

FUNDAMENTAL PROPERTIES OF CRYSTALLINE NANO-STRUCTURES CAUSED BY MECHANICAL AND THERMODYNAMICAL EXCITATIONS

M.Sc. Ana Šetrajčić Tomić¹, Prof. Dr. Siniša M. Vučenović², Prof. Dr. Tomislav M. Pavlović^{3,4}, Prof. Dr. Jovan P. Šetrajčić^{4,5}

University of Novi Sad, Faculty of Medicine, Novi Sad, Vojvodina – Serbia¹,
 University of Banja Luka, Faculty of Sciences, Banja Luka, Republic of Srpska, B&H²,
 University of Niš, Faculty of Sciences, Niš, Serbia³,
 Academy of Sciences and Arts of the Republic of Srpska, Banja Luka, Republic of Srpska, B&H⁴,
 University "Union – Nikola Tesla", Faculty of Sport, New Belgrade, Vojvodina – Serbia⁵;
 jovan.setrajcic@gmail.com

Abstract: Mechanical or thermodynamic excitations in solid state physics – phonons, cause all fundamental physical properties of materials and always are present, regardless of what is the main carrier of transport properties and ordering (for example, in electro-conductivity, it can be electrons / holes, ions, etc., and in magnetism – magnons). In particular, phonons play a different and more subtle role in low-dimensional nano-scale samples, because they, due to the confinement effects, influence the creation of completely unusual and altered characteristics in relation to large (bulk) samples of exactly the same material. Therefore, the possible phonon spectra and states in model of crystal nanostructures: ultrathin films, nano-wires and quantum dots were founded in the paper. The most noticeable phenomenon is the consequence of the dimensional quantization, but also the shape of the boundary surfaces, as well as the presence of the environment surrounding the nano-pattern. In addition to the analysis of the microscopic properties of the phonon subsystem, the calculation of the temperature dependence of the thermal capacity and entropy of these nano systems was also calculated and performed by comparisons with the same for bulk structure.

Keywords: PHONONS, GREEN'S FUNCTION, NANOSTRUCTURES, SPECTRA AND STATES, THERMODYNAMICS

1. Introduction

Over the last decade, we have been witness in rapid development of nanotechnology, i.e. production technologies of structures with nano-dimensions [1–3]. The trend of rapid development of nanotechnologies is not accidental since nanostructures possess physical characteristics that are substantially different from the physical characteristics of the structures, which are larger. Nanostructures have a number of qualitatively new effects. Superconductive, thermal insulating, acoustic and other features that characterize nanomaterials are better than in bulk structures. It is also expected that the usage of nanostructured elements may increase the instruments sensitivity for measuring, and that is leading to new experimental discoveries. All of the abovementioned leads to the conclusion that nanomaterials can be a good basis for further development of Physics [4–6]. In some way, nanostructure effects are connected to the effects in bulk structures, similarly to the relationship between quantum and classical effects. Therefore, further and even faster development of the science of nanostructure materials and nanotechnology is to be expected.

Application of nano-structures requires knowledge of their fundamental physical (mechanical, electro-magnetic, optical, etc.) characteristics. Thermodynamic properties associated with phonon displacements through the nano-samples are particularly interesting. Independent of the type of lattices, the thermodynamics of their subsystems (electrons, excitons, spin waves, etc.) is determined when the subsystem is in thermodynamic equilibrium with phonons. Phonons are quasiparticles that represent collective mechanical oscillations of molecules or atoms and they are the most important system of excitations [7–9]. Besides, the acoustical characteristics as well as conductive and superconductive properties etc. could not realistically being explained without knowing of phonons behavior. All quoted is well known and all applications of phonons in bulk structures have been intensively exploited for more than a century.

