48.79	-20.00	-21.75	-Ge	10	+14.76	+4.68	-44.48
Mn-Al	10	+16.20	+5.13	-11.89	-In	5.0	+36.66	+10.96	-42.87
-As	3.7	+24.70	+7.63	-27.08	-Mn	25	+23.20	+7.20	+7.16
-Co	13	+3.06	+1.01	+16.62	-Mo	22	+22.27	+6.93	-14.05
-Cr	8.0	-4.78	-1.62	-0.30	-Nb	8.0	+51.24	+14.79	-7.90
-Cu	16	+21.16	+6.60	+29.54	-Os	12	+7.71	+2.51	-15.71
-Fe	10	-3.72	-1.25	+3.20	-Pd†	30	+41.33	+12.21	+5.03
-Ga	20	+27.12	+8.32	-18.44	-Pt†	25	+45.68	+13.37	+5.54
-Ge	7.5	+34.51	+10.39	-25.54	-Ru	20	+28.76	+8.79	+4.35
-In	15	+88.11	+23.44	-9.27	-Sb	5.5	+21.32	+6.65	-56.08
-Ni	14	+16.90	+5.34	+34.79	-Si	12	-5.81	-1.98	-48.53
-Pd	18	+79.74	+21.59	+53.09	-Sn	10	+74.08	+20.29	-29.70
-Pt	11	+67.34	+18.72	+41.50	-Ti	9.0	+29.43	+8.97	-19.84
-Re	5.0	+20.27	+6.35	-0.23	-V	20	+13.34	+4.26	-11.69
-Ru	10	+58.34	+16.55	+42.36	-W	15	+36.93	+11.04	-5.76
-Si	14	-15.44	-5.44	-46.70	-Zn	23	+19.90	+5.24	-13.74
-Zn	18	+36.79	+11.00	+13.12	Np-Pu†	40	+5.58	+1.82	-7.51
Mo-Cr†	30	-17.87	-6.35	+7.08	-U	10	+11.14	+3.58	+2.87
-Hf	20	+25.77	+7.94	-11.56	Os -Mn	30	+10.83	+3.48	+23.10
-Ir	7.0	-6.98	-2.38	+2.49	-Mo	40	+10.23	+3.30	-0.95
-Nb†	20	+12.80	+4.09	-2.80	-Re†	40	+4.27	+1.40	-1.98
-Os	10	-9.62	-3.32	+0.58	-Ru†	50	-2.49	-0.84	+0.33
-Pd	5.0	-4.49	-1.52	+1.06	-Ta	20	+29.57	+9.02	+0.53
-Re	15	-5.56	-1.89	-0.76	-Tc†	40	+1.83	+0.60	-0.68
-Rh	20	-10.40	-3.59	+1.41	-W	20	+11.04	+3.35	-2.32
-Ru	18	-5.92	-1.98	+7.98	Pb -Bi	20	+7.04	+2.29	-8.20
-Ta†	40	+12.68	+4.05	-2.66	-Ca	1.0	-7.78	-2.66	-35.50
-Ti†	8.0	+0.56	+0.18	-11.62	-Cd	5.0	-43.11	-17.14	-19.87

