

Two-Parameter Scaling of Inverse Compressibility and Its Relation to Atome and Electron Concentrations of Main-Group Solid Elements

Seung-Am Cho^{1,2} and Maria G. Santana¹

¹ Department of Materials Science, Venezuelan Institute of Scientific Research (IVIC), Apartado 21827, Caracas 1020A, Venezuela

² School of Metallurgical Engineering and Materials Science, Central University of Venezuela, Apartado 50361, Caracas 1050A, Venezuela

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The scaling of the inverse compressibility (bulk modulus B) of the main-group solids with their valence Z and atomic volume V_a revealed the validity of a simple two-parameter function $B = b f(Z, V_a)$, regardless of the type of bond and lattice structure of the solid, with a unique constant $b = 3.0 \times 10^{-19}$ joules per electron.

Key words: Bulk modulus; Role of atomic volume and valence; Main-group solid elements.

1. Introduction

Failure of the applicability of the free electron theory on the calculation of the bulk modulus B (inverse compressibility β) of the alkali metals has been demonstrated [1–3]. Although it has become possible to describe the bulk modulus of elemental solids including transition metals by advanced theory with considerable confidence [4–13], a rigorous quantum mechanical treatment of the behavior of the electrons in a crystal is extremely difficult and, in practice, the details of the calculations involve various approximations and refinements, so that conclusions are still qualitative.

As the major variables in those calculations of B are mainly based on the valence Z and the atomic size either in radius r or in atomic volume V_a ,

$$B = b f(Z, V_a), \quad (1)$$

we have analysed in detail the validity and significance of (1) by scaling B with Z and V_a of the main-group (Group I through Group VI) solids that consist of s-block and p-block elements in the Periodic Table. The main-block solids have been selected because the valence of these common elements is definite, unlike that of transition elements, and the atomic volume of these solids is periodic and varies uniformly [14].

2. Scaling of Experimental Data

The unit of B is converted from pressure to energy density. Literature values of the experimental isothermal bulk modulus B are plotted in Figs. 1 and 2 according to the relations

$$B = b C_e \quad (2)$$

and

$$B = b Z C_a, \quad (3)$$

respectively, where $C_e = Z/V_a$ is the valence electron concentration and $C_a = 1/V_a$ the atome concentration. Both plots revealed linear correlations with a unique proportional constant $b = 3.0 \times 10^{-19}$ joules per electron. The deviations in the present correlations are smaller than the errors involved in some typical sophisticated theoretical calculations [11, 13, 15, 16].

3. Conclusions

The encountered dependence of B on Z testifies that the valence electrons are responsible for the bulk modulus. It further demonstrates that it is irrelevant whether the electrons are s-electrons or p-electrons. Rather, what matters is the number of valence electrons per atom. The present outcome also supports the role the atomic size plays in many physicochemical properties of solids [14].

An interesting observation is that the bulk modulus-volume relationship of many other solids (molecular solid hydrogen and deuterium [17], various inorganic

Reprint requests to Professor Dr. Seung-Am Cho, Venezuelan Institute of Scientific Research, (IVIC), Apartado 21827, Caracas 1020A, Venezuela.

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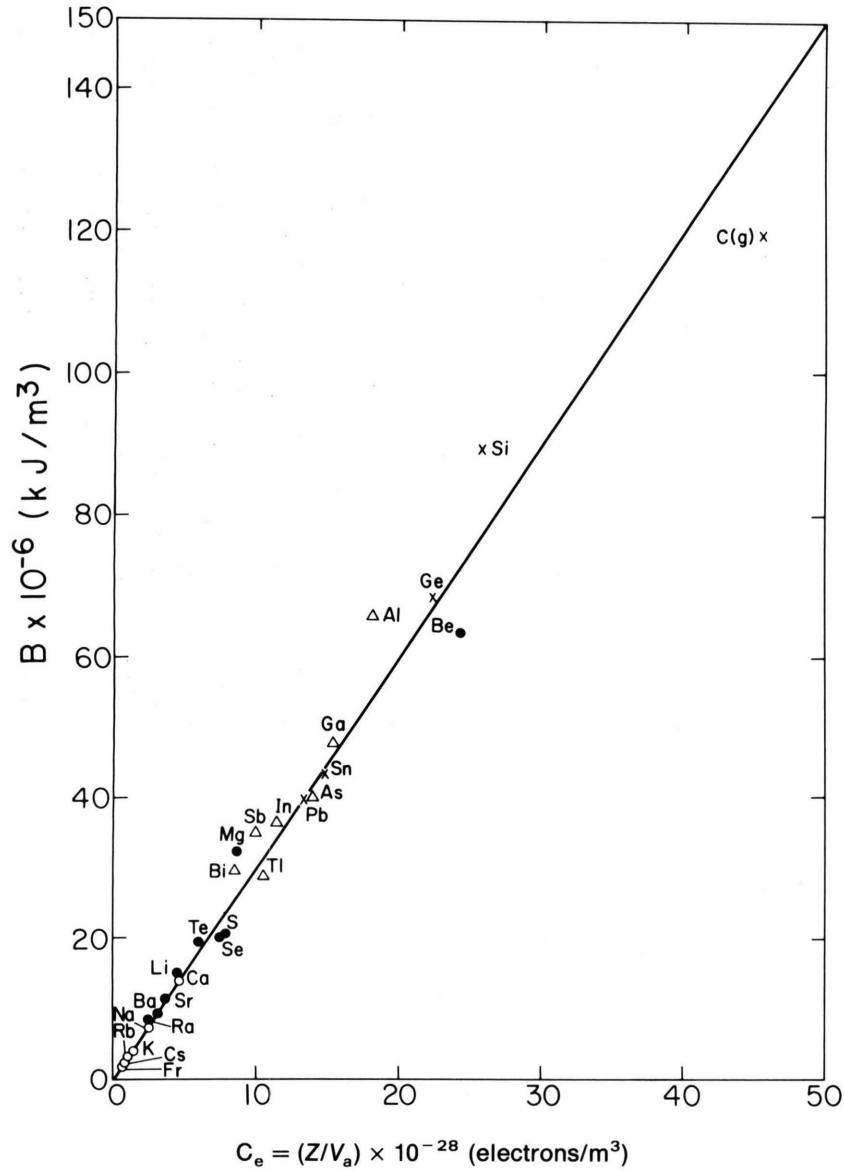