The fact, which must be especially pointed out, is that the role of phonons in nanostructures is much more impressive than in bulk structures. The main fact concerning phonon properties in nanostructures is the absence of the so-called acoustic phonons, i.e. phonons whose energy tends to zero when phonon momentum tends to zero. For the phonon excitation in nanostructures – activation energy different from zero is needed. These unexpected characteristics require revision of all conclusions obtained by bulk theories of phonons [10–12]. Therefore, the contribution of phonon subsystems to thermodynamic and energy transfer analysis is the first step in a research of nanostructure properties.

This paper describes a major aspect of the effort to understand nanostructures, namely the study of phonons and phonon-mediated effects in structures with nanoscale dimensional confinement in one or more spatial dimensions. During the last two decades, there has been a steady effort to understand the optical and acoustic phonons in nanostructures such as the superlattice, quantum wires, nanotubes and quantum dots. The central theme of this paper is the description of the acoustic phonons of the optical type in these nanostructures. Primarily, to describe the dispersion relations and mode structures for phonons in nanostructures, phonon amplitudes are quantized in terms of the harmonic oscillator approximation, and where anharmonic effects lead to phonon decay that is described in terms of the dominant phonon decay channels. These elastic and discontinued models are applied to describe the deformation potential and interactions in a variety of nanostructures. Dependence of energy on the wave vector is highly nonlinear and linear approximations of the dispersion laws of phonons in small size nanostructures make no sense. Changing the phonon dispersion law due to the confinement severely affects the kinetic effects conditioned by the interaction of acoustic phonons with electrons, dotted defects and phonon-phonon interactions. Managing transport properties of acoustic phonons through the modification of their energy spectrum in nanostructures was named phonon engineering.

2. Research method and models

Since quantum low-dimensional structures are of the great interest in science, we have investigated and researched the basic microscopic behavior of phonon subsystem in following models of nano-structures: ultra-thin films (UTF), nano-rods (NR) and quantum dots (QD). The influence of the phonons in these structures is decisive on macroscopic properties, especially from the aspect of their possible usage in nanotechnology. This paper is based on research from our group of researchers gathered around Department for theoretical Physic of University of Novi Sad in the last decades [12–15]. In the opposite of the films which are quasi-2D structures, limited by two surfaces parallel to XY planes, nano-rods and quantum dots are quasi 1D and 0D crystal systems limited in two or three directions: y and z, or x, y and z respectively, (Fig. 1.). It should be mentioned that we will, in here presented calculations, take into account only so called "cut of" models, where we don't consider influence of boundary parameters: $(\epsilon, \gamma, \sigma, \varphi) = 0$, i.e. we wanted to explore only the influence of quantum size effects.