QUANTITATIVE SIZE-FACTORS FOR METALLIC SOLID SOLUTIONS

Solution	c_{\max} (at. %)	Ω_{sf} (%)	l_{sf} (%)	VLF (%)	Solution	c_{\max} (at. %)	Ω_{sf} (%)	l_{sf} (%)	VLF (%)
-Hg	10	-5.25	-1.78	+22.59	Pu -Al	11	-46.00	-18.57	-18.83
-In	14	-11.16	-3.87	+2.29	-Ce	20	+13.54	+4.32	-17.63
-Na	9.0	-2.49	-0.84	-25.16	-Hf	8.0	+0.93	+0.29	+13.12
-Sb	0.2	-14.08	-4.93	-13.78	-In	2.0	+29.33	+8.95	+23.35
-Sn	5.0	-8.25	-2.83	+2.94	-Np†	60	-16.87	-5.97	-5.10
-Te	0.3	-28.89	-10.74	-36.54	-Sc	6.0	+12.45	+3.98	+14.23
-Tl	40	-4.53	-1.53	+1.28	-U	0.3	-8.41	-2.89	+10.15
Pd -Ag†	20	+13.12	+4.19	-2.29	-Zn	3.0	-39.47	-15.41	-0.69
-Au†	20	+16.31	+5.10	+8.43	-Zr	10	+0.48	+0.15	+7.62
-Bi	0.2	+52.59	+15.12	-36.70	Rb -Cs†	80	+24.43	+7.54	-1.02
-Cd	30	+21.63	+6.73	-16.92	Re -Os†	30	-7.08	-0.34	-2.24
-Co†	20	-15.37	-5.41	+11.07	-Pt	20	+15.35	+4.32	+4.62
-Cr	10	-1.45	-0.49	+20.94	-Ru†	25	-9.02	-3.10	-1.34
-Cu†	48	-18.60	-6.63	+1.54	-Tc†	40	-2.85	-0.86	-0.42
-Fe	20	-11.71	-4.07	+10.43	Rh -Au	2.4	+9.15	+2.95	-11.41
-Hg	12	+32.09	-9.72	-17.21	-Cr	8.0	-7.27	-2.46	+6.27
-Ir†	20	-5.68	-1.93	-1.82	-Ir†	100	+2.72	+0.89	Nil
-Mn	28	+3.68	+2.20	+21.18	-Mn	30	+5.73	+1.88	+15.57
-Mo	10	-4.40	-1.49	-9.69	-Mo	15	+8.03	+2.61	-4.67
-Nb	12	+6.00	+1.96	-13.28	-Pd†	50	+7.56	+2.46	+0.58
-Ni†	12	-14.41	-5.06	+15.17	-Pt†	100	+10.52	+4.84	Nil
-Pb	14	+38.72	+11.52	-32.63	-Sn	10	+35.94	+10.77	-30.77
-Pt†	40	+1.52	+0.49	-1.46	-Ta	8.0	+23.85	+7.38	-5.46
-Rh†	26	-4.97	-1.68	+1.63	-W	14	+9.60	+3.20	-5.20
-Ru	10	-8.27	-2.84	-1.23	Ru -Ir	30	+5.36	+1.94	+0.71
-Sn	26	+27.08	+8.31	-30.98	-Mo	41	+12.20	+3.91	-1.00
-Ta	14	+6.47	+2.11	-12.99	-Nb	2.4	+13.19	+4.21	-14.64
-U	11	+9.43	+3.04	+9.43	-Ni	45	-16.30	-5.76	+3.74
-V	20	-2.45	-0.82	+2.19	-Os†	30	+4.64	+1.52	+1.70
-Zn	20	-8.40	-2.98	-11.34	-Pd	3.0	+2.28	+0.74	-5.91
-Zr	21	+27.20	+8.35	-19.69	-Re†	42	+7.29	+2.36	-1.06
Pt -Ag	30	+8.88	+2.88	-4.01	-Rh	5.0	-0.37	-0.12	-1.65
-Al	10	-9.25	-3.18	-17.74	-Ta	25	+26.23	+8.07	-4.91
-Au†	25	+10.99	+3.52	-1.17	-Tc†	25	+4.46	+1.46	-1.07
-Cd	27	+16.99	+5.36	-17.96	-V	33	+1.48	+0.48	-2.08
-Co†	22	-18.65	-6.65	+9.26	-W	36	+19.95	+6.25	+1.76
-Cr	44	-16.16	-5.70	+5.53	-Zr	0.5	-4.13	-1.40	+29.24
-Cu†	38	-20.11	-7.21	+2.18	Sb -As†	80	-17.97	-6.39	+15.23
-Fe	40	-10.02	-3.46	+15.46	-Bi†	100	+16.45	+5.20	Nil
-Hg	10	+19.89	+6.23	-22.70	-Ge	2.5	-45.31	-18.22	-27.02
-Ir†	45	-6.76	-2.31	-4.45	-Sn	4.0	-15.10	-5.31	-5.19
-Mo	38	-0.55	-0.18	-3.95	Sc -Y†	22	+42.70	+12.58	+4.87
-Nb	22	+6.06	+1.97	-10.98	-Zr†	40	-8.67	-2.98	-2.01
-Ni†	18	-23.39	-8.50	+5.75	Si -Ge†	25	+4.68	-1.53	-6.10
-Pd†	20	-4.01	-1.36	-1.52	Sn -Bi	5.0	+22.40	+6.96	-6.43
-Re	42	+2.02	+0.66	+4.57	-Cd	1.0	-14.79	-5.20	+6.99
-Rh†	100	-8.86	-3.04	Nil					
-Ru	60	-7.05	-2.41	+3.84					
-Si	1.0	-14.56	-5.11	-35.55					
-Sn	8.0	-1.32	-0.44	-44.90					
-U	4.0	+77.88	+21.15	+29.24					
-Zn	25	-7.68	-2.63	-8.38					

