

Relationships between thermochemical properties, thermal expansion, and mechanical properties of the solid state of elements

F. KRÁLIK

ZVL Považské strojárne,
CS-01734 Považská Bystrica

Received 20 September 1988

Accepted for publication 13 April 1989

*Paper published on the occasion of the 60th anniversary
of the foundation of the factory*

The relationships between the ratio of molar enthalpy increase in the interval (0 K— T_f) to molar volume, the linear thermal expansion in the interval (273 K— T_f) and the fraction of atoms (molecules) of inorganic substances with molar enthalpy of the liquid state on the one hand and the mechanical properties of these substances such as hardness, tensile strength, and plasticity on the other hand have been analyzed. The ratio of molar enthalpy increase to molar volume has been used as a criterion of tensile strength and hardness of the solid substances. The plasticity of elements is interpreted from the viewpoint of the range of action of attractive forces in the solid state and of the value of the fraction of atoms with molar enthalpy of the liquid state.

Анализируется взаимосвязь между отношением прироста мольной энтальпии в интервале (0 К— T_f) к мольному объему, продольной растяжимостью в интервале (273 К— T_f) и отношением числа атомов (молекул) неорганических веществ с мольной энтальпией жидкого состояния с одной стороны и их механическими свойствами, такими, как твердость, прочность в растяжении и пластичность, с другой стороны. В качестве критерия прочности в растяжении и твердости твердых веществ было использовано отношение приростов мольной энтальпии к мольному объему. Пластичность элементов интерпретируется с точки зрения диапазона воздействия сил притяжения в твердом состоянии и величины отношения числа атомов с мольной энтальпией жидкого состояния.

The characteristic mechanical properties of inorganic substances in the solid state are represented by tensile strength, hardness, and plasticity. For better understanding these properties the following correlations are analyzed in this paper:

— The relationship between the ratio of molar enthalpy increase in the

interval ($0\text{ K} - T_f$) to molar volume of inorganic substances and their mechanical properties. The ratio $\Delta H/V_m$ is regarded as a criterion of cohesive forces among atoms in the solid state.

— The relationship between tensile strength at high temperatures and total linear expansion in the interval ($273\text{ K} - T_f$) for three pairs of elements with approximately equal melting temperature, different crystal structure, and different T_f and mechanical properties in the solid state. The range of action of interatomic forces in the solid state may be appreciated on the basis of these relationships.

— By using the theory of vacancies, the experimentally determined values of vacancies in the solid state and the Boltzmann statistical distribution of energy, the probable fraction of atoms with molar enthalpy of the liquid state was calculated for the three chosen pairs of elements. These atoms represent the defect sites in the crystal structure where the stress is concentrated owing to which the theoretical tensile strength is reduced to the real technical value.

These correlations also determine the basic mechanical properties of inorganic solid substances, especially the tensile strength, hardness, and plasticity and are operative in deformation of these substances.

In this paper the following values of molar enthalpy increase are used:

1. Increase in molar enthalpy in the interval ($298\text{ K} - T_f$)

$$H(T, f) - H(298\text{ K}) = \Delta H_1$$

2. Increase in molar enthalpy in the interval ($0\text{ K} - T_f$)

$$H(T, f) - H(0\text{ K}) = \Delta H_2$$

3. Increase in molar enthalpy in the interval ($0\text{ K} - T_f$) including enthalpy of fusion $H(T, f) - H(0\text{ K}) + \Delta H_f = \Delta H_3$

4. Increase in molar enthalpy in the interval ($0\text{ K} - T_b$) including enthalpy of fusion without enthalpy of evaporation

$$H(T, b) - H(0\text{ K}) = \Delta H_4$$

It is assumed in calculating particular increases that $H(0\text{ K}) = 0$.

The ratio of molar enthalpy increase in the interval ($0\text{ K} - T_f$) to molar volume and its relation to hardness and tensile strength of inorganic substances

Hardness and tensile strength of crystals result from the resistance of crystal structure to plastic deformation and thus they are functions of bond energy of atoms. The hardness of elements is a periodic function of atomic number. Every

modification of allotropic elements exhibits different value of hardness. *Grigorovich* [1] was concerned with the periodic dependence of hardness, melting temperature, melting enthalpy, and sublimation enthalpy of metals.