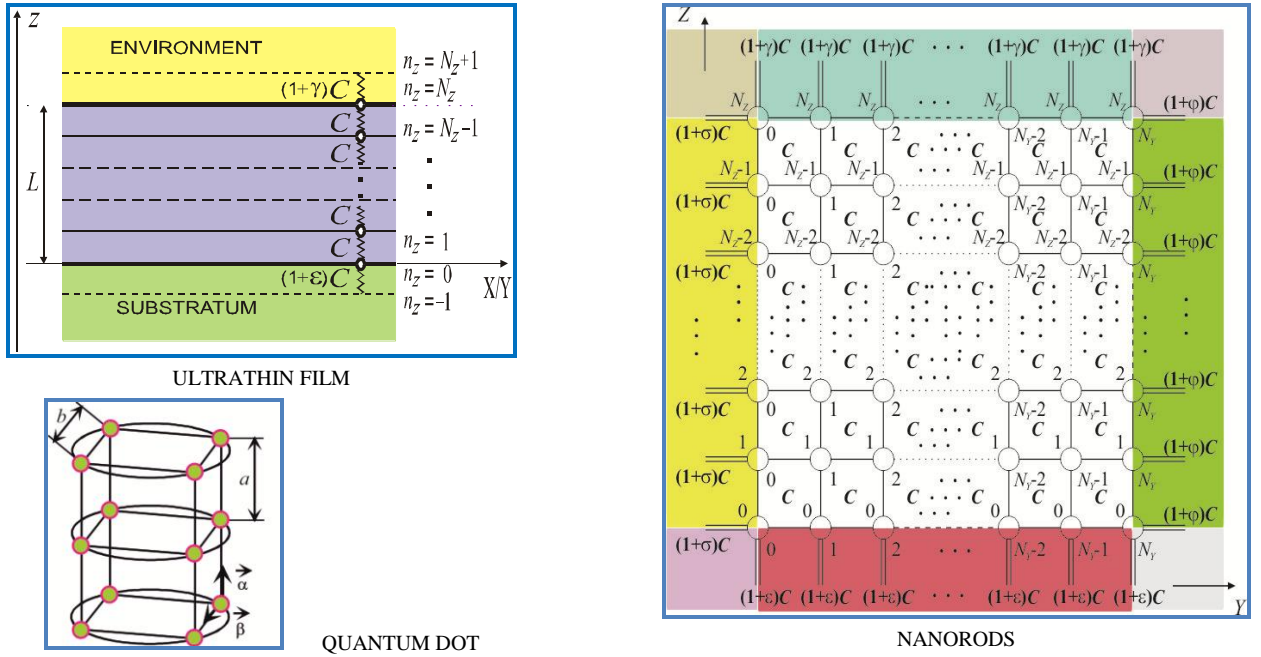


Fig. 1 Different models of crystalline quantum structures.

We have calculated dispersion law of the phonons using method of the Green's function [9,16]. Let us observe two-time temperature dependent retarded Green's function of displacement type:

$$G_{\bar{n},\bar{m}}^{\alpha\alpha}(t) \equiv \langle \langle u_{\bar{n}}^{\alpha}(t) | u_{\bar{m}}^{\alpha}(0) \rangle \rangle = Q(t) \langle [u_{\bar{n}}^{\alpha}(t), u_{\bar{m}}^{\alpha}(0)] \rangle_0, \quad (1)$$

where $u_{\bar{n}}^{\alpha}$ are displacement of atoms from the node $\bar{n} \equiv (n_x, n_y, n_z)$ in the direction $\alpha \in \{x, y, z\}$. Finding the second derivation we obtain equation of motion for the Green's function:

$$M_{\bar{n}} \frac{d^2}{dt^2} G_{\bar{n},\bar{m}}^{\alpha\alpha}(t) = -i\hbar \delta_{\bar{n}\bar{m}} \delta(t) + \frac{Q(t)}{i\hbar} \langle [[P_{\bar{n}}^{\alpha}, H(t)], u_{\bar{m}}^{\alpha}(0)] \rangle_0. \quad (2)$$

The Hamiltonian of the phonon subsystem in harmonic approximation and the approximation of the closest neighbor (with neglecting of the torsion constant $C^{\alpha\beta}$ (see in u [12–15]) is:

$$H = \frac{1}{4} \sum_{n_x, n_y, n_z; \alpha} [2M_{n_x, n_y, n_z} \dot{u}_{n_x, n_y, n_z; \alpha}^2 + C_{n_x, n_y, n_z; n_x \pm 1, n_y, n_z}^{\alpha\alpha} (u_{n_x, n_y, n_z}^{\alpha} - u_{n_x \pm 1, n_y, n_z}^{\alpha})^2 + C_{n_x, n_y, n_z; n_x, n_y \pm 1, n_z}^{\alpha\alpha} (u_{n_x, n_y, n_z}^{\alpha} - u_{n_x, n_y \pm 1, n_z}^{\alpha})^2 + C_{n_x, n_y, n_z; n_x, n_y, n_z \pm 1}^{\alpha\alpha} (u_{n_x, n_y, n_z}^{\alpha} - u_{n_x, n_y, n_z \pm 1}^{\alpha})^2]. \quad (3)$$

