Physica Macedonica **61**, (2012) p. 21-26
ISSN 1409-7168

PARTICIPATION OF MECHANICAL OSCILLATIONS IN THERMODYNAMICS OF CRYSTALS WITH SUPERLATTICE

S. K. Jaćimovski[1], D. Lj. Mirjanić[2,*] and J. P. Šetrajčić[3,*]

[1] *Academy of Criminology and Police, Cara Dušana 196, 11080 Zemun, Serbia*

[2] *University of Banja Luka, Faculty of Medicine, Save Mrkalja 11, 78000 Banja Luka, Republic of Srpska – B&H*

[3] *University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000 Novi Sad, Vojvodina – Serbia*

**Academy of Sciences and Arts of the Republic of Srpska, Bana Lazarevića 1, 78000 Banja Luka, Republic of Srpska – B&H*

Abstract. The superlattice, consisting of two periodically repeating films, is analyzed in proposal paper. Due to the structural deformations and small thickness, the acoustic phonons do not appear in these structures. The spontaneous appearance of phonons is possible in an ideal structure only. Therefore the thermodynamical analysis of phonon subsystems is the first step in investigations of superlattice properties. Internal energy as well as specific heat will be analyzed, too. Low-temperature behavior of these quantities will be compared to the corresponding quantities of bulk structures and of thin films. The general conclusion is that the main thermodynamic characteristics of superlattices are considerably lower than those of the bulk structure. Consequently, their superconductive characteristics are better than the superconductive characteristics of corresponding bulk structures. Generally considered, the application field of superlattices is wider than that of bulk structures and films.

PACS: 63.22.Np, 65.40.Ba, 65.80.-g, 68.65.Cd

1. INTRODUCTION

Possible applications of superlattices require knowledge of their thermodynamic characteristics [1]. Regardless of the type of superlattice, the thermodynamics of their subsystems (electrons, excitons, spin waves, etc) are determined when the subsystem is in thermodynamical equilibrium with the phonons [2–5]. Therefore the thermodynamical analysis of phonon subsystems is the first step in investigations of superlattice properties. Internal energy as well as specific heat will be analyzed, too. Low-temperature behavior of these quantities will be compared to the corresponding quantities of bulk structures and of thin films [6–9]. This should describe the approach which we would use for the book that deals with thermodynamics.

2. THE MODEL

It will be assumed that the symmetry is disturbed along the ***z***-direction. Translation symmetry of the cubic structure is conserved in ***XY*** planes. In the Fig.1 the scheme of a superlattice in the ***z***-direction, only, is given.

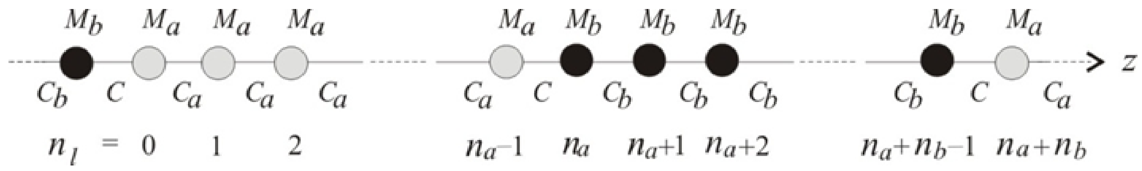

Fig. 1: The model of superlattice.

The Hamiltonian of the phonon subsystem [9] of a superlattice can be written as follows:

$$H=\frac{1}{2}\sum_{n,\alpha}\sum_{n_l=0}^{n_a+n_b-1}\left\{\sum_{n_l=0}^{n_a+n_b-1}\frac{\left[p^{(a/b)}_{n,n_l,\alpha}\right]^2}{M_{a/b}}+\frac{C_{\_/a/b}}{2}\left(u_n^{\alpha}-u_{n+\lambda}^{\alpha}\right)^2\right\};\quad \lambda=\pm 1; \tag{1}$$

All of these formulas are given in the nearest neighbor approximation. Taking into account that a superlattice is a periodic crystal structure, the following cyclic conditions for any configuration function are valid:

$$\begin{aligned} f_{m_x m_y m_z m_l+N_{x/y}} &= f_{m_x m_y m_z m_l}; \qquad \mathrm{e}^{iN_{x/y}k_{x/y}a_{x/y}}=\mathrm{e}^{i2\pi\nu_{x/y}};\\ f_{m_x m_y m_z m_l+(n_a+n_b)N_z} &= f_{m_x m_y m_z m_l}; \quad \mathrm{e}^{i(n_a+n_b)N_z k_z\tilde{a}}=\mathrm{e}^{i2\pi\nu_z}. \end{aligned} \tag{2}$$

