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THE FREQUENCIES OF LOCALIZED ACOUSTIC MODES IN Au/V NANOLAYERS WITH CAPPING LAYER

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Paper presents the results of theoretical analysis of localized acoustic modes, which can be generated in Au/V nanolayers with "heavy" capping layer. The transfer-matrix method was used to evaluate frequencies of localized acoustic modes in these nanostructures. Up to now the condition of generation of localized modes in nanolayer structure was that the acoustic impedance of capping layer is lower then the acoustic impedance of top (next) layer. This condition was in agreement with experimental results. This paper demonstrates the possibility of generation of localized acoustic modes in case of higher acoustic impedance of capping layer. The frequencies of localized modes for different thickness of capping layer were obtained.

Key words: picosecond acoustics, metallic nanolayers, localized acoustics modes.

1. Introduction

The periodical nanolayer structures have interesting elastic vibrational properties [1–3]. The vibrational modes of periodic multilayer structure are theoretically described by dispersion curve. Dispersion curve for such periodical structure exhibits a folding of the phonon branches in mini Brillouin zones [4]. The dispersion relation for periodical two component layered structure of infinite extent first was obtained by M. RYTOV [5]. Dimension of mini Brillouin zones depends on thickness of the period of nanolayer structure. Due to the mismatch of acoustic impedances of both component layers frequency gaps appear at the center and at the edge of these zones. In the frequency gap zones longitudinal and transversal acoustic modes cannot propagate.

In the previous papers [6–8] picosecond ultrasonic technique was used to study acoustic properties of nanolayers. In the Au/V nanolayers acoustic oscillations of high frequency were observed [7]. These oscillations are connected to acoustic localized modes. The theory of localized modes in layered structures was considered by DJAFARI–ROUHANI [9]. We have applied Djafari–Rouhani theory and transfer-matrix method [10], known from optics, to receive frequency dependences of localized acoustic modes for layered structures [11]. Frequency dependencies for Au/V nanolayers for case of vanadium capping layer were calculated numerically.

Experimental study has showed, that acoustic localized modes appears only in case when capping layer has smaller acoustic impedance then next layer [7, 12]. In this paper case of capping layer with heavier (bigger acoustic impedance) is examined theoretically. It was proved that existence of localized acoustic modes is also possible in considered case. The frequency dependences of localized acoustic modes in first and second gaps on thickness of capping layer for Au/V nanolayers were presented.

2. Theory of acoustical localized modes in periodical nanolayer

The considered nanostructure consists of alternative layers of two materials terminated by capping layer with thickness d_c. The geometry of semi-infinite nanostructure is shown in Fig. 1.

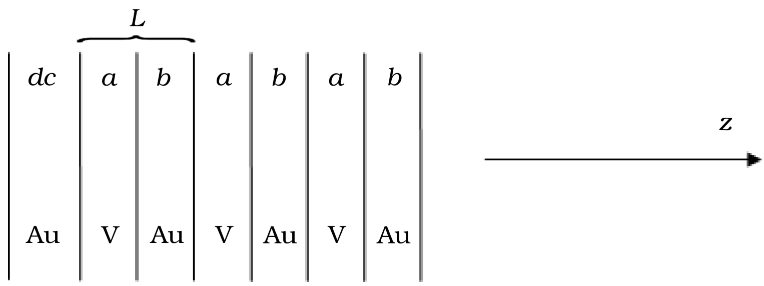

Fig. 1. Geometry of Au/V nanostructure.

We are looking for solution of elasticity equation:

$$\rho \frac{\partial^2 u(z,t)}{\partial t^2} = \frac{\partial \sigma(z,t)}{\partial z}\,, \tag{1}$$

where u – displacement, ρ – density, σ – stress.

We take solution of (1) in the form

$$u(z,t) = \left(A_{m,i} \sin[k_i(z - z_m)] + B_{m,i} \cos[k_i(z - z_m)]\right) e^{-i\omega t}, \tag{2}$$

where $A_{m,i}$, $B_{m,i}$ are constant amplitudes of the m-th bilayer, k_i – wave vector, $i = 1, 2$ denotes first or second layer, z_m – beginning of m-th bilayer. After applying continuity conditions dependences between constants $A_{m+1,i}$, $B_{m+1,i}$ and $A_{m,i}$, $B_{m,i}$ may be expressed by transfer matrix $\mathbf{T}$ as follows:

$$\begin{bmatrix} A_{m+1,1} \\ B_{m+1,1} \end{bmatrix} = \mathbf{T} \begin{bmatrix} A_{m,1} \\ B_{m,1} \end{bmatrix}. \tag{3}$$

