The three-dimensional considerations implicit in wall calculations are seldom mentioned. In fact, it is usual to assume that a minimum of G has been found when, in fact, all that has been found is a solution of the Euler equations (8). Nothing is said about the substitution of another boundary condition for the one that comes, just as unambiguously as does the differential equation, out of the formal variational procedure; and nothing is said about the sign of the second variation, which determines the stability. It does not follow from this that the usual calculations are necessarily not useful, but it does follow that they are lacking in completeness and consistency.

Finally, let us examine, from a three-dimensional point of view, a uniform state that was found stable under the constraint of one-dimensionality. If the magnetization has no component along Oz, the state is stable with respect to arbitrary three-dimensional variations; for every term in G is at a minimum with respect to such variations. But if there is a z component, removal of the constraint may allow a decrease of G by development of a structure nonuniform in x and y; for such nonuniformity can decrease the magnetostatic energy. Thus domain formation appears to be an essentially two- or three-dimensional phenomenon.

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Hardness of Nonmetallic Solids on an Atomic Basis

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Hardness values of 65 nonmetallic crystalline solids of 16 different structures are compared with data of a newly introduced concept: "the volumetric lattice energy." When such solids are classified according to a new interpretation of lattice anharmonicity, a set of linear interrelations is obtained which covers the entire hardness range. Thus, on the basis of interatomic cohesive forces, the over-all hardness of these solids becomes unambiguously defined. Hardness receives the dimension (ergs/cm³) or (kcal/cm³), and an absolute scale. Such hardness data become independent of anisotropy, structure type, and valency of the atoms. Conversion from relative to absolute hardness, as well as estimation of lattice energy data through appropriate hardness testing, becomes possible. For example, the extremely high hardness value of the rare type-II diamond could be determined to be 1.7 times that of the type-I diamond, purely from atomic data. Analogous treatment of the hardness of metallic solids poses additional problems.

I. INTRODUCTION

LL hardness measurements are relative, and the A data obtained by the many different methods of hardness testing are for the greater part not comparable with one another.¹ The hardness of a solid is defined by the resistance against lattice destruction and is considered to be a function of the interatomic forces.² Attempts towards a physical definition of hardness were made by Friedrich, Goldschmidt and others.³ Yet hardness has in general defied unambiguous physical

definition.⁴ This presentation intends to develop such a definition.

The vast majority of hardness data of crystals are given in numerical units according to Mohs (M scale). Therefore, the experimental hardness data of this study for the greater part refer to this M scale. As recent work shows, there is a sound physical basis upon which equal intervals of scratch-hardness can be constructed and, in fact, the M scale follows it surprisingly well up to the relative hardness H=9.5 About 99% of all known materials belong to a hardness range from H=1 to H=9, while the relative difference in hardness between successive materials is small within this range. Thus the *M* scale is quantitatively useful up to H=9.

However, the complementary range between corundum and diamond (corresponding to H=9 and 10 in

¹ H. Tertsch, Neues Jahrb. Mineral. Monatsh., p. 121 (1955). ² C. W. Stillwell, *Crystal Chemistry* (McGraw-Hill Book Company, Inc., New York, 1938), pp. 29, 225–239. R. C. Evans, *An Introduction to Crystal Chemistry* (Cambridge University Press, New York, 1948), pp. 21-23. H. Tertsch, Festigkeitserscheinungen der Kristalle (Springer-Verlag, Vienna, 1949), pp. 171–257. H. von Weingraber, Technische Haerlemessung (C. Hauser-Verlag, Muenchen, 1952). C. Zwicker, Physical Properties of Solid Mate-rials (Pergamon Press New York, 1954), pp. 258–261. H. G. F. Winkler, Struktur und Eigenschaften der Kristalle (Springer-Verlag, Derlig, 1955) np. 266–395

