Preface

As Honorary Chairman of the Executive Committee it is my great pleasure to present the selected refereed papers of the 8th Japanese-Mediterranean Workshop on Applied Electromagnetic Engineering for Magnetic, Superconducting, Multifunctional and Nano Materials, organized in 23-26 June 2013, in Athens, Greece, constituting a landmark in development of materials, manufacturing and electrical engineering.

This Conference, held every two years, is jointly organized this year by the Project Center for Nanotechnology and Advanced Engineering, a joint initiative of the Greek National Venter for Scientific Research "Demokritos" and the Russian Research Center "Kurchatov Institute", the Japan Society of Electromagnetics and Mechanics, the International Institute for Multifunctional Materials for Energy Conversion, a joint initiative of four American Universities, namely Texas A&M, Houston University, Georgia Tech and Penn State, and the Laboratory of Electrical Machines of the National Technical University of Athens.

The JAPMED has been originated from the very successful previous 1st and 2nd Japanese - Greek Joint Workshops, held in Athens, Greece in May 1999 and Oita, Japan in May 2001, respectively, and, subsequently, extended to further Mediterranean and International participation and cooperation, the 3rd event hosted in Athens, Greece in May 2003, the 4th in Cairo, Egypt in September 2005, the 5th in Larnaca, Cyprus in September 2007, the 6th in Bucharest, Romania, in July 2009 and the 7th in Budapest, Hungary in July 2011. This time, the 8th JAPMED has been organized in June 2013 in Athens, Greece. It provides a forum for specialists from universities, research centers and industry of various countries worldwide to establish cooperation, to share knowledge and experience and the cross-fertilization of new ideas and developments in the design, analysis, new materials utilization and optimization techniques in the areas of electromagnetics and manufacturing of advanced materials and their industrial applications in modern technologies in nanotechnology/ultraprecision engineering, electricity/electronics, transportation, bioengineering, energy and environment.

The high-temperature superconductivity constitutes the first preferential subject of the Conference, focusing on the recent progress in physics, mechanics, materials and applications of high- and low- temperature superconductors, with a projection to the emerging and future areas in science and technology.

Magnetic materials, such as magneto-resistance and ferroelectric materials, as well as conventional ferromagnetic materials and electromagnetics, constitute the second preferential subject, with results that appear to exhibit a breakthrough either conceptually or in the applications they generate.

The scope of the Conference has been further expanded to include the modern exciting areas, like nanotechnology, ultraprecision engineering, bioengineering and transport. In particular, this year, two additional topics are included: the multifunctional materials, in relation also to computational mechanics, i.e. the interests of IIMEC, and the shock loading of materials and structures as a part of the newly established Shockwaves Cluster, involving cooperation between Greece, Russia, USA, Germany, Japan, China, Hungary and Ukraine. The purpose of this international cooperation is the strong belief that we have to enhance our efforts and cooperation towards these advanced technologies, which may greatly affect our lives in the future.

Finally, as I have already announced in my initial invitation letter, this Conference is dedicated to the Former President of the Hungarian Academy of Sciences, Academician Professor Janos Prohászka, one of the greatest scientists in Materials Science, in particular, with his pioneering work on material texture and anisotropy. It was planned to present our recent common work on this topic in the Plenary Session of the Conference, however the Mighty God had other plans. Janos died a few months ago peacefully at his summer house in Magyarpolány Hungary, working on the paper; he was 93 years old. May Janos' soul rest in peace.

Academician Prof. Dr-ing, Dr.h.c. Prof.h.c. A.G. Mamalis
JAPMED'8 Honorary Chairman of the Executive Committee

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Prohászka's Approach to the Scatter of Material Properties of Solid Bodies

János Prohászka

Abstract. According to Prohászka, the scatter of the properties of solid materials cannot be eliminated, because, up to the current knowledge [1-4], identical thermodynamic state of different samples cannot be ensured.

Introduction

There is a permanent effort in the research and development of production processes to eliminate the scatter of properties of solid materials. With our current knowledge it can be decreased, however it is impossible to absolutely eliminate it. On the following pages the thermodynamic causes of the unavoidable nature of the scatter of material properties are discussed. These properties are affected by non-equilibrium crystal defects and due to their presence, no samples can be produced being in thermodynamic equilibrium and whose corresponding material properties are equal, and thus unscattered.

The properties of solid materials, in each instance, exhibit scatter to a certain degree, despite the most careful technological production processes. The magnitude of this scatter depends on the character of the given material property. For example, in metals the scatter of electrical resistivity is much smaller than the scatter of tensile strength because the former is a structure insensitive property and the second is a structure sensitive one.

In the following, it is presented that the cause of the scatter – besides the fluctuation of production conditions – is the thermodynamic dependence of measurable properties and the fact that these cannot be kept in constant level, even besides the most advanced technological circumstances.

