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REDUCTION OF THERMOELECTRIC MATERIAL LATTICE THERMAL CONDUCTIVITY USING SHAPE-FORMING ELEMENT OPTIMIZATION

Within the four different model approaches the lattice conductivity of Bi_2Te_3 was calculated for a physical model of shape-forming element of thermoelectric material structure, namely two hemispheres contacting in a circle with regard to phonon scattering on the contact boundary as applied to Bi_2Te_3. The calculated data is briefly discussed from the general physics and applied standpoints of thermoelectric material science.

Key words: thermoelectric material, extrusion, figure of merit, lattice thermal conductivity, shape-forming element, contact, boundaries, phonons, scattering, normal processes, *U*-processes.

Introduction

The most widely used thermoelectric materials nowadays are *Bi-Te* based alloys (Bi_2Te_3 compounds). They are prepared by different methods, namely zone recrystallization, Czochralski pulling and oriented crystallization process. These three methods yield thermoelectric figure of merit Z in the range of $(2.8 \div 3.1) \cdot 10^{-3}$ K^{-1}. Such Z values are achieved with heat flux and electric current orientations in the directions normal to Bi_2Te_3 trigonal axis. Whereas in the direction parallel to trigonal axis the Z values are essentially lower. This situation is due to the fact that Bi_2Te_3 is uniaxial anisotropic crystal whose conductivity values σ_{11} in the direction normal to trigonal axis are $\sigma_{11} = (800 \div 1000)$ Ω^{-1}cm^{-1} and are considerably higher than σ_{33} – conductivity along trigonal axis. The values of thermal conductivity χ_l are also anisotropic and make $\chi_{11} = 1.45$ W/m·K and $\chi_{33} = 0.58$ W/m·K. At the same time, the thermoelectric coefficients α_{11} and α_{33} are little different and make $210 \div 220$ µV/K. Therefore, $Z_{11} = (2.4 \div 2.5) \cdot 10^{-3}$ K^{-1}. For this reason, practical use is found by materials oriented normal to trigonal axis.

Thermoelectric instruments and devices are also manufactured with the use of Bi_2Te_3 based materials prepared by extrusion method whose thermoelectric figure of merit is about $3 \cdot 10^{-3}$ K^{-1}, that is, rather close to that of single crystal materials.

It should be noted that the macroscopic structure of extruded materials is a combination of arbitrarily oriented powder particles of size $(40 \div 80)$ µm whole properties are close to those of oriented crystalline thermoelectric materials. For extruded thermoelectric materials $\sigma_{ef} = \sqrt{\sigma_{11}\sigma_{33}}$ and $\chi_{ef} = \sqrt{\chi_{11}\chi_{33}}$. Therefore, thermoelectric figure of merit of extruded material must be lower than that of single crystal. Taking into account that electric conductivity anisotropy of Bi_2Te_3 depending on conductivity type is 2.7 for *p*-type and $4 \div 6$ for *n*-type, and thermal conductivity anisotropy is $2 \div 3$, the figure of merit can be reduced by a factor of $\sqrt{2} - \sqrt{3}$, that is, by $30 - 40$ %. However, in the best

case for *p*-type material it can even grow by about 5 %. In practice, no figure of merit reduction is observed. Hence, there must be a mechanism leading to thermoelectric figure of merit increase in going from single crystal to extruded material structure due to a change in the character of phonon and current carrier scattering. Research on this mechanism would provide for helpful information as to the ways of radical improvement of thermoelectric figure of merit of said materials.

The physical concept of thermoelectric figure of merit improvement in extruded material is that thermal conductivity in going from a bulk to porous or fine-dispersed structure is reduced considerably and the electric conductivity – essentially weaker.