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⁴ H. Tertsch, reference 2. D. Tabor, Endeavour 13, 27 (1954). W. F. de Jong, *General Crystallography* (W. H. Freeman & Com-pany, San Francisco, 1959), pp. 236. ⁵ E. Troeger, Neues Jahrb. Mineral. Monatsh. 233 (1954). D. Tabor, Proc. Phys. Soc. (London) **B67**, 249 (1954) (includes a compilation of pertinent literature). D. Tabor, Endeavour 13, 27 (1954).

the M scale) constitutes a much wider region with great differences in hardness between the few known materials within this range. Therefore, for the region above H=9, we employ the results of hardness testing according to Wooddell, who measured the relative resistance to abrasion during lapping.⁶ Wooddell fixed the hardness values of quartz and corundum at 7 and 9, (in agreement with the M scale), and extended the relative hardness scale in a linear-proportional sense. Consequently, Wooddell's linear-proportional hardness scale (W scale), ranging from corundum to diamond (H=42.5for South American diamonds) covers 80% of the known hardness region, although less than 1% of all solids have a hardness greater than that of corundum. A combina-

II. A PHYSICAL DIMENSION OF HARDNESS

tion of both the W scale and the M scale is justified

because of the overlapping interval.

The recent first determination of lattice energy data for a number of solids harder than corundum (such as SiC, BN, and the two types of diamond) from their respective infrared spectra,⁷ combined with a study on lattice anharmonicity,7 formed a basis for an examination of hardness from the atomic aspect. In technical hardness testing, hardness can be defined by a pressure or force per square centimeter (kg/cm^2) , and thus be conceived as an energy per volume (kgcm/cm³), e.g., the ratio between input energy and abraded volume.

Proceeding now to the atomic aspect, we should likewise have the dimension of an energy per volume for the resistance of the lattice against destruction during hardness testing. Thus we examine this resistance as a function of "the lattice energy per unit volume," and call it "volumetric lattice energy," U/V, having the dimension (ergs/cm³) or (kcal/cm³), where U = the total cohesive energy of the lattice (lattice energy) per

TABLE I. Data pertinent to A solids.

No.	Substance	Structure	X_m	<i>V</i> (cm³)	U (kcal/ mole)	U/V (kcal/ cm³)	H (combined <i>M-W</i> scale)
1	LiF	rock salt	0.27	11.3	246	21.8	3.5
2	LiCl	rock salt	0.31	20.2	203	10.0	3
- 3	LiBr	rock salt	0.34	25.2	203	8.0	3
4	NaF	rock salt	0.56	15.0	218	14.5	3.3
5	MgF_2	rutile	0.58	20.1	797	40	4.5
6	BeO	wurtzite	0.31	8.2	1055	129	8.5
7	MgO	rock salt	0.52	11.3	944	84	6.3
8	Al ₂ O ₃	α-corundum	0.54	24.5	3620	148	9
ġ.	SiO ₂	B-quartz	0.55	26.5	3090	116	7
10	CaO	rock salt	0.62	16.7	823	49	4.5
11	MnO	rock salt	0.67	13.0	923	71	5.5
12	NiO	rock salt	0.68	11.7	960	82	6
13	CaSO	harite ¹⁰	0.62	48.3	667	14	3.2
14	BN	zinc blende	0.33	10.8	54004	500	~195
15	SIC	zinc blende	0.45	12.7	42004	330	14
16	$\tilde{C} = C I$	type I diamond	0.32	6.0	0400a	1350	42 5
17	$\tilde{C} = \tilde{C}$	type II diamond	0.32	6.0	17 000a	2450	(71)
11	c - c n	cype-ii diamonu	0.32	0.9	11 000*	2130	(11)

* U data determined from pertinent infrared spectra.⁷ ^b The hardness of BN is known to be closer to the hardness of diamond than any other solid except BC, Therefore, it has been assumed that BN, whose U value was determinable,⁷ has approximately the same hardness as BC.⁶

TABLE II. Data pertinent to B solids.