The theoretical tensile strength of metals calculated from the values of sublimation enthalpy and surface energy is 45—70 times higher than the real tensile strength [2]. According to present views, this substantial decrease in real tensile strength is due to the presence of microfractures where the mechanical stress is concentrated and accelerates the expansion and increase in number of these microfractures. The hardness and tensile strength of solid inorganic substances decreases with increasing temperature down to zero value at the melting temperature. According to paper [3], the melting enthalpy of the solid—liquid transition at the melting temperature gives rise to about 10 % of vacancies. The increase in molar enthalpy of inorganic substances in the interval (0 K— T_f) ΔH_2 is utilized to the increase in kinetic energy of atoms and to the generation of different kinds of defects. Consequently, the hardness as well as the tensile strength of solid substances at the melting temperature practically drops to zero value. Therefore, we have chosen the ratio of molar enthalpy increase to molar volume $\Delta H_2/V_m$ as a criterion of hardness and tensile strength of solid substances in this work because the value of this ratio can be calculated for a great number of substances.

The molar enthalpy increase in the interval (0 K— T_f) is given by the following equation

$$\Delta H_2 = \int_0^{T_f} C_p dT$$

The values of molar enthalpy increases and molar volumes necessary for calculation were taken from literature [4—6]. The dependence of the ratio $\Delta H_2/V_m$ [7] as well as of the ratio of cohesion energy to molar volume $\Delta H_0^0/V_m$ [8] on atomic number at the temperature of 0 K is given in Fig. 1 for all investigated elements. In order to compare both ratios with each other, the scales on the axis of ordinates were so chosen that the values of both ratios for ruthenium were equal. This transformation has enabled us to compare the values of both ratios with each other for individual elements and to ascertain which relationship is the most convenient as a criterion of mechanical properties. It results from Fig. 1 that the values of the ratios are rather different for some elements, especially for gallium and indium. This difference is a consequence of relatively high boiling temperature of these elements, which is in connection with high value of their cohesion energy.

Furthermore, it is obvious from Fig. 1 that the value of $\Delta H_2/V_m$ is more appropriate for appreciating tensile strength and hardness. That follows mainly from a confrontation of the values of both criteria for Cd, In, Sn, Zn, Ga, Ge