Allowed values for the ***z***-component of the wave vector k_z are defined by integer $\nu_z\in\{0,\pm1,\pm2,\dots\ \dots\pm N_z/2\}$. In this way the boundaries of the first Brillouin's zone in ***z***-direction are defined as follows:

$$k_z\in\left[\frac{-\pi}{(n_a+n_b)\tilde{a}},\frac{\pi}{(n_a+n_b)\tilde{a}}\right],\quad \tilde{a}=\frac{(n_a-1)a^a+(n_b-1)a^b+2a}{n_a+n_b}, \tag{3}$$

We now introduce the symbolic notation: $\vec{n}\equiv\{n_x,n_y,n_z\},n_{x/y/z}\in\left[-N_{x/y/z}/2,N_{x/y/z}/2\right]$, where: $n_{x/y}$ is a counter of lattice nodes in ***x*** and ***y*** direction, n_z is a counter of positions along the basic motive of superlattice (***z*** direction), n_l is a counter of node positions within the basic motive.

3. DISPERSION LAW

The phonon dispersion law will be found using the Green's function [10]:

$$G_{\vec{n},n_l,\vec{m},m_l}(t-t')\equiv\left\langle\left\langle u_{\vec{n},n_l}(t)\middle|u_{\vec{m},m_l}(t')\right\rangle\right\rangle=\theta(t-t')\left\langle[u_{\vec{n},n_l}\,t),u_{\vec{m},m_l}(t')]\right\rangle \tag{4}$$

with the equation of the motion of the form:

$$-M_i\omega^2 G_{\vec{n},n_l;\vec{m},m_l}(\omega) = -\frac{i\hbar}{2\pi}\delta_{\vec{n},\vec{m}}\delta_{n_l,m_l} + \frac{1}{i\hbar}\left\langle\left\langle [p_{\vec{n},n_l}, H] \middle| u_{\vec{m},m_l} \right\rangle\right\rangle_\omega \tag{5}$$

where $M_i \in (M_a, M_b)$. After the calculation of the commutators from (5) and application of partial configurational Fourier's transformation (this transformation is applied to coordinates ***x***, ***y*** and ***z*** but not to coordinate ***l***, where the translation symmetry is disturbed):

$$G_{\vec{n},n_l;\vec{m},m_l}(\omega) = \frac{1}{N}\sum_{\vec{k}} G_{n_l,m_l}\,\mathrm{e}^{i[a_x k_x(n_x-m_x)+a_y k_y(n_y-m_y)+\tilde{a}_z(n_a+n_b)k_z(n_z-m_z)+J]} \tag{6}$$

where

$$J = \begin{cases} 1.\;\; a^a k_z(n_l - m_l), \quad n_l - m_l < n_a \\ 2.\;\; a^a k_z(n_a - 1) + ak_z, \quad n_l - m_l = n_a \\ 3.\;\; a^a k_z(n_a - 1) + ak_z + a^a k_z(n_l - m_l - n_a), \quad n_a < n_l - m_l < n_a + n_b \\ 4.\;\; a^a k_z(n_l - 1) + a^b k_z(n_b - 1) + 2ak_z, \quad n_l - m_l = n_a + n_b \end{cases},$$

we obtain the system of $n_a + n_b$ non-homogeneous algebraic-differential equations for Green's functions. This model can be reduced to the model of a simple cubic lattice (and in this way simplified) with the help of substitutions:

$$a^a = a^b = \tilde{a} = a = a_z;\;\; \Omega^2_{a_x} = \Omega^2_{a_y} = \Omega^2_{a_z} = \alpha\Omega^2_a;$$
$$a_x^{a/b} = a_y^{a/b} = a = a_z;\;\; \Omega^2_{b_x} = \Omega^2_{b_y} = \Omega^2_{b_z} = \beta\Omega^2_b$$

$$\rho_a = \frac{\omega^2}{\Omega_a^2} - 4\alpha(\sin^2\frac{ak_x}{2} + \sin^2\frac{ak_y}{2}) - 2\alpha;\quad \rho_b = \frac{\omega^2}{\Omega_b^2} - 4\beta(\sin^2\frac{ak_x}{2} + \sin^2\frac{ak_y}{2}) - 2\beta\,. \tag{7}$$