Derivation

The starting point is that that all of the properties of the substances of any material system are determined unambiguously by the thermodynamic state. The state variables determine the thermodynamic state. With their help it is possible to give the state equation or state function determining the properties of materials. One such state function is the

$$PV = nRT \tag{1}$$

in the case of specific thermodynamic circumstances
for the ideal gases of n molecules. It gives a very accurate result if the temperature T and the pressure P are far enough from the condensation of the gases.

This equation presupposes that the gas as a thermodynamic system is in the equilibrium state characterised by the minimum of the G free enthalpy. If the P pressure or the temperature T of gases varies with time, the gas goes to another equilibrium state changing the specific volume V in coincidence with equation (1). During the transition from one state to another, the gases are not in equilibrium state and consequently their free enthalpy G is higher than the minimum value and equation (1) does not correctly express the specific volume.

In solid states, materials always contain non-equilibrium crystal imperfections in indeterminable quantity. These imperfections increase the free enthalpy over the equilibrium quantity so that it is impossible to determine a state equation on the analogy of (1).

All materials have a given group of properties, which depend on their thermodynamic state. The degree of this dependence varies between different properties. If something changes these states, these material properties change also. In the following it will be proven that the thermodynamic state of materials may be different despite that the temperature T, pressure P, chemical composition c_k of the k_{th} constituent and free enthalpy G one by one have the same value. Normally, the

materials are in a metastable state, their free enthalpy G must be larger than $G_{min,}$, the ideal minimum, which corresponds to the free enthalpy of thermodynamic equilibrium.

Let G_i be the free enthalpy of a solid body being in ideal equilibrium characterised by the minimum of G:

$$G_i = U_i - TS_i + PV_i \tag{2}$$

Where U is the internal energy, S is the entropy and V is the specific volume. The indices i are related to the ideal solid body having minimal free enthalpy. In ideal equilibrium the material must contain only equilibrium crystal defects. The G_r free enthalpy of real solid bodies is:

$$G_r = U_r - TS_r + PV_r \tag{3}$$

r relates to the real states and, as we mentioned formerly, they gave at all times some ΔG free enthalpy excess and its value is:

$$\Delta G = G_r - G_i \tag{4}$$

This emanates from the fact that free enthalpy increases effects of crystal imperfection over the equilibrium quantity. ΔG can be regarded as the measurement of metastability of the material.

It is supposed that it is possible to take a sample A from a material having a certain chemical composition and its free enthalpy is G_r^A, and a similar one B with the same composition and its free enthalpy, G_r^B is equal to the free enthalpy of A.

$$G_r^A = G_r^B \tag{5}$$

In this case two equations can be written for the free enthalpy of the two materials, as follows:

$$\begin{aligned} \Delta G^A &= \Delta U^A - T\Delta S^A + P\Delta V^A = \\ &\Delta U^B - T\Delta S^B + P\Delta V^B = \Delta G^B \end{aligned} \tag{6}$$

Where ΔU, ΔV and ΔS should be interpreted as ΔG defined in (4). The equations in (6) can hold also in the cases that the following inequalities are present:

$$\begin{aligned} \Delta U^A &\neq \Delta U^B \\ \Delta S^A &\neq \Delta S^B \\ \Delta V^A &\neq \Delta V^B \end{aligned} \tag{7}$$

Let it be supposed that sample A contains crystal defects belonging to n different types and sample B contains these n types of defects also. Let the density of different kinds of the defects be $\rho_1^A, \rho_2^A \ldots \rho_i^A \ldots \rho_n^A$ and $\rho_1^B, \rho_2^B \ldots \rho_i^B \ldots \rho_n^B$ respectively. With these quantities it can be written:

$$\Delta U^A = \Delta U_1^A + \Delta U_2^A + \ldots + \Delta U_n^A$$
$$\Delta S^A = \Delta S_1^A + \Delta S_2^A + \ldots + \Delta S_n^A$$
$$\Delta V^A = \Delta V_1^A + \Delta V_2^A + \ldots + \Delta V_n^A$$

and

(8)

$$\Delta U^B = \Delta U_1^B + \Delta U_2^B + ... + \Delta U_n^B$$
$$\Delta S^B = \Delta S_1^B + \Delta S_2^B + ... + \Delta S_n^B$$
$$\Delta V^A = \Delta V_1^B + \Delta V_2^B + ... + \Delta V_n^B$$

From the above equation the subsequent equations can be derived:

$$\Delta G^A = \sum_k^n \Delta U_k^A - T\sum_k^n S_k^A + P\sum_k^n V_k^A =$$

$$= \sum_h^n \Delta U_h^B - T\sum_h^n S_h^B + P\sum_h^n V_h^B = \Delta G^B \tag{9}$$

In agreement with the above mentioned facts, to determine the *ΔG* free enthalpy excess of a given solid body one needs *3n* data if the temperature *T* and the pressure *P* are known. Then *n* is the number of the types of special crystal defects. But the *3n* data are not independent of each other, because the following equations can be written:

$$\Delta U_i = f(\rho_i)$$
$$\Delta S_i = f(\rho_i)$$
$$\Delta V_i = f(\rho_i) \tag{10}$$

This means that every increment of free enthalpy caused by the k_{th} kind crystal defect depends only on its density. The effects of different crystal defects to the uncertainty of the thermodynamic system have been overviewed, but the interactions of crystal defects - which result in an excess of free enthalpy – were not taken into account. However this does not weaken the validity of the consideration; in contrast it supports it while these interactions make the control of the real thermodynamic state even more obscure.