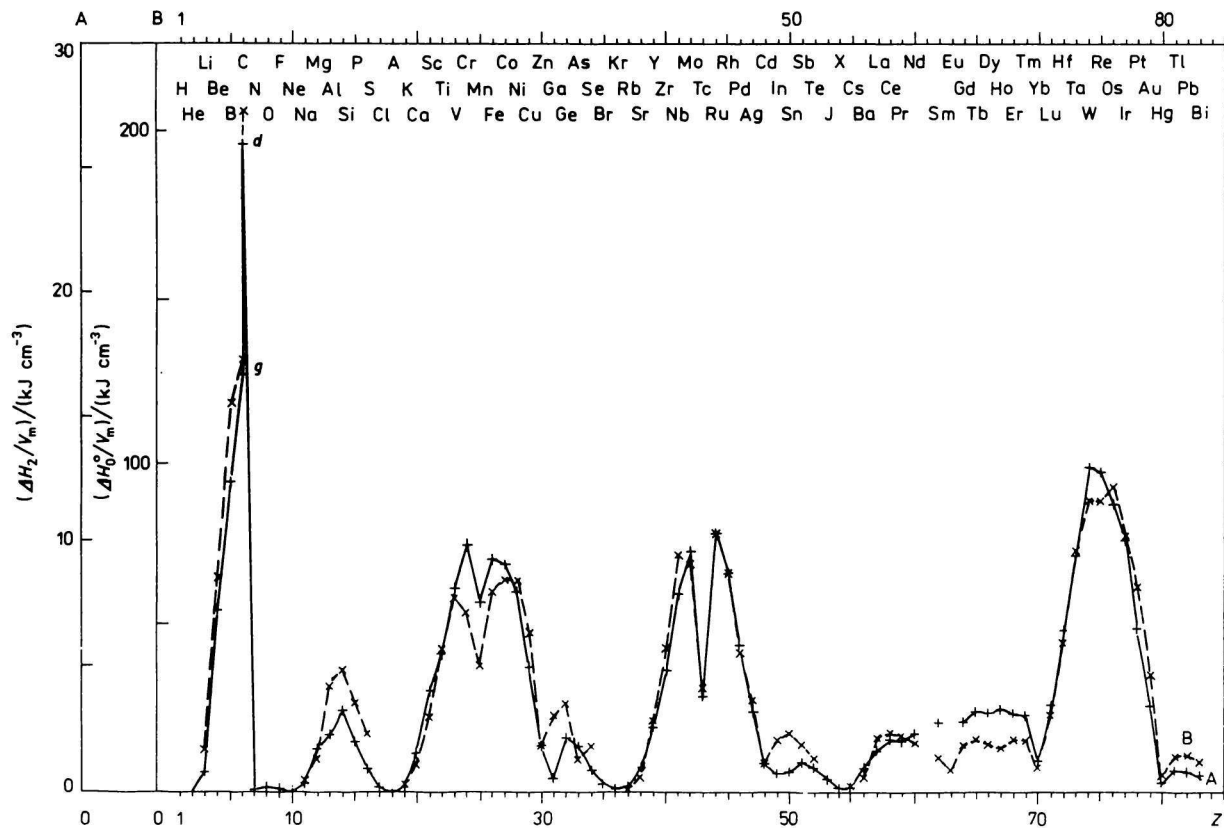


Fig. 1. Periodic relationship between atomic number Z and the ratio of increase in molar enthalpy (from 0 K to melting point) ΔH_2 to molar volume when compared with the relationship between atomic number and the ratio of cohesion energy ΔH_0 to molar volume.

and others because the values of the ratio $\Delta H_2/V_m$ are more consistent with the real technical values of hardness and tensile strength. The criterion $\Delta H_2/V_m$ is more convenient for appreciating tensile strength and hardness in the class of rare-earth elements, especially for La and Ce. The correlation between criterion $\Delta H_1/V_m$ and hardness is represented in Fig. 2 where the dependence of this criterion, microhardness and Vickers hardness on the hardness according to Mohs scale is given for some selected members of this scale (NaCl, CaF₂, SiO₂, Al₂O₃, and C) (cooking salt, fluorspar, quartz, corundum, and diamond). The scales on the axis of ordinates were so transformed that the values of the ratio $\Delta H_1/V_m$ and microhardness of corundum coincided into single point. Fig. 2 shows a good correlation of both quantities.

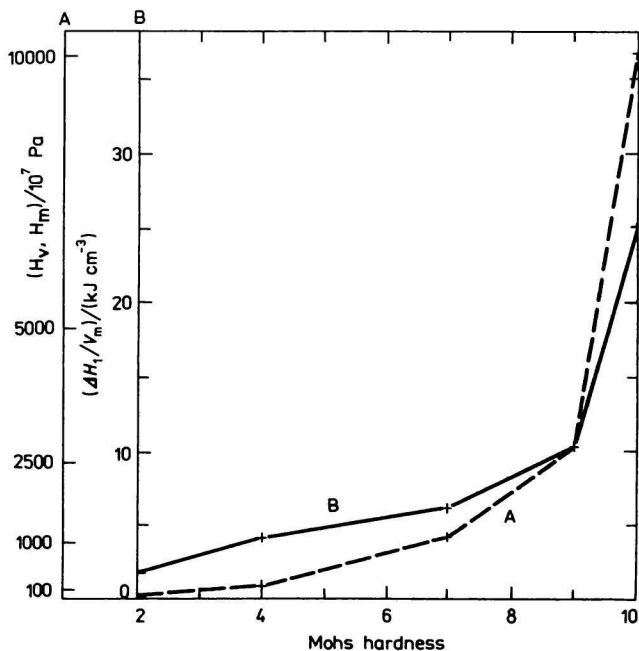


Fig. 2. Dependence of the Mohs streak hardness, Vickers hardness and microhardness on the ratio of molar enthalpy (from 298 K to melting point) ΔH_1 to molar volume.