Using Bloch's theorem we obtain:

$$\begin{bmatrix} A_{m+1,1} \\ B_{m+1,1} \end{bmatrix} = \lambda \begin{bmatrix} A_{m,1} \\ B_{m,1} \end{bmatrix}. \tag{4}$$

Taking trace of matrix $\mathbf{T}$ it is easy to obtain Rytov equation [5, 11]:

$$\cos(qL) = \cos\left(\frac{\omega a}{c_1}\right)\cos\left(\frac{\omega b}{c_2}\right) - \frac{1+p^2}{2p}\sin\left(\frac{\omega a}{c_1}\right)\sin\left(\frac{\omega b}{c_2}\right), \tag{5}$$

where q – wave vector for whole nanostructure, c_1 and c_2 – sound velocities for first and second layers of bilayers, L – bilayer thickness, a and b – thickness of first and second layers, p – ratio of acoustic impedances of bilayer components.

After applying boundary condition on capping layer (stress equals zero) solution of Eq. (4) is obtained [11]:

$$\tan\left(\frac{\omega b}{c_2}\right) + p\tan\left(\frac{\omega a}{c_1}\right)\left(\frac{\cos^2\left(\frac{\omega d_c}{c_2}\right) + p^{-2}\sin^2\left(\frac{\omega d_c}{c_2}\right) - \frac{1-p^2}{p^2}\tan\left(\frac{\omega b}{c_2}\right)}{\sin\left(\frac{\omega d_c}{c_2}\right)\cos\left(\frac{\omega d_c}{c_2}\right)}\right) = 0, \tag{6}$$

$$\begin{aligned}\lambda \;=\; & \cos\left(\frac{\omega a}{c_1}\right)\cos\left(\frac{\omega b}{c_2}\right) - p\sin\left(\frac{\omega a}{c_1}\right)\sin\left(\frac{\omega b}{c_2}\right) \\ & - p^{-1}\tan\left(\frac{\omega d_c}{c_2}\right)\left(\sin\left(\frac{\omega a}{c_1}\right)\cos\left(\frac{\omega b}{c_2}\right) + p\cos\left(\frac{\omega a}{c_1}\right)\sin\left(\frac{\omega b}{c_2}\right)\right).\end{aligned} \tag{7}$$

Solution for localized mode of Eq. (6) exists only for $|\lambda| < 1$.

3. Results of calculation and discussion

The dispersion dependence for Au/V nanostructure with thickness of both vanadium and gold layers equal to 100 Å obtained from Eq. (5) is presented in Fig. 2.

The values of the densities and sound velocities were used $\rho = 19320$ kg/m^3, $c = 3154.9$ m/s and $\rho = 6110$ kg/m^3, $c = 6108.7$ m/s for Au and V, respectively [13, 14]. The frequency f is calculated in THz $(f = \omega/2\pi)$.

The parameters of calculated frequency for first and second gaps are shown in Table 1.

Table 1. Values of lower, upper edges and width of first and second gaps for Au/V nanolayers.

gap	f_- [GHz]	f_+ [GHz]	Δ [GHz]
1	89	117	28
2	195	223	28

The area of existence of solution for localized modes can be obtained from Eq. (7). This region in the plane frequency versus thickness of capping layer (Au) for nanolayers Au/V (100 Å/100 Å) is presented in Fig. 3.

While basing on Eq. (6) frequency dependences of acoustic localized modes on thickness of capping layer in first and second frequency gaps are shown in Fig. 4.

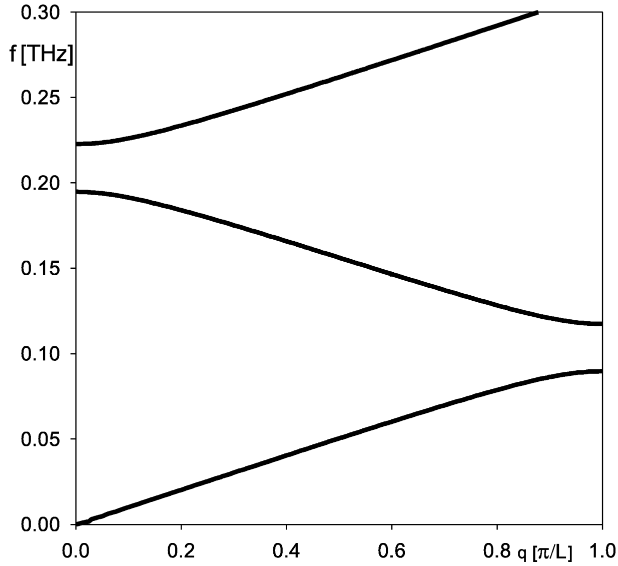

Fig. 2. Dispersion curve for longitudinal acoustic waves propagating in Au/V (100 Å/100 Å) multilayer structure.