Substance	Structure	X_m	V (cm²)	U (kcal/ mole)	U/V (kcal/ cm ³)	H (M scale)
Substance TiO ₂ MnO ₂ Cu ₂ O ZnO Y ₂ Fe ₃ O ₁₂ SrO CdO SnO ₂ BaO PbO ₂ KF CaF ₂ ZnF ₂ CdF ₂ BaF ₂ PbO ₂ KF MgS CdF ₂ BaF ₂ PbF ₂ MgS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS CaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS BaS SrS CdS SrS SrS CdS SrS SrS CdS SrS SrS CdS SrS SrS CdS SrS SrS CdS SrS SrS CdS SrS SrS Cd	structure rutile tenorite cuprite wurtzite garnet rock salt rock salt rock salt fuorite fluorite zinc blende rock salt zinc blende rock salt cock salt cock salt cock salt cock salt fluorite rock salt	X_m 0.65 0.69 0.69 0.73 0.76 0.78 0.76 0.78 0.76 0.78 0.76 0.78 0.79 0.79 0.79 0.74 0.94 0.74 0.94 0.74 0.94 0.74 0.94 0.74 0.94 0.73 0.75 0.76 0.73 0.75 0.79 0.79 0.79 0.79 0.73 0.75 0.79 0.79 0.79 0.79 0.73 0.76 0.79 0.79 0.79 0.73 0.76 0.79 0.79 0.79 0.74 0.74 0.74 0.74 0.74 0.75 0.76 0.79 0.79 0.74 0.74 0.74 0.74 0.74 0.74 0.74 0.74	V (cm ³) 21.0 18.2 12.5 22.0 15.1 145 22.0 23. 24.3 24.3 21.3 36.5 22.5 36.5 25.8 22.4 22.5 36.5 22.5 36.5 22.4 22.5 30.5 25.4 22.5 30.5 25.5 25.4 25.5 26.8 21.5 25.5 26.8 21.5 25.8 25.	U (kcal/mole) 2900 3100 920 740 952 25000 740 25000 740 2800 740 2800 740 2800 740 2800 740 2800 740 2800 740 2800 740 2800 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 740 740 2800 740 740 740 740 740 740 2800 740 740 740 740 740 2800 740 740 740 740 2800 740 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 740 740 2800 772 564 599 597 804 804 805 805 805 805 805 805 805 805 805 805	U/V (kcal/ cm ³) 138 170 73 31 63 170 73 31 63 27 27 5 75 27.5 27.5 27.5 27.5 27.5 27.	H (M (M 3.5 4 4.5 4 4.5 7 4.2 6 3.5 5.3 2.8 4 4.3 3.2 4.2 3.8 4 4.3 3.2 4.2 3.3 3 3.3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
KBr CuBr AgBr NaI KI CuI AgI	rock salt rock salt rock salt rock salt rock salt zinc blende zinc blende	$ 1.42 \\ 1.92 \\ 2.45 \\ 1.05 \\ 1.61 \\ 2.30 \\ 3.20 $	43 31 29.3 41 53 33.8 41.5	160 232 212 167 152 231 211	4 7.5 7 4 3 7 5	2.4 2.4 2 2.3 2.3
	Substance TiO ₂ MnO ₃ CuO CuO CuO CuO SnO ₂ SrO ₂ Solution SnO ₂ BaO PbO ₂ KF CaF ₂ SrF ₂ CdF ₂ BaF ₂ PbO ₂ KF MgS CdF CaS MnS FeS Cu ₂ S SrS CdS BaS SrSO ₄ BaSO ₄ PbSO ₄ Si-Si Ge-Ge NaCl KCl CaCl ₂ CaCl ₂ SrSO ₄ PbSO ₄ Si-Si Cu ₂ S SrS CdS BaS SrSO ₄ PbSO ₄ Si-Si Cu ₂ S SrS Cu ₂ S SrS SrS Cu ₂ S SrS Cu ₂ S SrS Cu ₂ S SrS Cu ₂ S SrS Cu ₂ S SrS SrS Cu ₂ S SrS Cu ₂ S SrS SrS Cu ₂ S SrS SrS Cu ₂ S SrS Cu ₂ S SrS Cu ₂ S SrS Cu	Substance Structure TiO2 rutile MO2 rutile CuO tenorite CuO tenorite CuO tenorite CuO tenorite CuO tenorite CuO tenorite CuO wurtzite SrO rock salt CdO rock salt BaO rock salt CaF2 fluorite SrF3 fluorite SrF4 fluorite BaF2 fluorite MnS zinc blende FeS nickel arsenide CuS zinc blende FeS nickel arsenide CuS zinc blende SrS rock salt SrS0. barite BaS0. barite SrS0. barite PbS0. barite SrS0. barite SrCl3 fluorite NaCl rock salt CaCl	