The authors of [1] who were among the first who paid attention to this fact, made evaluation calculations of the electric and thermal conductivity of model structure of thermoelectric material rods divided by vacuum gaps. From the evaluation formulae it follows that if the characteristic dimensions of the rods are small, then the electric and thermal conductivity of the structure is proportional to these dimensions. However, with the large rod dimensions said characteristics tend to parameters of the bulk material. Moreover, in the estimation of thermoelectric figure of merit in this work it was considered that the lattice conductivity of such structure is zero. The electric and thermal conductivity of the structure caused by free charge carriers is essentially dependent on the coefficient of electrons passage through the vacuum gap which does not affect, however, the thermoelectric figure of merit. Said approach did not yield quantitative estimates of rod dimensions and gaps between them that are optimal in terms of thermoelectric figure of merit. In [2] it is shown that in going from single-crystal to fine-dispersed germanium with the average grain radius $2.0 \div 2.5$ μm (of which samples with porosity 70 % were made), the ratio of electric conductivity to thermal conductivity increased by a factor of 100 as compared to single crystal, and thermoelectric figure of merit – only by a factor of $4 - 6$, which, in the authors' opinion is attributable to incomplete restoration of negative thermoEMF after annealing. In [3], formulae were obtained for the determination of the electric and thermal conductivity of a dispersed medium comprising spherical particles of thermoelectric material, but electron and phonon scattering on the boundaries of spheres and contacts between them was not considered.

Paper [4] is a theoretical study of the thermal conductivity of the bulk nanostructured bismuth telluride samples which, nevertheless, does not take into account that phonon scattering on the boundaries of individual nanoparticles occurs at all phonon frequencies, rather than at "selected" ones.

In patent [5] for the efficient phonon drag it is proposed to use small-area contacts between relatively large parts of thermoelectric material. In so doing, said contacts must have dimensions of the order of several nanometers.

There were also considered the possibilities of creating such thermoelectric materials that would be "phonon glasses", remaining in this case "electron crystals" due to the fact that lattice thermal conductivity with a large concentration of structural defects is reduced more than the electric conductivity owing to the peculiarity of electron density of states [6]. The researchers' attention is also focused on the whiskers of organic conductors of the type TTF-TCNQ and the like [7, 8]. It is considered that a high degeneracy level of free charge carriers gas is attainable in these crystals, owing to which lattice thermal conductivity cannot affect considerably the thermoelectric figure of merit of material, and the latter can be regarded as the integral characteristic of free charge carriers subsystem in material [9], that is, the lower limit of thermal conductivity in these crystals has already been achieved, and the only opportunity of thermoelectric figure of merit improvement is the Lorentz number increase.

In the manufacture of thermoelectric modules of conventional material powders by hot pressing or extrusion methods, a question arises as to the optimal in terms of thermoelectric figure of merit size of powder grains and contacts between them. According to [10], particles of source powder can be adequately considered spherical. In the course of pressing they can acquire the shape of hemispheres

with a circular contact between them. The shape-forming element of such structure can be approximated by two equal-radius hemispheres contacting in a circle. Research on the generalized conductivities of such shape-forming element should be a preliminary to a research on the above mentioned characteristics of structure as a whole. It is this that motivates the relevance of the problem solved in this work.

Our purpose in this work is to calculate changes in the lattice thermal conductivity of shape-forming element of extruded thermoelectric material structure due to phonon scattering on the boundaries of contact between two osculating hemispheres, and estimate the radius of contact necessary for 30 – 40 % reduction of lattice thermal conductivity of shape-forming element.

Consideration of the problem of phonon scattering on the boundaries of shape-forming element in the approximation of constant relaxation time

As will be shown below, for consideration of this problem it is reasonable to involve a model of unit sphere placed in a heat flux. This will enable a more transparent physical interpretation of quantitative estimates. With a constant phonon relaxation time, the following expression for the resulting phonon mean free path in a limited sample is valid [11]:

$$l_{tp} = \frac{l_p L}{l_p + L}. \tag{1}$$

In this formula, l_p is phonon mean free path in material caused by all scattering mechanisms, except for the boundaries of contact spot or sample as a whole; L is effective phonon mean free path due to sample boundaries. As long as the effective mean free paths in a sample due to the boundaries are not equal for all the phonons, the thermal conductivity of material at boundary scattering is:

$$\chi_l^{ef} = \frac{1}{3}\rho v c_V l_p \left\langle \frac{L}{L + l_p} \right\rangle. \tag{2}$$