Relationship between tensile strength at high temperatures and linear thermal expansion in the interval (273 K— T_f) for three selected pairs of elements

Three pairs of elements with near melting points and different plasticity and crystal structure were selected for investigating the relationship between tensile

strength and thermal expansion. Thus each pair of elements lost its mechanical properties at almost equal temperature.

The dependence of tensile strength at raised temperature on total linear expansion in the temperature interval ($293\text{ K}—T_f$) is represented in Fig. 3. The needed data were taken from literature [4, 9—11]. For confronting the decrease in tensile strength of individual metals, the normalized scale on the axis of ordinates has been used (tensile strength at $20\text{ }^\circ\text{C} = 100\%$, at melting point = 0%). The values of linear thermal expansion of the elements Sb, Si, Al, Mg, Ni, Cu, and Ta in the interval ($273\text{ K}—T_f$) were taken from literature [9, 12].

Sylwestrowicz [13] has stated that the tensile strength of monocrystalline silicium at $1100\text{ }^\circ\text{C}$ (homologous temperature 0.81) is equal to $6 \times 10^7\text{ Pa}$ while this value is equal to $2 \times 10^7\text{ Pa}$ at $600\text{ }^\circ\text{C}$. That indicates different course of tensile strength at increased temperature when compared with that one observed

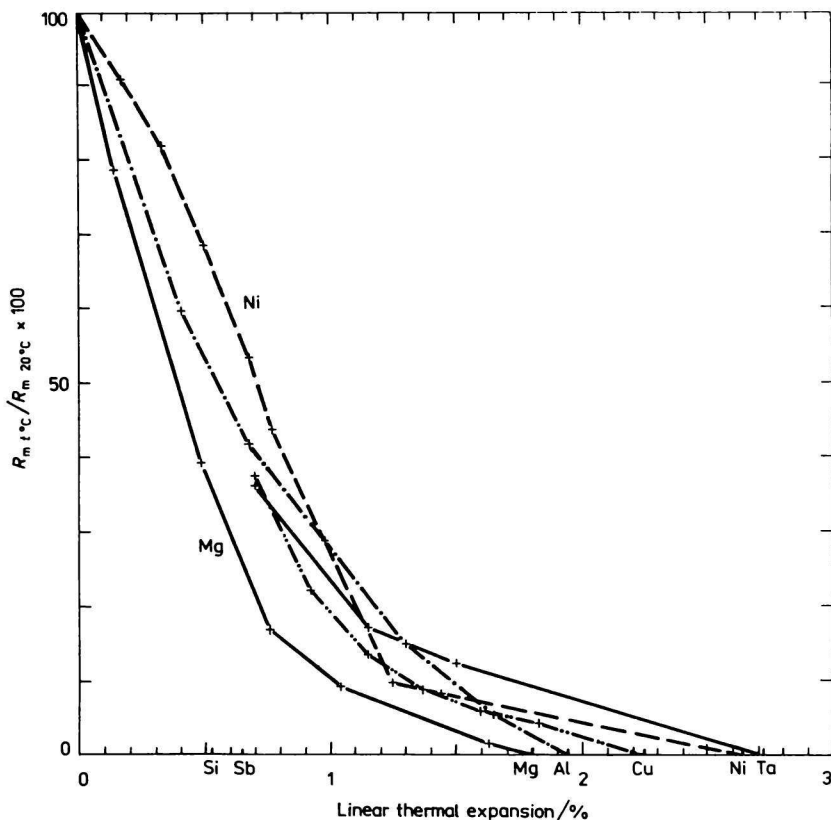


Fig. 3. Dependence of tensile strength at high temperatures on total linear expansion between $0\text{ }^\circ\text{C}$ and testing temperature of elements Al, Mg, Cu, Ni, Ta.

for the above-mentioned metals. A substantial increase in plasticity of silicium appears only at higher temperatures, which is accompanied by significantly higher values of tensile strength. It ensues from curves in Fig. 3 that the decrease in tensile strength at high temperature as a function of linear expansion exhibits similar character and is the most conspicuous in the range of homologous temperatures from 0 to 0.7. But the total linear expansion up to the melting point is essentially higher for metal elements than for Sb, Ge, and Si. The value of tensile strength gradually decreases with increasing temperature and attains the zero value at melting temperature. Simultaneously, the dimensions of sample increase owing to expansion. Though the influence of temperature on tensile strength is predominant, we may compare the elements exhibiting approximately equal melting points with each other and estimate the relative range of interatomic forces by means of Table 1. The values of mean relative distances of interatomic forces action are proportional to total expansion from 0 °C to the melting point.