SubstanceStructure X_m TiO2rutile0.65MnO2rutile0.67CuOtenorite0.69CuOcuprite0.69CuOwurtzite0.69SrOrock salt0.73CdOrock salt0.73CdOrock salt0.73CdOrock salt0.76BaOrock salt0.76BaOrock salt0.70SrF2fluorite0.70SrF2fluorite0.70CdF2fluorite0.70CaF2fluorite0.80KFrock salt0.70ZnF2fluorite0.81CdF2fluorite0.96MnSzinc blende1.09FF2fluorite0.96MnSzinc blende1.10CuSzinc blende1.13ZnSzinc blende1.40SrSrock salt0.77PbS04barite0.77PbS054barite0.77PbS054barite0.77PbS054barite0.77SrS04barite0.77ShaSO4barite0.77ShaSO4barite0.77ShaSO4barite0.77ShaSO4barite0.77ShaSO4barite0.77ShaSO4barite0.77ShaSO4barite0.78ShaClrock salt1.36AgClrock salt1.35 <tr< td=""><td>$\begin{array}{c ccccccccccccccccccccccccccccccccccc$</td><td>Substance Structure X_m (cm^3) $mole$ TiO2 rutile 0.65 21.0 2900 MnO2 rutile 0.67 18.2 3100 CuO tenorite 0.69 12.5 920 CuO cuprite 0.69 13.1 952 YaFeeJO12 garnet 0.70 145 25 000 StO rock salt 0.73 12.5 910 SnO1 rutile 0.76 145 25 000 BaO rock salt 0.73 22.0 790 CdO rock salt 0.73 22.0 790 CdO rock salt 0.73 22.0 790 SnO2 rutile 0.80 29.0 2830 KF rock salt 0.76 21.3 670 Strf2 fluorite 0.81 36.4 597 GdS zock salt 0.76 21.3 670</td><td>SubstanceStructure$X_m$$U$$U/V$$U/V$SubstanceStructure$X_m$$(cm^3)$mole)$cm^3$TiO2rutile0.6521.02900138MnO2rutile0.6912.592073Cuotemorite0.6912.592073Cuocuprite0.6923.974031ZnOwurtzite0.6921.592073SrOrock salt0.7314525 000*172SrOrock salt0.7518.591149SnO2rutile0.8029.0283097KFrock salt0.7624.366227.5ZnF2fluorite0.7923.656415.6PbO2rutile0.8136.459716.4CdF2fluorite0.8136.556415.6PbF2fluorite0.9429.779932.2MgSrock salt0.7419.577840CaSrock salt0.7419.577840CaSrock salt0.7419.484043CusSzinc blende1.0922.89440Resnickel arsenide1.1019.484043CusSzinc blende1.6527.538017ZnF2fluorite0.7346.364714Sinoszinc blende1.0922.894<</td></tr<>	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Substance Structure X_m (cm^3) $mole$ TiO2 rutile 0.65 21.0 2900 MnO2 rutile 0.67 18.2 3100 CuO tenorite 0.69 12.5 920 CuO cuprite 0.69 13.1 952 YaFeeJO12 garnet 0.70 145 25 000 StO rock salt 0.73 12.5 910 SnO1 rutile 0.76 145 25 000 BaO rock salt 0.73 22.0 790 CdO rock salt 0.73 22.0 790 CdO rock salt 0.73 22.0 790 SnO2 rutile 0.80 29.0 2830 KF rock salt 0.76 21.3 670 Strf2 fluorite 0.81 36.4 597 GdS zock salt 0.76 21.3 670	SubstanceStructure X_m U U/V U/V SubstanceStructure X_m (cm^3) mole) cm^3 TiO2rutile0.6521.02900138MnO2rutile0.6912.592073Cuotemorite0.6912.592073Cuocuprite0.6923.974031ZnOwurtzite0.6921.592073SrOrock salt0.7314525 000*172SrOrock salt0.7518.591149SnO2rutile0.8029.0283097KFrock salt0.7624.366227.5ZnF2fluorite0.7923.656415.6PbO2rutile0.8136.459716.4CdF2fluorite0.8136.556415.6PbF2fluorite0.9429.779932.2MgSrock salt0.7419.577840CaSrock salt0.7419.577840CaSrock salt0.7419.484043CusSzinc blende1.0922.89440Resnickel arsenide1.1019.484043CusSzinc blende1.6527.538017ZnF2fluorite0.7346.364714Sinoszinc blende1.0922.894<