In this formula, ρ is material density, v is sound velocity in it, c_V is specific heat of material with a constant volume. The angular brackets mean averaging of respective expression over possible effective lengths L of phonon mean free path in a sample, including the shortest ones, because theirs is the major contribution to general possibility of phonon scattering [11]. In the case of a circular contact which is small as compared to hemisphere diameters, it can be considered that phonon drag takes place only in its vicinity. Moreover, all points of contact boundary are equivalent by virtue of its symmetry. Hence, formula (2) implies the following ratio between thermal conductivity of shape-forming element and that of the bulk sample:

$$\chi_l^{ef} \Big/ \chi_l = \pi^{-1} \int_0^1 \int_0^{2\pi} x \frac{k\sqrt{1 + x^2 - 2x\cos\varphi}}{1 + k\sqrt{1 + x^2 - 2x\cos\varphi}} \, d\varphi dx . \tag{3}$$

In this formula, $k = r/l_p$, l_p is phonon mean free path. As it must be, at $k = 0$ formula (3) gives zero, and at $k \to \infty$ – thermal conductivity of a bulk sample. The results of these calculations are shown in Fig. 1.

From the results of calculations it follows that for thermal conductivity reduction, for instance, by 30 – 40 %, the contact radius must not exceed $(1.3 \div 2.5) \, l_p$. Taking into account that according to

[12] the phonon mean free path corresponding to a greater thermal conductivity value is 4.16 nm, we obtain that contact radius must not exceed $(5 \div 10)$ nm. The mean free path corresponding to the lower thermal conductivity value is, however, 1.4 nm. Therefore, for the same reduction of the lower thermal conductivity value the contact radius must not exceed $(1.8 \div 3.3)$ nm. By analogy, this problem can be solved for a unit sphere. The respective formula is given by:

$$\chi_l^{ef} \Big/ \chi_l = 1.5 \int_0^1 \int_0^{2\pi} x^2 \frac{k\sqrt{1 + x^2 - 2xy}}{1 + k\sqrt{1 + x^2 - 2xy}} \, dy dx. \tag{4}$$
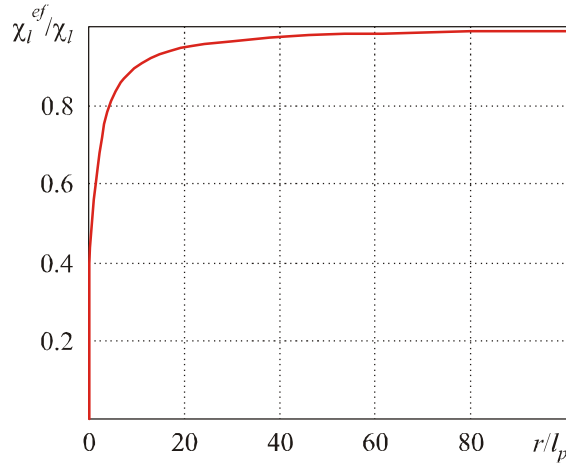

*Fig. 1. Dependence of thermal conductivity of a system of two hemispheres
contacting in a circle on the contact radius.*

Double integral in this formula is caused by averaging the expression for thermal conductivity over the effective phonon mean free paths inside the sphere. In this formula, $k = R/l_p$, where R is sphere radius. The corresponding plot is presented in Fig. 2
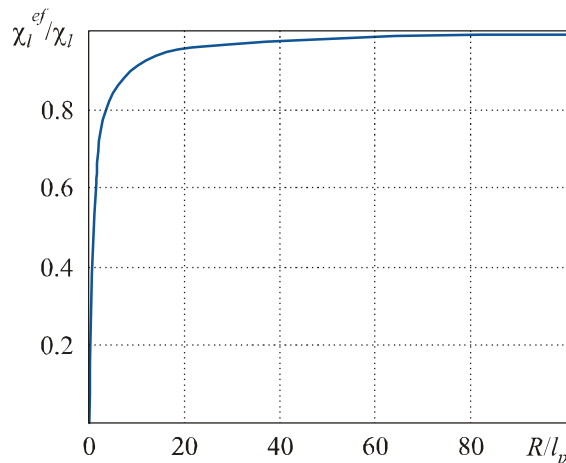

*Fig. 2. Sphere radius dependence of a relative decrease
in lattice thermal conductivity due to phonon drag size effect.*

It is seen that for the above discussed thermal conductivity reduction the sphere radius should not exceed $(1.2 \div 2.2)$ l_p. For a greater thermal conductivity value it makes $(5.1 \div 9.3)$ nm, and for the lower – $(1.6 \div 2.9)$ nm.