The values listed in Table 1 were obtained by interpolation or extrapolation of the values taken from literature [4, 9, 12, 14, 15]. The total volume change due to transition from the solid state to the liquid state has been calculated by means of the equation

$$\Delta V_{m, T_f} / V_m = (V_{m, T_f} - V_m) / V_m - \Delta V(273 \text{ K} - T_f) / V_m$$

where V_{m, T_f} is the molar volume of the liquid phase at melting point, V_m molar volume at 20 °C, and $\Delta V(273 \text{ K} - T_f)$ volume thermal expansion from 273 K to the melting point. The necessary data were taken from papers [9, 12]. It is evident from the data listed in column C of Table 1 that the difference in the range of interatomic forces action in the solid state is considerable for all pairs.

The dependence of technical tensile strength on total linear expansion is represented in Fig. 3. It results from this figure that the decrease in relative tensile strength of the compared metals at higher temperatures is very similar. A decrease in relative tensile strength to an approximately 10 % value can be observed for Mg, Cu, Ni, and Ta at the homologous temperature of about 0.7. *Grigorovich* [1] presented the temperature dependence of relative hardness of Ti, Zr, U, Ca, Mn, and Sr. It can be correlated with the analogous dependence of tensile strength. In general, the decrease in relative hardness of the above elements to 10 % value appears at homologous temperatures 0.7—0.8, which is comparable with the course represented in Fig. 3.

It results from Fig. 3 and Table 1 that the values of total linear expansion in the temperature interval (273 K— T_f) are considerably higher for Al, Ag, and Ni than for Sb, Ge, and Si. Both groups of elements exhibit quite different crystal structure. The melting of Sb, Ge, and Si is accompanied by a decrease in volume,

Table 1

Linear and volume changes from 273 K to boiling point of the selected pairs of elements

Element	Relative linear change $\Delta l(0\text{--m. p.}/^\circ\text{C})/l_0$ %	Relative volume change $\Delta V(0\text{--m. p.}/^\circ\text{C})/V_0$ %	Relative volume change due to melting ΔV_m , m. p. %	Relative volume change in liquid state $\Delta V(\text{m. p.}\text{--b. p.}/^\circ\text{C})/V_0$ %	Relative total volume change $\Delta V(0\text{--b. p.}/^\circ\text{C})/V_0$ %	Relative total linear change $\Delta l(0\text{--b. p.}/^\circ\text{C})/l_0$ %
A	B	3B	C	D	3B + C + D	$\frac{3B + C + D}{3}$
Al	1.95	5.85	8.15	25.7	39.70	13.25
Sb	0.65	1.95	−0.32	9.9	11.53	3.84
Ag	2.20	6.60	6.24	13.6	26.44	8.81
Ge	0.80	2.40	−5.48			
Ni	2.70	8.10	7.94	25.39	41.43	13.81
Si	0.53	1.59	−9.38			

while the melting of Al, Ag, and Ni makes the volume increase. This difference can be explained by a rise in coordination number of Ge and Si accompanying the transition from the solid state to the liquid state [9]. The ratios of total linear expansion in the temperature interval (273 K— T_f) for individual pairs of elements are as follows

$$\begin{aligned}\Delta l(\text{Al})/\Delta l(\text{Sb}) &= 3 \\ \Delta l(\text{Ag})/\Delta l(\text{Ge}) &= 2.7 \\ \Delta l(\text{Ni})/\Delta l(\text{Si}) &= 5\end{aligned}$$

Feschotte [16] came to similar conclusion on the basis of linear expansion of some selected elements.