In "cut-off" case ($\alpha = \beta = 1,\;\; \rho_a = \rho_b = \rho$), the system of equations of phonon Green's functions in superlattices in individual layer is:

$$\rho G_s + e^{ix}G_{s+1} + e^{-ix}G_{s-1} = R_s \tag{8}$$

were are $x \equiv ak_z$. We seek for the solution equations in the form $G_s = Pe^{isx}$. Since $G_{s\pm1} = G_s\mathrm{e}^{\pm ix}$, for Green's function we obtain the following expression:

$$G_s = \frac{R_s}{\rho + \cos 2x}\,. \tag{9}$$

The poles of Green's function determine value ρ, where from (9) following dispersion law of phonon was obtained:

$$\omega_{\vec{k}} = 2\Omega\sqrt{\sin^2\frac{ak_x}{2} + \sin^2\frac{ak_x}{2} + \sin^2\frac{ak_s}{2}};k_s = 2k_z\,. \tag{10}$$

In small wave-vector approximation: $\omega_{\vec{k}} = \Omega a k;\quad k = \sqrt{k_x^2 + k_y^2 + k_z^2}$, the maximal wave-vector value is determined as:

$$ak_M = a\sqrt{\frac{2}{3}k_D^2 + k_{\max}^{\ 2}} = \sqrt{\frac{2}{3}\sqrt[3]{6\pi^2} + \left(\frac{2\pi}{n_a + n_b}\right)^2} \ .$$

4. THERMODYNAMICAL BEHAVIOUR

Internal energy of the system is [10]:

$$U_s = \frac{3}{(2\pi)^3} N a^3 \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \int_0^{k_{\max}} dk k^2 \frac{\hbar\Omega k a}{\mathrm{e}^{\frac{\hbar\Omega a k}{\theta}} - 1} \tag{11}$$

where phonon dispersion law is given by $\hbar\Omega ak$. Introducing substitution: $\hbar\Omega ak_{\max} / \theta$ after partial integration we obtain the following expression for internal energy

$$\begin{aligned} U_s = \frac{3N}{2\pi^2}\theta\{6\varsigma(4)\frac{\theta^3}{(\hbar\Omega)^3} - [a^3 k_M^3 Z_1(\frac{\Delta_m}{\theta}) + 3\frac{\theta}{\hbar\Omega} a^2 k_M^2 Z_2(\frac{\Delta_m}{\theta}) + \\ + 6(\frac{\theta}{\hbar\Omega})^2 a k_M Z_3(\frac{\Delta_m}{\theta}) + 6(\frac{\theta}{\hbar\Omega})^3 Z_4(\frac{\Delta_m}{\theta})]\} \end{aligned} \tag{12}$$

Since the specific heat is given by [9]:

$$C_{vs} \equiv C_s = \frac{k_B}{N}\frac{\partial U}{\partial \theta} , \tag{13}$$

using (12) we find that:

$$\begin{aligned} C_s = \frac{3k_B}{2\pi^2}\{a^3 k_M^3 \frac{\Delta_m}{\theta}\frac{1}{1 - \mathrm{e}^{\Delta_m/\theta}} - 4a^3 k_M^3 Z_1(\frac{\Delta_m}{\theta}) - 12\frac{\theta}{\hbar\Omega} a^2 k_M^2 Z_2(\frac{\Delta_m}{\theta}) - (3.2) \\ -24(\frac{\theta}{\hbar\Omega})^2 a k_M Z_3(\frac{\Delta_m}{\theta}) + 24(\frac{\theta}{\hbar\Omega})^3[\varsigma(4) - Z_4(\frac{\Delta_m}{\theta})]\}. \end{aligned} \tag{14}$$

Temperature dependence of the thermal capacity is determined by two specific terms. First term is: $\approx (1 - \mathrm{e}^{\Delta_m/\theta})^{-1} / \theta$ which is "responsible" for behavior of the system at extremely low and extremely high temperatures. Second term containing zeta functions characterizes temperature behavior in middle temperature range. Graphical presentation of the temperature dependence of relative thermal capacity $C_{bfs} \equiv C_{bfs}(x)/C_0$; $C_0 = k_B/2(\Delta/E_0)^3$; $x \equiv \theta / \theta_D$ is given on Fig.2.