The equations (10) reduce the 3n variables to n. Let us consider the case when sample *A* containing m_v vacancies above the equilibrium quantity. The surplus of the internal energy ΔU_v^A due to excess vacancies is:

$$\Delta U_v^A = m_v Q_v = fv(m_v) \tag{11}$$

where Q_v is the forming energy of one vacancy.

The ΔS_v^A entropy caused by the m_v vacancies is:

$$\Delta S_v^A = k \ln \frac{N!}{(N - m_V)! m_V!} = g_v(m_v) \tag{12}$$

where the equilibrium vacancy concentration is:

$$\frac{n_v}{N} = e^{-\frac{Q_v}{kT}} \tag{13}$$

here n^v is the number of equilibrium vacancies, m^v is the number of non-equilibrium vacancies, N is the number of total lattice points of the system, hence $N - m^v - n^v$ is the number of atoms in the samples and k is the Boltzmann constant.

Finally the excess of the specific volume caused the surplus of the vacancies are:

$$\Delta V_v = V_0^v(m_v) = h_v(m_v) \tag{14}$$

where V_0^v is the volume of the primitive cell of crystal structure in which there are z atoms embedded. (For example in the b.c.c. structure z equal to 2 and in the f.c.c. cell it is 4.)

With the previous functions, the (9) summarisations can be overwritten as follows:

$$\begin{aligned}\Delta G^A &= \sum_k^n f_k(\rho_k^A) - T\sum_k^n g_k(\rho_k^A) + P\sum_k^n p_k(\rho_k^A) = \\ &= \sum_h^n f_h(\rho_h^B) - T\sum_h^n g_h(\rho_h^B) + P\sum_h^n p_h(\rho_h^B) = \Delta G^B\end{aligned} \tag{15}$$

From the last two equations it follows, that if the samples have the same chemical composition and their temperature T and pressure P are the same and their free enthalpy excesses are equal, than these conditions are only a necessary, but not a fully satisfactory requirement for an identical thermodynamic state. The last two equations can also be equal in those cases if the following inequality exists:

$$\rho_k^A \neq \rho_h^B \tag{16}$$

Discussion

The statement described above can be demonstrated by the following theoretical example. Let us consider two single crystal copper samples, whose composition and free enthalpy is assumed to be identical. Let the orientation of the samples be the same. Furthermore, let these samples be identical in every aspect, even regarding the dislocations indeed of the real life experience. Suppose that the free enthalpy excess of sample A is increased by ΔG^A with neutron bombing. Let us deform Sample B with plastic deformation which increases the free enthalpy by ΔG^B. Let these free enthalpy increments be equal. Note, that point defects change material properties in a different manner than dislocations caused by plastic deformation. In this case the material properties of the crystals are different instead of their free enthalpy excesses being equal.

The above written equations prove that the scatter of material properties is derived from the fact that their thermodynamic states are not identical instead of their free enthalpy excesses are equal. With our current knowledge, two or more samples having the identical thermodynamic state cannot be produced. Namely, for an identical thermodynamic state, the two samples must have the same chemical composition, temperature T, pressure P and moreover the different kinds of crystal defect must have the same density. The samples can only have the same properties if all of the crystal defects have the same density. It can be concluded that the usual technological steps which are applied to enhance various material properties (ex. material strength, etc) are increasing the scatter of material properties, while they are increasing the free enthalpy excess. Therefore, the effort to produce materials with unvaried properties is contradictory to practical material engineering requirements.

Conclusions

In conclusion, from all the above mentioned, the following remarks can be drawn:

- The cause of the scatter of properties of solid materials is that their thermodynamic states are not identical, even if the integrated thermodynamic measures of their states are equal.
- For identical thermodynamic states, the chemical composition, temperature T, pressure P is only a necessary but not the satisfactory requirement.
- The thermodynamic states of solid materials are only identical in the cases when not only the composition temperature T and pressure P are the same, but it must also be true that

$$\rho_k^A = \rho_k^B \tag{17}$$

i.e., all kinds of crystal defects one by one must have the same density.

- The satisfaction of the last requirements depends on the precision of the production processes and by advancing these the scatter can be decreased but it is impossible to eliminate in the strictest sense. The interactions of crystal defects have not been considered, while their effects are increasing the differences between the investigated materials.
- The magnitudes of scatter are growing with the free enthalpy excess ΔG, which is a measure of metastability.

Typical production processes of metals resulting in desired material properties, such as hardening, rolling, etc., are increasing the free enthalpy, thus, as a side effect; these methods increase the scatter of material properties. Therefore, by usual production methods there is a level of scatter which cannot be lowered.

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