The values of thermal expansion of the elements in the temperature interval (273 K— T_f) are proportional to the relative distance within which the interatomic cohesive forces are operative. The slipping of two adjoining atomic planes with interplanar distance a results in the fact that the most distant position of an atom from the position of an atom in the adjacent plane is

$$b = \sqrt{a^2 + \left(\frac{a}{2}\right)^2} = \sqrt{\frac{5a^2}{4}} = 1.118a$$

i. e. this distance is by 11.8 % longer than the distance of two vicinal atoms. In this position the atom has the lowest cohesion energy with respect to the atoms of the adjacent plane. The cohesive forces determining tensile strength must be in operation as far as to this distance lest a microfracture should come into existence.

The second model approach is based on approximate determination of total volume and linear change in the condensed phase at temperature varying within the interval (273 K— T_b). It results from the last column of Table 1 that these values vary within the range 9—14 % for plastic elements, which is in good agreement with the values obtained by using the first model approach. We were not able to determine the total volume and linear changes in the above temperature interval for Sb, Ge, and Si because the necessary data were not available. Moreover, the melting of these elements is accompanied by a decrease in volume [17].

Relationship between tensile strength, plasticity, and the fraction of atoms with molar enthalpy of the liquid state

At every temperature, there are atoms in solid substances, the energy of which is much higher or lower than the mean energy corresponding to the law of the equipartition of energy [2]. As a consequence of thermal vibration of atoms in crystal structure there is an equilibrium state which is characterized by

the equilibrium portion of the Schottky defects. The molar enthalpy of the Schottky defects in most metals corresponds to *ca.* 1 eV [18].

The existence of the vapour pressure of elements below melting point suggests that a certain portion of atoms has the enthalpy higher than 1 eV even at these temperatures. The mechanoluminescence of metals [19] also indicates that processes involving a change in energy higher than 1 eV take place in the course of plastic deformation.

An interesting information is provided by the value of equilibrium portion of the atoms in the solid state, the molar enthalpy of which corresponds to the molar enthalpy of the liquid state. The molar enthalpy of the atoms in the liquid state corresponds to a rather lower value than 1 eV and that is why the portion of these atoms must be significantly higher than the equilibrium portion of the Schottky defects.

The mechanical properties of solid substances such as tensile strength and hardness are dependent on the fraction of the atoms in the solid phase the molar enthalpy of which corresponds to the liquid state (n). Its minimum value corresponds to the increase in molar enthalpy in the temperature interval (0 K— T_f) augmented by the enthalpy of melting ΔH_3 . These atoms exhibit decreased values of cohesive forces in the solid phase and consequently they bring about a decrease in mechanical properties. The relative proportion of these atoms may be calculated from the Boltzmann law of the energy distribution.

$$\frac{n(\Delta H_3)}{N} \doteq \exp(-\Delta H_3/RT)$$

The maximum increase in molar enthalpy in the liquid state at the boiling temperature has been denoted ΔH_4 . For this second limiting value of the increase in molar enthalpy and a certain temperature of the solid state we may calculate the ratio $n(\Delta H_4)/N$. Both terminal values of the increase in molar enthalpy as well as the values between them are dependent on the difference between melting temperature and boiling temperature of the elements.

For instance, it is valid $\Delta H_3 = 34.69 \text{ kJ mol}^{-1}$ for aluminium, which corresponds to 0.36 eV and the molar enthalpy of the Schottky defects varies in the range from 0.65 to 0.75 eV. The difference between both the values indicates that the fraction $n(\Delta H_3)/N$ of atoms must be by decimal order higher than that of the Schottky defects.

The values of $n(\Delta H_3)/N$ and $n(\Delta H_4)/N$ calculated for three pairs of the compared elements at 300 K and at melting temperature are given in Table 2. The increase in values of the mentioned fractions due to the temperature rise from 300 K to melting temperature corresponds to the range of decimal orders from 4 to 13 for ΔH_3 and to the range of decimal orders from 8 to 19 for ΔH_4 . These increases are the most characteristic of the above examples. The differ-

Table 2

Fractions n/N of the atoms with the increase in molar enthalpy from 0 K to melting point including heat of fusion ΔH_3 as well as with the increase in molar enthalpy from 0 K to boiling point without heat of vaporization ΔH_4 . Both values are given for 300 K and melting point of the selected pairs of elements