Solution	c_{\max} (at. %)	Ω_{sf} (%)	l_{sf} (%)	VLF (%)	Solution	c_{\max} (at. %)	Ω_{sf} (%)	l_{sf} (%)	VLF (%)
Sn -Hg	7.2	-17.46	-6.20	-4.70	-V	8.0	-15.40	-5.42	-6.57
-In	6.0	-3.14	-1.06	+0.12	-Zr†	30	+30.08	+9.16	-1.34
-Pb	1.0	+29.05	+8.87	+15.33	Tl -In	6.5	-7.06	-2.41	+1.61
-Sb	8.2	+5.47	+1.79	-5.56	U -Cr	1.4	+4.03	+1.33	+89.14
-Zn	0.7	-5.70	-1.94	+67.67	-Nb†	30	-24.49	-8.94	-11.73
Sr -Ba	20	+21.65	+6.74	+6.98	-Os	12	+15.99	+5.06	+15.99
-Ca†	100	-23.38	-8.49	Nil	-Pu	20	+1.41	-0.46	-15.82
Ta -Mo†	35	-16.56	-5.86	-3.40	-Ti	3.0	-8.00	-2.74	+8.06
-Nb†	100	-0.23	-0.08	-0.23	V -Al	50	+8.84	+2.87	-8.74
-Os	10	-28.47	-10.57	-7.82	-Cr†	40	-15.91	-5.61	-2.73
-Ru	25	-28.44	-10.56	-5.62	-Fe†	10	-18.86	-6.73	-4.34
-Ti	28	-3.59	-1.21	-1.64	-Mo†	50	+9.83	+3.18	-1.03
-V†	20	-10.02	-3.46	+15.43	-Nb†	20	+27.93	+8.55	-1.44
-W†	75	-13.13	-4.58	-1.43	-Ru	20	-14.56	-5.11	-12.30
-Zr	22	+12.91	+4.12	-12.67	-Ta†	70	+36.06	+10.80	-14.70
Tb -Lu†	23	-6.12	-2.08	+1.87	-W†	50	+12.64	+4.04	Nil
Tc -Co	40	-27.24	-10.06	-6.34	W -Cr†	20	-21.73	-7.84	+3.61
-Ir	15	-2.43	-2.19	-5.30	-Mo†	25	-1.55	-0.52	+0.18
-Ni	30	-24.32	-8.87	-0.99	-Nb†	25	+7.33	+2.39	-5.15
-Os†	50	-2.97	-1.00	-0.53	-Os	7.5	-7.82	-2.68	+1.09
-Pt	34	+0.38	+0.12	-4.50	-Pt	4.0	-2.71	-0.91	+2.09
-Re†	60	+2.24	+0.73	-0.26	-Ru	12	-5.35	-1.82	+10.54
-Rh	50	-6.61	-2.28	-2.88	-Si	20	+0.81	+0.27	-80.03
-Ru†	25	-6.39	-2.18	-1.16	-Ta†	45	+11.01	+3.54	-1.68
Th -Ce†	25	-1.21	-0.41	-5.47	-U	2.0	-0.82	-0.74	-24.23
-Pu	40	-19.71	-7.06	+5.76	-V†	30	-10.60	-3.66	+1.09
-Rh	1.0	-5.78	-1.89	+152.77	Y -Gd†	25	+0.65	+0.20	+0.39
-Ru	1.0	+3.65	+1.19	+151.19	-La†	25	+17.30	+5.46	+3.30
-U	5.0	-6.09	-2.07	+48.66	-Sc†	22	-20.95	-7.54	+7.57
-Y	30	+0.20	-0.05	-0.50	-Th	27	-2.38	-0.80	+0.18
-Zr	10	-7.68	-10.25	+2.06	Zn -Ag	5.5	-10.19	-3.52	-19.91
Ti -Ag	5.0	-9.28	-3.20	-6.03	-Al	1.5	-6.25	-2.13	-16.93
-Al	27	-20.09	-7.20	-13.92	-Au	5.5	-10.98	-3.80	-20.17
-Cr	20	-37.71	-14.60	-8.32	-Cd	1.2	+49.23	+14.27	+5.38
-Fe	20	-53.62	-22.59	-30.35	-Cu	3.0	-54.57	-23.13	-41.49
-Hf	25	+3.91	+1.28	-17.31	-Ga	2.0	+25.33	+7.79	-2.74
-Mn	13	-51.17	-21.25	-31.48	-Hg	4.0	+39.52	+11.74	-9.59
-Mo†	40	-20.96	-7.64	-11.09	Zr -Dy	7.5	+26.92	+8.27	-6.21
-Re	50	-30.16	-11.28	-16.10	-Nb†	2.0	-6.40	-2.18	+21.15
-Rh	15	-32.15	-12.13	-12.94	-Sc†	24	+4.51	+1.48	-2.59
-Ru	20	-33.75	-12.82	-15.83	-Th	50	+51.67	+14.89	+8.52
-Sn	11	+13.60	+4.26	-25.97	-Ti†	10	-22.33	-8.08	+2.41
-Ta	5.5	+0.28	+0.08	-1.69					