Problem consideration with regard to frequency dependence
of phonon relaxation time

All previous calculations have been valid in the approximation of constant phonon relaxation time. Next, we consider the problem with regard to frequency dependence of phonon relaxation time.

If we normalize phonon relaxation time to the time of normal processes, then, taking into account [11], components of thermal conductivity tensor of the bulk sample of such layered material as bismuth telluride can be written as:

$$\chi_{l\|,\perp} = \frac{3\hbar M v_{\|,\perp}^4 k_B}{32\gamma^2 a_{\|,\perp}^3 \left(k_B T_D^2\right)\theta^3\pi} \int_0^1 \frac{x^4 \exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2}\left(\frac{1}{Q_{l\|,\perp}(x)}+\frac{2}{Q_{t\|,\perp}(x)}\right)dx. \tag{5}$$

In these formulae, χ_l is lattice thermal conductivity; M is average atom mass in bismuth telluride; v is sound velocity in it; k_B is the Boltzmann constant; γ is the Gruneisen parameter; T_D is the Debye temperature of material; $\theta = T/T_D$, $Q_l(x)$ and $Q_t(x)$ are frequency polynomials introduced by one of the authors (P.V. Gorsky) that are to a power not higher than the fourth and caused by scattering mechanisms for the longitudinal and transverse phonons, indexes $\perp$ and $\|$ refer to thermal conductivity and sound velocity normal and parallel to the layers.

At room temperatures and higher the thermal conductivity of thermoelectric material is mainly determined by Umklapp processes (U-processes). Therefore, polynomials $Q_l(x)$ and $Q_t(x)$ are determined as:

$$Q_{l\|,\perp}(x) = Q_{t\|,\perp}(x) = \mu_{\|,\perp} x. \tag{6}$$

Coefficient μ in the analytical form was calculated by Leibfried and Shleman [11] for a cubic lattice. However, according to experimental data [11], the value μ is not universal. Therefore, we will "retrieve" $\mu_\|$ and $\mu_\perp$ coefficients from the real values of components of thermal conductivity tensor of bismuth telluride [12], on condition of their coincidence with the theoretical values (5) and (6). At $\chi_{l\perp} = 0.58$ W/m·K, $\chi_{l\|} = 1.45$ W/m·K, $M = 158.8$ a.m.u., $a_\perp = 3\cdot10^{-9}$ m, $v_\perp = 1867$ m/s, $a_\| = 7\cdot10^{-10}$ m, $v_\| = 2952$ m/s, $T_D = 155$ K and $T = 300$ K we obtain $\mu_\| = 0.131$, $\mu_\perp = 6.657\cdot10^{-4}$.

Based on these coefficients, it is easy to calculate a relative reduction of thermal conductivity due to scattering on the boundaries of circular contact and sphere. By analogy with formula (3) in the case of a circular contact:

$$\chi_{l\|,\perp}^{ef}\Big/\chi_{l\|,\perp} = \pi^{-1}\int_0^1\int_0^1\int_0^{2\pi}\frac{zx^4\exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2}\left(\frac{k_{\|,\perp}^*\sqrt{z^2-2z\cos\varphi+1}}{1+k_{\|,\perp}^*Q_{l\|,\perp}(x)\sqrt{z^2-2z\cos\varphi+1}}+\right.$$

$$+\frac{2k_{\|,\perp}^*\sqrt{z^2-2z\cos\varphi+1}}{1+k_{\|,\perp}^*Q_{t\|,\perp}(x)\sqrt{z^2-2z\cos\varphi+1}}\Bigg)d\varphi dz dx\left\{\int_0^1\frac{x^4\exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2}\left(\frac{1}{Q_{l\|,\perp}(x)}+\frac{2}{Q_{t\|,\perp}(x)}\right)dx\right\}^{-1}. \tag{7}$$

In so doing, $k_{\|,\perp}^* = \frac{r_{\|,\perp}\gamma^2}{a_{\|,\perp}}\left(\frac{k_B T_D a_{\|,\perp}}{\hbar v_{\|,\perp}}\right)^4\left(\frac{k_B T_D}{M v_{\|,\perp}^2}\right)$.