• U data determined from pertinent infrared spectra.? • In determining X_m for the SO₄ compounds, only adjacent metal and oxygen ions are taken into consideration, since the S ions **ar**e shielded by the O ions, as a result of their tetrahedral coordination.

mole, V = the mole volume, defined as M/s, M = the molecular weight, and s = the specific weight. Tables I and II show values of "volumetric lattice energy" and relative hardness for 65 minerals and inorganic crystals (semiconductors and nonconductors) of 16 different structure types, for which pertinent data are on hand.^{3,8} The vast majority of them are binary compounds and some are either ternary compounds or elements. The number of these crystalline substances is limited by the requirement that data for both relative hardness and lattice energy be known. It should be noted that the above solids have H values from 2 to 42.5. In Figs. 1 and 2 the H values of these solids are plotted against their respective U/V values.

⁶ C. E. Wooddell, Trans. Electro. chem. Soc. 68, 11 (1935).

⁷ J. N. Plendl, Phys. Rev. 123, 1172 (1961).

⁸ H. H. Landolt and R. Boernstein, Zahlenwerte und Funktionen ⁶ H. H. Landolt and K. Boernstein, Zahlenwerte und Funktionen (Springer-Verlag, Berlin, 1955), Vols. I and IV/1: A Kaputinsky and B. Weselowsky, Z. physik Chem. **B22**, 261 (1933). Dana's Manual of Mineralogy, revised by C. S. Hulbert (John Wiley & Sons., Inc., New York, 1960), 17th ed. A. N. Winchell and H. Winchell, Elements of Optical Mineralogy (John Wiley & Sons, Inc., New York, 1951), 4th ed., Part II. The pertinent volumes of *Carding: Hardbuck der Ausganischen Chemie* (Verlag Chemie Gmelins Handbuch der Anorganischen Chemie (Verlag Chemie, GmbH., Berlin).



FIG. 1. Proportionality between relative hardness (H) and "volumetric lattice energy" (U/V) for A solids. $(M \text{ scale}: H \leq 9, W \text{ scale}: H \geq 9)$.