Using time Fourier transformation and when simplify ($M_{\bar{n}} \equiv M$ and $C_{\bar{n}, \bar{n} \pm \vec{\lambda}_{\alpha}/2}^{\alpha\alpha} \equiv C_{x/y/z}^{\alpha\alpha}$), and calculating of commutators $[P_{\bar{n}}^{\alpha}, H]$, equation of motion (2) turn into (see in [12–15]):

$$M \omega^2 G_{n_x, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha}(\omega) = \frac{i\hbar}{2\pi} \delta_{n_x, m_x} \delta_{n_y, m_y} \delta_{n_z, m_z} + \left[C_x^{\alpha\alpha} (G_{n_x, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha} - G_{n_x \pm 1, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha}) + C_y^{\alpha\alpha} (G_{n_x, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha} - G_{n_x, n_y \pm 1, n_z; m_x, m_y, m_z}^{\alpha\alpha}) + C_z^{\alpha\alpha} (G_{n_x, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha} - G_{n_x, n_y, n_z \pm 1; m_x, m_y, m_z}^{\alpha\alpha}) \right]. \quad (4)$$

This equation has general character and it has the same form for all structures (as for the bulk too). To adjust equation to nanostructures it has to be modified to the spatial limitations of the observed systems:

$$u_{n_x, n_y, n_z}^{\alpha\alpha} = 0, \quad G_{n_x, n_y, n_z; m_x, m_y, m_z}^{\alpha\alpha}(\omega) = 0 \quad (5)$$

- a) films: for $n_z < 0$ and $n_z > N_z$
- b) wires: for $n_y < 0$ and $n_y > N_y$; $n_z < 0$ and $n_z > N_z$
- c) dots: for $n_x < 0$ and $n_x > N_x$; $n_y < 0$ and $n_y > N_y$; $n_z < 0$ and $n_z > N_z$.

Because of spatial modifications, equation (4) turns into the system of $N_z + 1$, $(N_y + 1) \times (N_z + 1)$, or $(N_x + 1) \times (N_y + 1) \times (N_z + 1)$

equations, respectively. Using partially spatial Fourier transformation (due to the brake of translational invariance along (z) , (y, z) and (x, y, z) axes, see in [12–15]), we obtain system of $N_z + 1$, $(N_y + 1) \times (N_z + 1)$, or $(N_x + 1) \times (N_y + 1) \times (N_z + 1)$ nonhomogeneous algebraic difference equations. The obtained Green's function from the system we present as $G_{l f/w/d} \equiv D_{l f/w/d}(\omega) / D_{f/w/d}$, where $D_{f/w/d}$ are determinants of the system from this equations, and $D_{l f/w/d}(\omega)$ – corresponding substitute determinants. As poles of the Green's function define allowed energies of the phonons [16], this problem comes down to the finding the roots of the characteristic polynomials of these determinants.

3. Phonon spectra

Numerical and analytical results for phonon spectra in ideal ultra-thin films (UTF), nano-rods (NR) and quantum dots (QD) are already obtained in previous works [12–15]:

$$E_{k_x, k_y, v_z / f} \equiv \frac{\hbar \omega_{k_x, k_y, v_z / f}}{\hbar \Omega_b} = 2 \left[\sin^2 \frac{a k_x}{2} + \sin^2 \frac{a k_y}{2} + \sin^2 \frac{\pi v_z}{2(N_z + 2)} \right]^{1/2}, \quad (6)$$

$$E_{k_x, v_y, v_z / w} = 2 \left[\sin^2 \frac{a k_x}{2} + \sin^2 \frac{\pi v_y}{2(N_y + 2)} + \sin^2 \frac{\pi v_z}{2(N_z + 2)} \right]^{1/2}, \quad (7)$$

$$E_{v_x, v_y, v_z / d} = 2 \left[\sin^2 \frac{\pi v_x}{2(N_x + 2)} + \sin^2 \frac{\pi v_y}{2(N_y + 2)} + \sin^2 \frac{\pi v_z}{2(N_z + 2)} \right]^{1/2}. \quad (8)$$

Quantum numbers v_{α} , ($\alpha = x, y, z$) in expressions (6-8) take values: $v_{\alpha} \in [1, N_{\alpha} + 1]$. One can see that solutions have form of Pythagoras theorem and that discretization of the spectra along one direction is independent from discretization along other two directions.