[See Table III on following page

TABLE III Atomic volumes (Ω) and Seitz radii (r_0) of the elements at room temperature

Element	Atomic Number	$\Omega(\text{\AA}^3)$	$r_0(\text{\AA})$	Element	Atomic Number	$\Omega(\text{\AA}^3)$	$r_0(\text{\AA})$
Ac	89	37.48	2.076	Nd	60	34.18	2.013
Ag	47	17.06	1.598	Ni	28	10.94	1.377
Al	13	16.60	1.582	Np	93	19.22	1.662
Am	95	33.77	2.005	Os	76	13.99	1.495
As	33	21.54	1.726	P	15	16.59	1.582
Au	79	16.96	1.594	Pa	91	24.94	1.812
B	5	7.67	1.22	Pb	82	30.33	1.949
Ba	56	62.59	2.463	Pd	46	14.72	1.521
Be	4	8.112	1.246	Po	84	37.43	2.075
Bi	83	35.38	2.036	Pr	59	34.15	2.013
C	6	5.678	1.107	Pt	78	15.10	1.534
Ca	20	43.48	2.181	Pu	94	23.4	1.77
Cd	48	21.58	1.726	Rb	37	92.67	2.80
Ce	58	34.37	2.017	Re	75	14.70	1.520
Co	27	11.13	1.385	Rh	45	13.77	1.487
Cr	24	12.00	1.423	Ru	44	13.57	1.480
Cs	55	115.17	4.865	S	16	25.52	1.826
Cu	29	11.81	1.413	Sb	51	30.20	1.932
Dy	66	31.52	1.960	Sc	21	23.41	1.775
Er	68	30.64	1.941	Se	34	27.27	1.863
Eu	63	48.86	2.268	Si	14	20.02	1.669
Fe	26	11.77	1.411	Sm	62	33.01	1.990
Ga	31	19.59	1.672	Sn	50	27.65	1.862
Gd	64	33.10	1.992	Sr	38	56.32	2.378
Ge	32	22.64	1.755	Ta	73	18.01	1.626
Hf	72	22.16	1.743	Tb	65	31.14	1.954
Hg*	80	23.42	1.775	Tc	43	14.213	1.503
Ho	67	31.12	1.951	Te	52	33.98	2.005
In	49	26.15	1.841	Th	90	32.86	1.987
Ir	77	14.14	1.500	Ti	22	17.65	1.614
K	19	75.31	2.618	Tl	81	28.58	1.892
La	57	37.12	3.335	Tm	69	30.10	1.930
Li	3	21.61	1.728	U	92	20.81	1.706
Lu	71	29.50	1.917	V	23	13.88	1.491
Mg	12	23.23	2.853	W	74	15.85	1.549
Mn	25	12.21	1.428	Y	39	33.01	1.990
Mo	42	15.58	1.550	Yb	70	33.02	1.990
Na	11	39.50	2.113	Zn	30	15.24	1.538
Nb	41	17.98	1.625	Zr	40	23.27	1.771

*Measured at sub-zero temperature.

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