III. HARDNESS AND "VOLUMETRIC LATTICE ENERGY"

A striking experimental phenomenon is discovered when correlating the H and U/V values. An unambiguous linear relationship between both H and U/Vis established for the entire hardness range of the solids, if properly classified. The maximum limits of error are about ± 0.5 unit in the H and ± 5 percent in the U/Vdata. In detail, we obtain from Tables I and II two distinct hardness characteristics: $A-\bar{A}$ and $\bar{B}-B$, as is shown in Figs. 1 and 2, respectively. They correspond to different classes of solids which result from a recent study on lattice anharmonicity by one of us.⁷ The mechanical properties of solids appear to be controlled by the amount of anharmonicity of the respective cohesive forces. If the related mass values X_m of adjacent atom or ion partners9 decrease substantially below unity, a strong increase of mutual interpenetration or interlinking of the atoms occurs with a corresponding increase of the lattice anharmonicity, represented by $X_m^{-1/p}$ (see Fig. 3). This results in a very strong resistance against lattice destruction or very high hardness values. (Figure 3 indirectly relates $X_m^{-1/p}$ to the electronic configurations of the rare gases: $X_m = \frac{2}{3}$ indicates the neon configuration, $X_m =$ unity defines the argon configuration.) Thus, depending upon whether they do or do not have the neon configuration, the nonmetallic solids were divided as follows:

(I) Class-A Solids. The atom partners do not have

the electronic configuration of neon. These solids are defined by related mass values $X_m < 0.64$ (= X_m value of Sc₂O₃) if the atom partners in the solid display different valencies, and $X_m < 0.69$ (= X_m value of KF) if they have equal valencies. Pertinent data for 17 *A*-solids are compiled in Table I and graphically represented by the lines *A* and \overline{A} in Figs. 1 and 2. The *A* solids exhibit the steepest hardness characteristic that exists. Since in this case we employ the two relative scales *M* and *W*, *two* linear relations result:

3),

$$U/V = 24(H - 2.7)$$
 (kcal/cm

and

$$U/V = 36(H - 4.8)$$
 (kcal/cm³),

corresponding to line \overline{A} . (2)

corresponding to line A (1)

Equation (2) covers the W scale between the coordinates (H=9, U/V=150) and (H=42.5, U/V=1350), while Eq. (1) covers values from H=3 to H=9. The change from the first to the second relation (or from the M scale to the W scale) results in different slopes of the lines A and \overline{A} . A variety of 20 additional \overline{A} and Asolids (borides, carbides, nitrides), for which H data but no U data are available, are tabulated in Table III.

(II) Class-B Solids. The atom partners have the electronic configuration of neon. These solids are defined by related mass values $X_m \ge 0.64$ if the atom partners have different valencies among one another, and $X_m \ge 0.69$ if they display equal valencies. Pertinent data of 48 B solids are compiled in Table II and graphically represented by the lines B and \overline{B} in Fig. 2. The B solids exhibit a medium hardness characteristic. Since, according to Troeger,⁵ the progression ratio increases within the M scale by a factor $\sqrt{3}$ when H < 4, we again



FIG. 2. Proportionality between relative harndess (H) and "volumetric lattice energy" (U/V). Line A : A solids as in Fig. 1, lines $B-\overline{B}: B$ solids.

⁹ The "related mass" X_m is a dimensionless quantity which represents the reduced mass of the vibrating ion (atom) partners related to the reduced mass of the ions of K and Cl (electronic configuration of argon).⁷