Element	$\frac{\Delta H_3}{\text{kJ}}$	$\frac{\Delta H_4}{\text{kJ}}$	$\exp\left(-\frac{\Delta H_3}{RT}\right)$ for 300 K	$\exp\left(-\frac{\Delta H_4}{RT}\right)$ for 300 K	$\exp\left(-\frac{\Delta H_3}{RT}\right)$ for m. p./K	$\exp\left(-\frac{\Delta H_4}{RT}\right)$ for m. p./K
Al	34.69	91.68	1.01×10^{-6}	1.42×10^{-16}	1.17×10^{-2}	7.91×10^{-6}
Sb	42.31	73.84	4.84×10^{-8}	1.72×10^{-17}	3.71×10^{-3}	5.74×10^{-7}
Ag	44.27	81.04	2.22×10^{-8}	9.78×10^{-18}	1.38×10^{-2}	3.93×10^{-7}
Ge	67.39	121.83	5.80×10^{-9}	8.68×10^{-19}	1.31×10^{-3}	6.17×10^{-8}
Ni	70.77	127.81	5.84×10^{-9}	8.02×10^{-19}	7.52×10^{-3}	1.46×10^{-8}
Si	89.60	138.77	3.24×10^{-10}	1.00×10^{-24}	1.75×10^{-3}	5.35×10^{-9}

ences incident to individual pairs considerably decrease at melting temperature. As a matter of fact, the values of the proportion $n(\Delta H_3)/N$ are always lower for brittle elements. It means that in the case of Sb, Ge, and Si the equilibrium state at both temperatures involves a significantly lower portion of the atoms with molar enthalpy corresponding to the liquid state. The result is a lower plasticity and higher tendency of these elements to generate microfractures. Simultaneously, the decrease in volume during melting explained for Ge and Si by an increase in coordination number facilitates the formation of defects and vacancies in the solid state.

The differences between the values of $n(\Delta H_3)/N$ and $n(\Delta H_4)/N$ corresponding to the pairs of elements Ge, Ag and Si, Ni are not convincing enough for explaining the essential differences in their behaviour during deformation. The magnitude of these differences is probably affected by an increase or decrease in coordination number during melting. As for the compared elements Al, Ag, and Ni, their behaviour during melting differs owing to the fact that their volume increases (Table 1) and the coordination number decreases.

At equal thermodynamic temperature the concentration of the atoms with the values of ΔH_3 in the solid state must be by decimal orders lower in the case of elements with high melting points. Simultaneously, the probability of a short-termed increase in content of the above-mentioned atoms promoting the plasticity which are generated during deformation significantly falls. Particularly, the metals with low melting point and low melting enthalpy will preserve plasticity down to very low temperatures.

The plasticity of elements significantly depends on their purity, especially small amounts of specific admixtures, and their structure and exhibits irregularities in some cases, especially in the region of low or higher temperatures.

Discussion

The preceding considerations have led to the conclusion that the value of the increase in molar enthalpy of solid substances in the temperature interval (0 K— T_f) and the value of the ratio of this quantity to molar volume $\Delta H_2/V_m$ may be used as criteria of properties of the solid state, in particular, of hardness and tensile strength. At all temperatures up to melting temperature the ratio

$$\frac{\Delta H_2 - (\Delta H_T - H_{0K})}{V_m}$$

is a measure of cohesive forces in a given element at the testing temperature T . According to *Epifanov* [2], the critical length of microscopic cracks determining the technical strength of metal materials is equal to 8×10^{-6} m, which approxi-

mately corresponds to 2×10^3 up to 3.5×10^3 atomic diameters. The gradual increase in number of the microcracks and their size during deformation is responsible for the difference between theoretical and technical tensile strength. The Griffith cracks in solid substances preferentially are growing from the atoms the energy of which is equal to the value of increase in enthalpy in the temperature interval ($0 \text{ K} - T_f$) including the enthalpy of melting. The relative proportion of these atoms may be calculated on the basis of the Boltzmann law of the energy distribution (Table 2). These atoms also represent the weakened points in the crystal structure where the slipping sets in and the dislocations are generated.