The afore-mentioned figures of thermal conductivity reduction for its greater value are obtained at $k^* = 17.37 \div 33.02$. With the above defined problem parameters we get $r_\| = (3.5 \div 6.7)\cdot10^{-9}$ m. The same figures of thermal conductivity reduction for its lower value are obtained at $k^* = 3419 \div 6498$.

Therefore, $r_\perp = (0.6 \div 1.2) \cdot 10^{-9}$ m. Such radii of contacts between particles of diameter $60 \div 80$ μm are hardly feasible.

In the case of a sphere, by analogy with formula (4) we have:

$$\chi_{l\|,\perp}^{ef} \Big/ \chi_{l\|,\perp} = 1.5 \int_0^1 \int_0^1 \int_{-1}^1 \frac{z^2 x^4 \exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2} \left(\frac{k_{\|,\perp}^* \sqrt{z^2-2zy+1}}{1+k_{\|,\perp}^* Q_{l\|,\perp}(x)\sqrt{z^2-2zy+1}} + \right.$$

$$\left. + \frac{2k_{\|,\perp}^* \sqrt{z^2-2zy+1}}{1+k_{\|,\perp}^* Q_{t\|,\perp}(x)\sqrt{z^2-2zy+1}} \right) \mathrm{d}y \mathrm{d}z \mathrm{d}x \left\{ \int_0^1 \frac{x^4 \exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2} \left(\frac{1}{Q_{l\|,\perp}(x)} + \frac{2}{Q_{t\|,\perp}(x)} \right) \mathrm{d}x \right\}^{-1}. \tag{8}$$

where $k_{\|,\perp}^* = \dfrac{R_{\|,\perp} \gamma^2}{a_{\|,\perp}} \left(\dfrac{k_B T_D a_{\|,\perp}}{\hbar v_{\|,\perp}} \right)^4 \left(\dfrac{k_B T_D}{M v_{\|,\perp}^2} \right)$.

Hence, in case of a sphere, to obtain the above reduction of greater thermal conductivity value, there must be $k^* = 15.57 \div 29.07$, whence $R_\| = (3.2 \div 5.9) \cdot 10^{-9}$ m. To obtain the same reduction of lower thermal conductivity value, there must be $k^* = 3420 \div 6500$, whence $R_\perp = (0.6 \div 1.2) \cdot 10^{-9}$ m. Such particle dimensions are realizable only in nanostructured thermoelectric materials. Thus, the approach that takes into account only U-processes, cannot explain yet a small change in thermoelectric figure of merit in going from a single crystal to extruded thermoelectric material.

Therefore, it is worthwhile to consider phonon scattering on the boundaries of a circular contact and sphere with regard to not only U-processes, but normal processes as well. For this purpose, frequency polynomials $Q_l(x)$ and $Q_t(x)$ may be written as follows:

$$Q_{l\|,\perp}(x) = x^4 + \mu_{\|,\perp} x, \tag{9}$$

$$Q_{t\|,\perp}(x) = \left(\mu_{\|,\perp} + 3.125\theta^3 \right) x. \tag{10}$$

Hence we get $\mu_\| = 4.142 \cdot 10^{-5}$, $\mu_\perp = 5.917 \cdot 10^{-12}$. In this case, to obtain the above reduction of greater thermal conductivity value with phonon scattering on the boundaries of a circular contact, there must be $k^* = (1.52 \div 4.37) \cdot 10^5$. Thus contact radius $r_\| = 31 \div 89$ μm. To obtain the same reduction of lower thermal conductivity value, there must be $k^* = (1.839 \div 5.454) \cdot 10^{14}$, whence $r_\perp = 32 \div 97$ m. Quite similarly, in the case of phonon scattering on the boundaries of a sphere, to obtain the above reduction of greater thermal conductivity value, there must be $k^* = (1.37 \div 3.90) \cdot 10^5$, whence $R_\| = 28 \div 80$ μm. For the same reduction of lower thermal conductivity value, there must be $k^* = (1.66 \div 4.88) \cdot 10^{14}$, whence $R_\perp = 29 \div 87$ m.