No.	Substance	Structure	X_m	V (cm ³)	H (M scale)	U/V (kcal/cm ³)	U (kcal/mole)	Hardness type
1	B4C	CsCl (deformed)	0.31	22.1	19.7 (W scale)	540	12 000	\bar{A} solids
2	SiB ₆		0.43		9–10			
3	TiB		0.48		9-10			
4	VB		0.48		9-10			
5	ZrB		0.52		9-10			
6	VC	rock salt	0.53	10.9	9-10			
7	NbC	rock salt	0.57	13.4	9-10			
8	VN	rock salt	0.59	10.6	9-10			
9	TaC	rock salt	0.60		9-10			
10	W ₂ C		0.61	22.1	9-10			
11	WC	(hexagonal)	0.61	12.6	12 (W scale)	260	3300	
12	BeS	zinc blende	0.38	17.4	7.5	115	2000	A solids
13	TiC	rock salt	0.52	12.2	8-9	139	1700	
14	Cr_3C_2	$D5_{10}$	0.53	27.0	8-9	139	3800	
15	ZrC	rock salt	0.57	15.3	8-9	139	2100	
16	MoC	(hexagonal)	0.58	12.3	8	127	1600	
17	ScN	rock salt	0.58	13.4	8	127	1700	
18	TiN	rock salt	0.58	11.4	8-9	139	1600	
19	ZrN	rock salt	0.60	14.8	7-8	115	1700	
20	NbN	rock salt	0.60	12.7	9	151	1900	
21	GeO ₂	rutile	0.71	16.7	5	82	1400	B solids
22	Y2O3	$D5_3$	0.73	45.2	6	129	5800	
23	ZrO ₂	fluorite	0.74	21.7	7-8	202	4400	
24	Ce ₂ O ₃	$D5_2$	0.78	47.0	5	82	3900	
25	Yb ₂ O ₃	$\overline{D5_3}$	0.79	43.0	6	129	5600	
26	WO ₂	rutile	0.80	17.8	56	106	1900	
27	ThO ₂	fluorite	0.81	26.4	6-7	153	4000	
28	V ₂ Si	β tungsten (A15)	0.98	23.7	7-8	202	4800	
29	M ₂ Si	iron silicide (B28)	1.00	22.3	6	129	2900	
30	$ZrSi_2$	C49	1.15	30.4	4	33.6	1000	

TABLE III. Hardness type classification and lattice energy values (U) which are estimated from the data of scratch-hardness (M scale) or abrasion-hardness (W scale).

obtain two linear relations:

$$U/V = 48(H-3.3)$$
 (kcal/cm³),
corresponding to line B (3)

and

$$U/V = 16(H-2.0)$$
 (kcal/cm³),
corresponding to line \overline{B} . (4)

Equation (3) covers the M scale between the coordinates (H=4, U/V=35) to (H=8, U/V=225), while Eq. (4) covers values from H=2 to H=4. The change from the first to the second relation is again indicated by the different slopes of the lines B and \overline{B} . The increase of slope from B to \overline{B} (by a factor 3 at H<4) corresponds to the increase of the above mentioned progression ratio (by the factor $\sqrt{3}$). The line \overline{B} may be conceived as to substitute the real curve, a cubic parabola: $U/V = H^3/2$, for which $H \to 0$ when $U/V \to 0$. A similar relationship does not appear with the A solids, however, since their H values remain ≥ 3 . A small variety of 10 additional B solids (oxides and silicides), of which only the H data were known,³ are tabulated in Table III.

The remaining metallic solids have the flattest hardness characteristic that exists for inorganic crystals. They include the metallic and transition elements, their alloys and the conducting compounds. A total examination of these solids, however, poses additional problems, such as a determination of their true lattice energy and a definition of the indentation hardness on the basis of interatomic forces. Therefore, this subject will be treated as a whole in a forthcoming paper.



FIG. 3. The two hardness types (A and B) of nonmetallic solids as a consequence of lattice anharmonicity $(X_m^{-1/p})$ and related mass (X_m) .⁷ $X_m = 1.0$ corresponds to the electronic configuration of argon, and $X_m = \frac{2}{3}$ corresponds to the electronic configuration of neon; where $X_m < \frac{2}{3}$ defines the region of the A solids, and $X_m \ge \frac{2}{3}$ defines the region of the B solids.

