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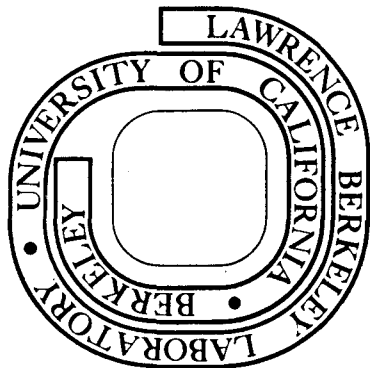
Charles W. Krause and J. W. Morris, Jr.

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ON THE DETERMINANTS OF THE STABILITY OF METALLIC PHASES

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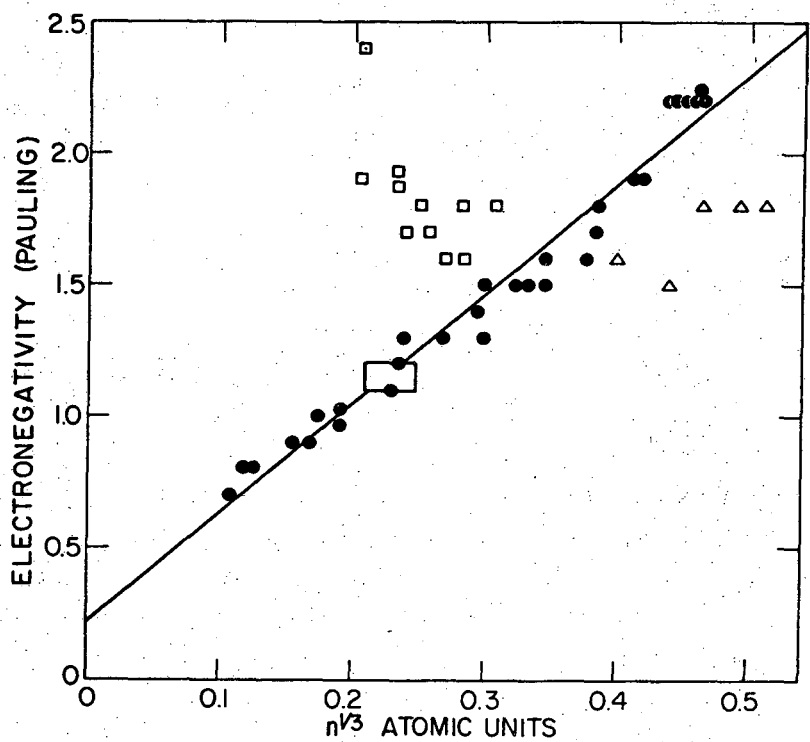
The phase stability of metallic alloys is often discussed in terms of three factors (1): the electron-atom ratio, the size factor, and the electrochemical effect. Three variables commonly used to quantify these factors are the valence (Z), the atomic volume (Ω), and the electronegativity (χ), respectively, of the metallic elements composing an alloy. The description of phase stability in terms of these three parameters would have maximum utility, if they were independent variables. However, it is shown below that, for a commonly used scale of electronegativities, the three parameters are not independent for a large number of metallic elements. In fact, such an interdependence is suggested by a number of expressions for χ in terms of Z and measures of atomic or molecular size (2). The expression obtained below uses the atomic volume derived from the elemental, metallic solids.

The interdependence of Z , Ω and χ for a large number of alloy systems is indicated in Fig. 1, in which are plotted the electronegativities of Pauling (3) for the metallic elements from groups IA through IVB of the periodic chart (4) and the lanthanides as a function of $n^{1/3}$, where n is what may be called the bonding electron density, $n = Z/\Omega$, with Z equal to the number of bonding electrons per atom for the element, and Ω equal to the atomic volume as determined from the elemental solid. The values of Z were taken as the group numbers (4) from the periodic chart, except for the cobalt and nickel groups and the lanthanides for which the values nine, ten and three were used. Values of Ω were taken from Barrett and Massalski (5).

The only elements which are metals in the solid state and are not included in Fig. 1 are francium, radium and the actinides. The other metals divide themselves into three classes in Fig. 1: 1) the metals from groups IA through VIIIIC, aluminum and the lanthanides; 2) the magnetic transition metals: chromium, manganese, iron, cobalt and nickel; and 3) the metals from groups IB through IVB. The three classes are shown with distinct symbols and contain forty-four, five and eleven elements respectively. The linear trend of the electronegativities with $n^{1/3}$ for the first class of metals establishes a relation between χ and n , or χ , Z and Ω , for these elements. The straight line in the figure is expressed by

$$\chi = 4.2 n^{1/3} + .2 = 4.2 \left(\frac{Z}{\Omega} \right)^{1/3} + .2$$

and was found by a least squares fit for the elements from groups IA through VIIIC (excluding the magnetic transition metals) and aluminum.



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FIG. 1

The electronegativities of the metals according to Pauling plotted versus $n^{1/3}$.

- - Metals from groups IA-VIIIC and aluminum.
- ▲ - Cr, Mn, Fe, Co, and Ni.
- - Metals from groups IB-IVB.

The box represents the lanthanides.

This interdependence between χ , Z and Ω indicates that the through factors are not independent for alloys of the forty-four elements included in class 1. Admittedly, use of these parameters is arbitrary, but at least the value of efforts (6) to find an independent set of variables with which phase stability can be studied is indicated.

Acknowledgement

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References

1. C. S. Barrett and T. B. Massalski, Structure of Metals, 3rd ed., McGraw-Hill, New York (1966).
2. H. O. Pritchard and H. A. Skinner, Chem. Revs., 55, 745 (1955).
3. L. Pauling, The Nature of the Chemical Bond, 3rd ed., Cornell, Ithaca, 88 (1960).
4. Reference to the periodic chart will be as in W. Hume-Rothery and G. V. Raynor, The Structure of Metals and Alloys, 3rd ed., The Institute of Metals, London (1954).
5. C. S. Barrett and T. B. Massalski, Structure of Metals, 3rd ed., McGraw-Hill, New York, p. 626 (1966).
6. C. H. Hodges and M. J. Stott, Phil. Mag., 26, 375 (1972); A. R. Miedema, J. Less Common Metals, 32, 117 (1973); A. R. Miedema, F. R. de Boer and P. F. de Chatel, J. Phys. F, 3, 1558 (1973).

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