A considerable increase in number of dislocations during deformation of plastic elements at lower temperatures and a decrease in density after deformation also indicate that the cohesive forces exhibit a relatively long range. The marked differences in plasticity of the three investigated pairs of elements (Al—Sb, Ag—Ge, Ni—Si) are due to the fact that the cohesive forces determining the value of tensile strength are operative in plastic elements in 3 times up to 5 times longer range than they are in brittle elements. At the ending of every Griffith microcrack the interatomic distances are always larger than in the crystal structure. The different effect of the cohesive forces of atoms manifests itself in these places, too. Owing to local changes in temperature during deformation, the concentration of the atoms which possess the molar enthalpy corresponding to the liquid state — during deformation at lower temperatures when the tensile strength is high in particular — instantaneously increases. This short-time increase in concentration of these atoms is much greater in plastic elements where a lower energy is necessary for exciting them. Because of a decrease in coordination number and an increase in volume, these atoms occupy a larger space, which also affects the range of action of cohesive forces. It results that the concentration of the atoms endowed with the mentioned increases in molar enthalpy and the volume change caused by melting are further parameters characterizing the plastic or brittle behaviour of elements during deformation, especially at temperatures lower than $0.5 T_f$. The relative proportion of the atoms endowed with the above increase in molar enthalpy is also a quantity that determines the linear expansion of solid substances which is significantly higher in the case of plastic elements.

References

1. Grigorovich, V. K., *Tverdosť i mikrotverdosť metallov*. Nauka, Moscow, 1976.
2. Epifanov, G. I., *Solid State Physics*. Mir, Moscow, 1979.
3. Górecki, T., *Z. Metallkd.* 65, 426 (1974).
4. Landolt, H.—Börnstein, R., *Physikalisch-Chemische Tabellen, Makrophysik und Chemie*, Vol. II, Part IV. Springer-Verlag, Berlin, 1961.

- Collective of authors. *Termicheskie konstanty* *izshchestv.* Vol. I–X. Izd. Akad. Nauk SSSR, Moscow, 1965.
6. Barin, I., Knacke, O., and Kubaschewski, O., *Thermochemical Properties of Inorganic Substances*. Springer-Verlag, Berlin, Verlag Stahleisen, Düsseldorf, 1973, Supplement 1977.
 - Dykyj, J. et al., *Fyzikálně-chemické tabulky*. (Physicochemical Tables.) Státní nakladatelství technické literatury (State Publishing House of Technical Literature), Prague, 1953.
 8. Gschneider, K. A., Jr., *Solid State Physics*, Vol. 16, p. 275. Academic Press, New York, 1964.
 9. *Gmelin's Handbuch der Anorganischen Chemie*. System Nr. 15 Si, Teil B; 18 Sb, Teil B, Lfg 1; 27 Mg, Teil A, Lfg 1–2; 39 Rare-Earths Elements, Teil B 3; 45 Ge, Erg. Bd., 50 Ta, Teil A, Lfg 2; 57 Ni, Teil A II, Lfg 1; 61 Ag, Teil A 2. Verlag Chemie, Berlin.
 10. Zholobov, V. V. and Zverov, G. I., *Pressovanie metallov*. Metallurgizdat, Moscow, 1971.
 11. Wilkins, R. A. and Bunn, E. S., *Copper and Copper Base Alloys*. McGraw Hill, New York, 1943.
 12. Goldsmith, A., Watermann, T. E., and Hirschorn, H. J., *Armour Research Foundation: Handbook of Thermophysical Properties of Solid Materials*, Vol. I. The MacMillan Company, New York, 1961.
 13. Sylwestrowicz, W. D., *Philos. Mag.* 7, 1825 (1962).
 14. Shimoji, M., *Liquid Metals*. Academic Press, London, 1977.
 15. Darken, L. C. and Gurry, R. V., *Fizicheskaya khimiya metallov*. (Russian translation.) Gosudarstvennoe nauchno-tehnicheskoe izdatel'stvo, Moscow, 1960.
 16. Feschotte, P., *Z. Metallkd.* 68, 448 (1977).
 17. Siethoff, H. and Schröter, W., *Z. Metallkd.* 75, 475 (1984).
 18. Hume-Rothery, W. and Raynor, V., *The Structure of Metals and Alloys*. The Institute of Metals, London, 1954.
 19. Molotskii, M. Yu., *Fiz. Met. Metalloved.* 55, 43 (1983).

Translated by R. Domanský