Dispersion law (6-8) in thin films, quantum wires and quantum dots formally has the same form as for corresponding spatially unlimited crystalline structures. Significant difference is in appearing of discrete phonon energies along the direction of spatial confinement. We have numerically analyzed and calculated dispersion law for the 4-layered UTF ($N_z = 4$) and quadratic surface NR with 5 crystalline planes ($N_y = N_z = 4$), with the results showed on Fig. 2 (for the ideal infinity structures – with the dashed lines, between is continual and for the nanostructures – with the full lines, which is discrete one). Thereby, introduced are following labels: $X \equiv \sin(a k_x/2)$ and $Y \equiv \sin(a k_y/2)$. On the graphs are clearly visible gaps (E_{\min} and E_{\max}), as well as $N_z - 1$ (for UTF) and $(N_z - 1) \times (N_y - 1)$ – for NR, allowed discrete values between the gaps.

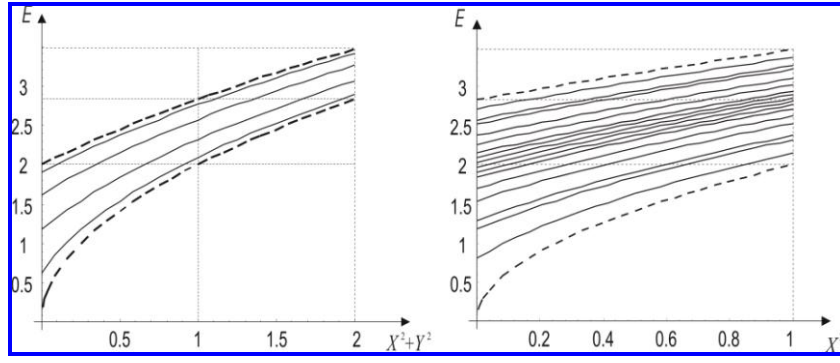


Fig. 2 Phonon spectra in ultrathin films (left) and in quantum wires (right)

Shown cases doesn't include out of bulk localizes states of the phonons. These especially interesting states are processed in [17]. The most imported result of this analysis is existence of the energy gaps in finite structures. Because of the fact that their appearance is caused by the broken translational symmetry (along boundary axes), the gaps are more expressed in quantum dots then in quantum wires, and in thin films, while in unlimited crystals they practically don't exist. From the (6-8) we have calculated expression for the energy gaps in the form as:

$$\Delta_{f/w/d} \approx \pi \left[\sum_{\beta \in \{x,y,z\}} \left(\frac{v_{\min}^{\beta}}{N_{\beta} + 2} \right)^2 \right]^{1/2}, \quad (9)$$

where are: $v_{\min}^x = v_{\min}^y = 0; v_{\min}^z = 1$ (for UTF), $v_{\min}^x = 0; v_{\min}^y = v_{\min}^z = 1$ (for NR) and $v_{\min}^x = v_{\min}^y = v_{\min}^z = 1$ (for QD). On can see from (9) that the magnitude of the gaps rashly decreases (approximately hyperbolically), with the increasing of the dimension of the system, i.e. with the increase of N_{α} .

Existence of the gaps in the phonon spectra couldn't be explained with the absence of the acoustic and appearance of the optic phonons, then as the appearance of the acoustic phonons – of the optic type [13], whose support calculated statistical limit:

$\lim_{N_{x/y/z} \rightarrow \infty} \Delta_{f/w/d} = 0$. Existence of the phonon gaps could be interpreted with appearance of activation temperature $T_{ac}^{f/w/d} = \hbar \Delta_{f/w/d} / k_B$. The phonon subsystem in these nanostructures appears only if temperature of these structures is higher than T_{ac} . Below these temperatures system behavior is like "frozen" and represents ideal electrical conductor. Accordingly with the results of this analysis (9), the best properties have quantum dots.