From the absurd, on the face of it, results for $r_\perp$ and $R_\perp$ parameters it follows that thermal conductivity anisotropy of macroscopic (e.g. meter long) samples cut from Bi_2Te_3 single crystal must be essentially dependent on their size, which is not the case. So, such an approach needs to be modified. Its main disadvantage introducing an excessive error lies in a forced replacement of real crystal lattice of material by a simple cubic lattice with one atom in the unit cell. However, in this case it is clear that neither $a_\|$ nor $a_\perp$ can serve as cube edges, since $M/a_\|^3$ and $M/a_\perp^3$ quantities yield evidently understated material density values.

In conclusion, we consider an approach based on the substitution of a real Bi_2Te_3 crystal lattice by a simple cubic lattice of the same density. According to this approach, the value of dimensionless

parameter $k_{\parallel,\perp}^{*}$ for the case of a circular contact should be redefined as:

$$k_{\parallel,\perp}^{*} = \frac{r_{\parallel,\perp}\gamma^2}{\rho}\left(\frac{k_B T_D}{\hbar v_{\parallel,\perp}}\right)^4\left(\frac{k_B T_D}{v_{\parallel,\perp}^2}\right),$$ (11)

and for the case of a sphere as:

$$k_{\parallel,\perp}^{*} = \frac{R_{\parallel,\perp}\gamma^2}{\rho}\left(\frac{k_B T_D}{\hbar v_{\parallel,\perp}}\right)^4\left(\frac{k_B T_D}{v_{\parallel,\perp}^2}\right).$$ (12)

As to formula (5), it must be re-written as:

$$\chi_{l\parallel,\perp} = \frac{3\hbar\rho v_{\parallel,\perp}^4 k_B}{32\gamma^2\left(k_B T_D^2\right)\theta^3\pi}\int_0^1\frac{x^4\exp(x/\theta)}{\left[\exp(x/\theta)-1\right]^2}\left(\frac{1}{Q_{l\parallel,\perp}(x)}+\frac{2}{Q_{t\parallel,\perp}(x)}\right)\mathrm{d}x.$$ (13)

Just as before, with regard to formulae (9) and (10), we obtain $\mu_{\parallel} = 0.022$, $\mu_{\perp} = 2.177\cdot10^{-3}$. According to this approach, for the reduction of either thermal conductivity values by $30 - 40\,\%$ in the case of phonon scattering on the circular contact boundaries, $k_{\parallel}^{*}$ must be $69.6 \div 167.7$ and $k_{\perp} - 1008 \div 2691$. Therefore, contact radius must be $0.4 \div 1.1\,\mu m$. In the case of phonon scattering on the sphere boundaries, $k_{\parallel}^{*}$ must be $62.5 \div 149.1$ and $k_{\perp} - 908 \div 2400$. Therefore, the sphere radius is $0.35 \div 1\,\mu m$.

Contacts of said dimensions can occur between particles of diameter $40 \div 80\,\mu m$ at extrusion, which can account for the absence of a considerable decrease in thermoelectric figure of merit in going from a single crystal to extruded material.

Conclusions and recommendations

1. Based on the model of a shape-forming element of thermoelectric material structure in the form of two hemispheres contacting in a circle, it is shown that one of possible mechanisms of thermoelectric material lattice conductivity reduction in going from a single crystal to extruded material can be additional phonon scattering on the boundaries of contacts or spherical particles themselves.

2. In the approximation of constant phonon relaxation time it is shown that for the reduction of lattice thermal conductivity of a shape-forming element by $30 - 40\,\%$ as compared to that of the bulk material the radius of contact between the particles should not exceed $1.3 \div 2.5$ of the mean free path of phonon in material. With the use of a drag on the boundaries of spherical particles themselves, their radius should not exceed $1.2 \div 2.2$ of the mean free path of phonon in material.

3. With a substitution of a real crystal lattice of bismuth telluride by a model simple cubic lattice with unchanged material density and account of both *U-* and normal processes, the above discussed reduction of both components of thermal conductivity tensor is obtained with contact or particle radii within $0.3 \div 1\,\mu m$. As long as such contacts may be created between particles in the process of extrusion, it is exactly phonon scattering on their boundaries that can account for a slight change in thermoelectric figure of merit in going from a single crystal to extruded material.

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Submitted 23.01.2013.