5. CONCLUSIONS

The superlattice, consisting of two periodically repeating films, is analyzed in proposal paper. Due to the structural deformations and small thickness, the acoustic phonons do not appear in these structures. The spontaneous appearance of phonons is possible in an ideal structure only. The general conclusion is that the main thermodynamic characteristics of superlattices are considerably lower than those of the bulk structure. Consequently, their superconductive characteristics are better than the superconductive characteristics of corresponding bulk structures. Generally considered, the application field of superlattices is wider than that of bulk structures and films.

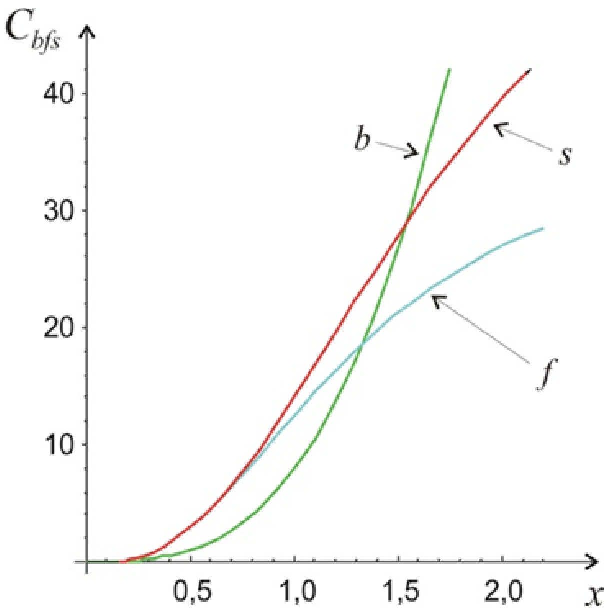

Fig. 2: Specific heats of bulk (b), films (f) and superlattice (s).

From the Fig.2 it can be concluded the behavior of thermal capacity of superlattice is similar to that of film (it is higher then in bulk structure) while difference is more expressive in middle temperature range. So, it can be concluded that the superlattices in low temperature range are somewhat better heat conductors than the bulk structures. In the same time the heat conduction of films is higher than that of superlattices. On the other hand in high temperature range superlattices are better heat isolators than film structures and the corresponding infinite crystal structures.

Acknowledgment

This work was partially supported by the Ministry of Education and Science of the Republic of Serbia (Grand No: 171039) and the Provincial Secretariat for Science and Technological Development (Grand No: 114-451-2048).

REFERENCES

[1] M.G.Cottam, D.R.Tilley: Introduction to Surface and Superlattice Excitations, Univ. Press, Cambridge (1989).
[2] C.Kittel: Quantum Theory of Solids, Wiley \& Sons, New York (1963).
[3] B.S.Tošić and D.Popov, J.Phys.Chem.Sol. **61**, 1561 (2000).
[4] B.S.Tošić, J.P.Šetrajčić, D.Lj.Mirjanić and Z.V.Bundalo, Physica A **184**, 354 (1992).

[5] J.P.Šetrajčić, V.M.Zorić, N.V.Delić, D.Lj.Mirjanić and S.K.Jaćimovski: Phonon Participation in Thermodynamics and Superconductive Properties of Thin Ceramic Films, Chapter 15, pp. 317-348, In „Thermodynamics”, Ed.M.Tadashi, ISBN: 978-953-307-544-0, InTech, Vienna (2011).

[6] S.K.Jaćimovski, J.P.Šetrajčić, B.S.Tošić and V.D.Sajfert, Materials Science Forum **453-454**, 33-36 (2004).

[7] S.G.Davison and M.Steslicka: Basic Theory of Surface States, Clarendon, Oxford (1996).

[8] S.Lazarev, M.R.Pantić, S.M.Stojković, B.S.Tošić and J.P.Šetrajčić, J.Phys.Chem.Sol. **61**, 931 (2000).

[9] J.P.Šetrajčić, V.M.Zorić, N.V.Delić, D.Lj.Mirjanić and S.K.Jaćimovski, Phonon Participation in Thermodynamics and Superconductive Properties of Thin Ceramic Films, Chapter 15, pp. 317-348, In „Thermodynamics”, Ed.M.Tadashi, ISBN: 978-953-307-544-0, InTech, Vienna (2011); Available from: http://www.intechopen.com/articles/show/title/phonon-participation-in-thermodynamics-and-superconductive-properties-of-thin-ceramic-films

[10] G.Mahan: Many Particle Physics, Plenum Press, New York (1990).