4. Phonon states

For the case of the observed film, using the same reason as with thermodynamically analysis of spatially unlimited systems [7–9], we use next approach (for the number of allowed values \vec{k} for volume unity of \vec{k} -space) and overall number of states in the frequency region between ω and $\omega + d\omega$:

$$\left(\frac{L}{2\pi} \right)^3 \Rightarrow \frac{N_x N_y (N_z + 1)}{k_x^m k_y^m k_z^m} \Rightarrow N = \frac{N_x N_y (N_z + 1) a^2 k^2}{4\pi^2},$$

and density of states is:

$$D_f(\omega) = \left(\frac{dN}{d\omega} \right)^{-1} \frac{N_x N_y (N_z + 1) a^2 k^2}{2\pi} = \frac{a^2 N_x N_y (N_z + 1)}{v^2} \frac{1}{2\pi} \omega. \quad (10)$$

Generally, from the norming conditions, now adjusted to the model,

$$N_f \equiv N_x N_y (N_z + 1) = \int_0^{\omega_b^f} D_f(\omega) d\omega = \frac{a^2 N_x N_y (N_z + 1)}{v^2} \frac{1}{2\pi} (\omega_b^f)^2,$$

we can obtain relation for the Debye frequency in the film structures $\omega_b^b / \omega_b^f = \sqrt[3]{3\pi/4}$ and when compared with the same in

ideal and unlimited structure, show that $\omega_b^f < \omega_b^b$, i.e. Debye frequency has somewhat lower value in film (about 10 %) in respect to the ideal bulk crystal. With the same procedure for NR and QD [18], follows: $\omega_b^d < \omega_b^w < \omega_b^f < \omega_b^b$, and obtained is known as "softening of the nano-phonons". With finding the ratio of the phonon states in bulk structures [7–9]) and UTF, but exactly on Debye frequencies, follows:

$$\frac{D_b(\omega_b^b)}{D_f(\omega_b^f)} = \frac{6}{\sqrt[3]{6\pi}} \frac{N_z}{N_z + 1}, \quad (11)$$

therefore, we obtain that population of phonons in film is smaller, i.e. $D_f(\omega_b^f) < D_b(\omega_b^b)$. With the same procedure applied on NR and QD (as in [18]), finally follows:

$$D_d(\omega_b^d) < D_w(\omega_b^w) < D_f(\omega_b^f) < D_b(\omega_b^b).$$

5. Phonon thermodynamics

Regarding the fact that the properties of anisotropic structures are conditioned with the change of dispersion law, it is needed to observe behavior of some thermodynamic values in order to get complete picture of this properties. Accordingly, we will analyze heat capacity of the observed models of nanostructures, but before we need to calculate internal energy of this system, starting from standard form [7–9]:

$$U = 3 \sum_{k_x, k_y, k_z} E(\vec{k}) \left[e^{E(\vec{k})/\theta} - 1 \right]^{-1}; \quad \theta = k_B T.$$

Taking into account that when $k \rightarrow 0$ (in long wave approximation) energies of all three phonon branches stay different from zero, we could use dispersion relation (6) is somewhat simplified form:

$$E_{f/w/d}(\vec{k}) = \sqrt{a^2 k_{f/w/d}^2 E_0^2 + \Delta^2}; \quad k_f^2 = k_x^2 + k_y^2; \quad k_w^2 = k_x^2; \quad k_d^2 = 0,$$