Fig. 1. Scaling of bulk modulus B vs. valence electron concentration $C_e = (Z/V_a)$.

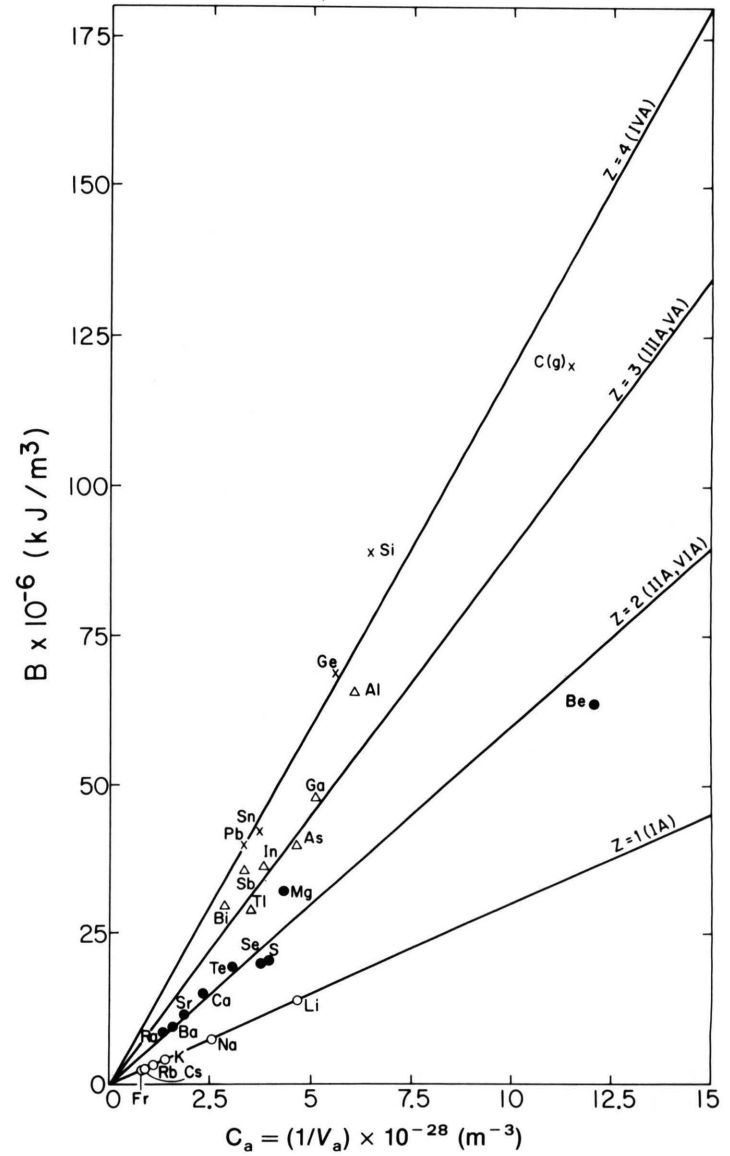


Fig. 2. Scaling of bulk modulus B vs. atomic concentration C_a (inverse of atomic volume V_a^{-1}).

compounds [18, 19], glass [20] and polymers [21]) is similar to that of our present examples. This similarity leads us to think that the voluminous valence electron clouds surrounding the core ions of solids act as fluid regardless of the bond type of the substance. This view of a solid is different from that of harmonic oscillators

of thermally vibrating atoms [22] interconnected by conceptual springs with force constants [23] in Lindemann's mechanical theory of fusion of solids. These two views of a solid may, however, be reconcilable if one regards the bulky interionic clouds of the electron gas in the solid body as interionic elastic springs.

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