IV. COMPILATION OF THE RESULTS

Summarizing the above results, we find that the definition of hardness by means of the "volumetric lattice energy" provides unambiguous scales. Moreover, it gives to hardness the dimension (kcal/cm³). Thus instead of using relative hardness scales, such as the combined Mohs-Wooddell scales, we may now employ, with appropriate classification, the new U/V scales. As for the A solids, the obtained maximum hardness so far is $(U/V)_A = 1350$ kcal/cm³, while for the B solids the corresponding $(U/V)_B$ values extend to about 225 kcal/cm³ only. When compared to the combined M-W scales, the U/V scales resolve hardness by a factor of 24 for A, 36 for \overline{A} , 48 for B, and 16 for \overline{B} .

The U/V scales give strictly comparable hardness values and avoid any change of the progression ratio. Such a definition of hardness eliminates selective hardness properties (anisotropy), which generally result from differences between the cohesive forces in various crystallographic directions, since the U values integrate these forces. The U/V hardness data also appear independent of lattice structure and valency of the atoms, the two already being taken into consideration with U.⁷ Thus, the U/V hardness, properly classified, could be deemed the absolute over-all hardness.

Hardness data can now be obtained from mole volume and lattice energy values. Vice versa, lattice energy data can be estimated by appropriate scratch or abrasive hardness testing which adds to the various existing methods of lattice energy determination from ionic and structural properties. Table III shows the U values of 19 A and B solids, estimated from hardness data ≤ 9 , using Eqs. (1) and (3). The \overline{A} solids of Table III (H>9), however, require a determination of their W hardness, in order to enable estimation of their Uvalues in an analogous manner by Eq. (2).

It should be emphasized that the vast majority of the examined solids are binary compounds, except for some ternary compounds and elements, and are all either semiconductors or nonconductors. An investigation of the more complicated compounds was hampered by the fact that either their U or H data, or both were unknown. A study of the hardness of the metallic, conducting, solids on an atomic basis is in progress.

Impurities in samples of tested minerals and inorganic crystals may cause some differences in relative hardness values and other experimental data. Consequently, the impurities reduce somewhat the accuracy of the results and thus may cause the experimental values to deviate from purely linear relationships.

V. PRACTICAL APPLICATIONS AND CONCLUSIONS

A recent first determination of the lattice energy for the rare type-II diamond from its infrared spectrum gave⁷ U=17~000 kcal/mole which results in U/V=2450kcal/cm³. Using Eq. (1), the relative hardness of the rare type-II diamond is obtained as $H_{D \text{ II}}=71$ which is 1.7 times the relative hardness of the type-I diamond. On the basis of these data we obtain the full range of the U/V scale for the $A-\overline{A}$ solids as about 10 times larger than that for B solids. Since the $H_{D \text{ II}}$ value is extrapolated from line \overline{A} , a confirmation by testing according to Wooddell's abrasive method seems desirable.¹⁰

Effects of structure modifications on hardness could not as yet be examined on an atomic basis for substances other than diamond because of lack of pertinent data. However, since data of either U or V are known to vary when the modification changes, we may assume until later confirmation that the U/V values change in accordance with the H values. The same reasoning should for the time being be applied to temperature effects.

Shortcomings within the M scale, such as considerable changes in the progression ratio, are indicated by changes of slopes (as for the lines $A-\overline{A}$ at H=9, or the lines $\overline{B}-B$ at H<4) and to a lesser degree by deviations from the straight line relation (e.g. line B at H=7 and H=8). Because of this fact, it appears desirable to subject additional \overline{A} , A, and B solids (see Table III) to hardness testing according to Wooddell and to determine their U values (e.g., from their infrared spectra⁷). The samples should be of high purity and the accuracy of measurements of such a degree that the slopes of all curves can be even more accurately fixed. Such work will allow us to form and confirm a uniform experimental scale for the entire hardness range, of nonconducting solids.

An investigation of \overline{A} solids on the basis of interatomic forces would supply data of value for the ultimate preparation of materials capable of withstanding extreme environmental conditions.

¹⁰ It seems rather unlikely that the very rare type-II diamond was among Wooddell's test specimens, since the differences in the hardness of his diamonds are much less than those observed in the diamond cutting industry.