$\Delta \equiv \Delta_{f/w/d} = a k_{f/w/d}^{\min} E_0$; $E_0 = \hbar \Omega$ and $\varepsilon \equiv \sqrt{1 + (E_D / \Delta)^2}$. We will execute this calculation with transition from summation to integration (more detailed in [12–15]), and after doing this, we obtain:

$$U_{f/w/d} = \frac{3N_{f/w/d}}{2\pi} \left(\frac{\Delta}{E_0} \right)^2 \theta \left\{ \left[Z_1 \left(\frac{\Delta}{\theta} \right) - \varepsilon^2 Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 2 \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 2 \left(\frac{\theta}{\Delta} \right)^2 \left[Z_3 \left(\frac{\Delta}{\theta} \right) - Z_3 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\}, \quad (12)$$

where $Z_r(X) = \sum_{j=1}^{\infty} j^{-r} e^{-jX}$ – represents Dyson function. To obtain

expression for the heat capacity per elementary cell (here, per atom), we start from standard form [7–9]:

$$C = \frac{1}{N} \frac{\partial U}{\partial T} = \frac{k_B}{N} \frac{\partial U}{\partial \theta}.$$

and after that we obtain:

$$C_{f/w/d} = \frac{3k_B}{2\pi} \left(\frac{\Delta}{E_0} \right)^2 \left\{ \frac{\Delta}{\theta} \left[(e^{\Delta/\theta} - 1)^{-1} - \varepsilon^3 (e^{\varepsilon\Delta/\theta} - 1)^{-1} \right] + 3 \left[Z_1 \left(\frac{\Delta}{\theta} \right) - \varepsilon^2 Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 6 \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 6 \left(\frac{\theta}{\Delta} \right)^2 \left[Z_3 \left(\frac{\Delta}{\theta} \right) - Z_3 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\}. \quad (13)$$

With analysis of this expression, we could observe that it contain two essential terms. The first one has inverse exponential dependence from the reciprocal temperature: $(e^{\Delta/\theta} - 1)^{-1}$, that is $(e^{\varepsilon\Delta/\theta} - 1)^{-1}$, and that term is responsible for the heat capacity behavior on extreme temperatures (very low and very high temperatures). The second term, expressed over Dyson function Z_r (Δ/θ) and $Z_r(\varepsilon\Delta/\theta)$, show the heat capacity behavior in the region of medium temperatures (significant lower from the faze transition temperature). This term represent linear dependence of the heat capacity from temperature.

Along with the internal energy and heat capacity, it could be observed temperature behavior of the free energy and entropy. Based on the definition of free energy [7-9]:

$$F = \theta \sum_{\alpha, \vec{k}} \ln \left[1 - e^{-E_\alpha(\vec{k})/\theta} \right],$$

and with the same procedure as just has been explained, for the case of observed nanostructures upper expression comes down to:

$$F_{f/w/d} = -\frac{3N_{f/w/d}}{4\pi} \left(\frac{\Delta}{E_0} \right)^2 \theta \left[\ln(1 - e^{-\Delta/\theta}) - \varepsilon^2 \ln(1 - e^{-\varepsilon\Delta/\theta}) \right] - \frac{1}{2} U_{f/w/d}. \quad (16)$$

Using standard defined form [7-9]:

$$S = -\frac{1}{N} \frac{\partial F}{\partial T} = -\frac{k_B}{N} \frac{\partial F}{\partial \theta},$$

for the phonon contribution to the entropy of the crystalline film, we obtain next expression:

$$S_{f/w/d} = \frac{3k_B}{2\pi} \left(\frac{\Delta}{E_0} \right)^2 \left\{ \left[\ln(1 - e^{-\Delta/\theta}) - \varepsilon^2 \ln(1 - e^{-\varepsilon\Delta/\theta}) \right] + 3 \left[Z_1 \left(\frac{\Delta}{\theta} \right) - \varepsilon^2 Z_1 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 6 \frac{\theta}{\Delta} \left[Z_2 \left(\frac{\Delta}{\theta} \right) - \varepsilon Z_2 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] + 6 \left(\frac{\theta}{\Delta} \right)^2 \left[Z_3 \left(\frac{\Delta}{\theta} \right) - Z_3 \left(\varepsilon \frac{\Delta}{\theta} \right) \right] \right\}. \quad (17)$$

In entropy expression we could notice that, similar to specific heat, exist two fundamental terms. The first one has logarithm dependence from reciprocal temperature and it determines entropy behavior on low and high temperatures. The second term is defined with Dyson functions and determines entropy behavior on medium temperatures.

Graphic representation of the low-temperature dependence of the heat capacity and entropy is shown on Fig.3, where we introduce next labels: i, f for indices ideal (bulk) and finite modeled nanostructures, respectively, as well as $x = \theta / \Delta \equiv k_B T / \Delta$. It is clearly visible that specific heat of nanostructures below values for the bulk, but with entropy is opposite situation.

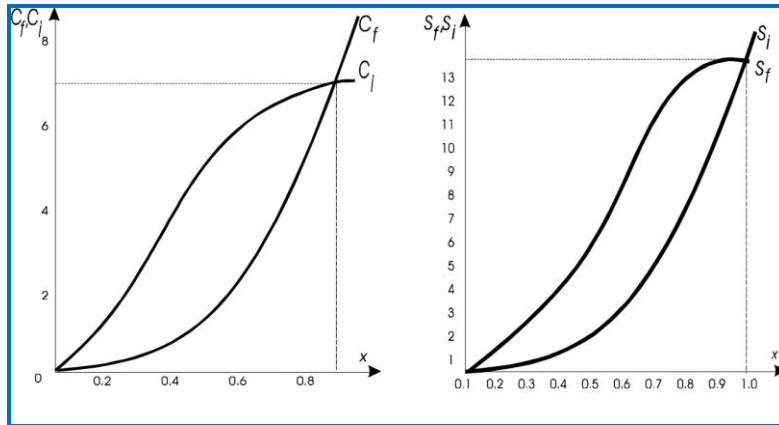


Fig. 3 Temperature behavior of phonon participation in heat capacities (left) and entropies (right) bulk and nanostructures

6. Conclusion

On relatively low temperatures the heat capacity and entropy of massive samples is changing with temperature as T^3 , while in nanostructures that dependence is: $T^{-1} \exp(\text{const}/T)$. Until some temperature T^* , the heat capacity in nanostructures has lower values in than in massive samples. Until that temperature T^* , it has to load more energy (per volume) to heat up nanostructure, which is in agreement with the fact that energy of phonon excitation is bigger in nanostructures than in massive (bulk) samples.

Until temperature T^* , entropy in nanostructures has higher values than in bulk structures, which implies that nanostructures are more unordered structures than bulk, up to T^* , and closer to equilibrium. This corresponds to the fact that in nanostructures is better achieved phonon collectivization and that they have longer-range influence onto physical properties of materials. Regarding that dominant part in these differences between bulk and nanostructures is existence and magnitude of gaps, it is not hard to conclude that these differences will be most evident with QD (~ 3 times bigger than corresponding UTF), than with NR (~ 2 times bigger).

As we know that, on Debye frequencies, phonons are responsible for electric and heat transport properties of materials, follows that nanostructures will be weaker electric ($\sigma_{f/w/d} < \sigma_b$) and heat ($C_{f/w/d} < C_b$) conductor in comparison to corresponding bulk structures, so far as between them there are no chemical or crystallographic differences. That mean that phonon excitation in nanostructures occur more difficult. Certainly, this effect is most evident in QD, than in NR and only then in UTF.

All these results are in agreement with the fact that superconducting samples (in form of quantum nanostructures) has better superconductive properties and higher critical temperatures than corresponding massive samples [19]. It is very interest to mention that high-temperature superconductors are distinctly fine grained structures [20] and that quantum dots could connect with the Josephson tunnel junctions.

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