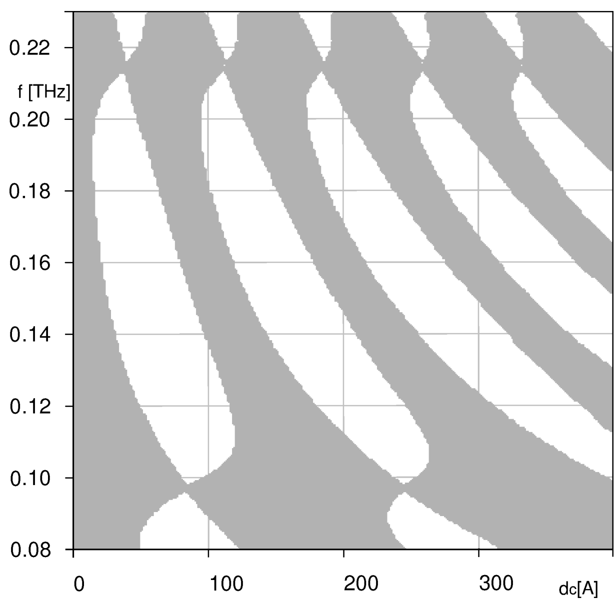

Fig. 3. Region of existence of solution for localized modes (grey color) in plane top layer thickness-frequency.

The exact view of frequency dependences on thickness of capping layer from 0 to 140 Å are exposed in Fig. 5. The analysis of these dependences allows existence of localized modes for some interval of capping layer thickness simultaneously in both frequency gaps. Moreover for certain values of thickness localized mode exist only in one gap and there are also such values of thickness where localized modes not exist. It is worth to note that when thickness of capping layer is equal to thickness of equivalent internal layer (Au) of nanostructure Au/V localized mode is not present. Up to now only this

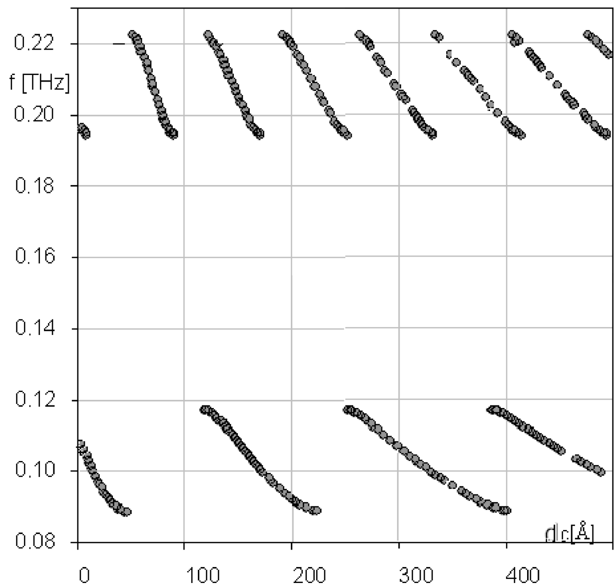

Fig. 4. Frequency of localized acoustic modes as function of thickness capping layer for Au/V (100 Å/100 Å) nanolayer with Au capping layer for first and second gap.

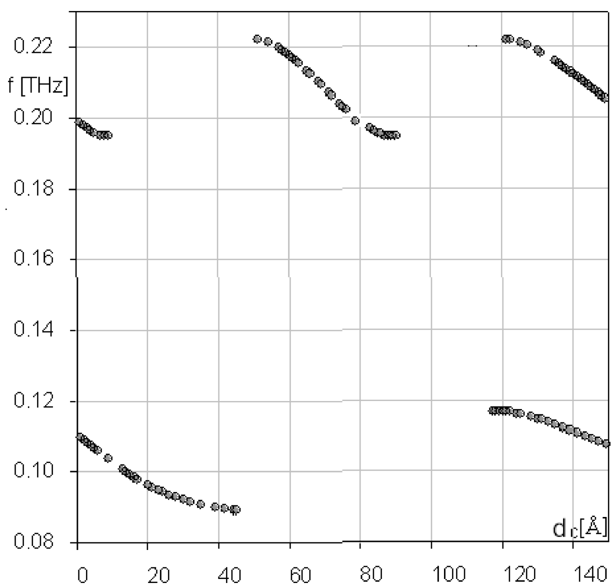

Fig. 5. Frequency of localized acoustic modes as function of thickness capping layer for Au/V (100 Å/100 Å) nanolayer with Au capping layer for d_c in range: 0–150 Å.

case was experimentally confirmed in the literature while theoretical considerations related to no existence of localized modes for nanolayers with “heavy” capping layer were in general not correct.

For the thin Au capping layer (thickness up to 0.5 of internal layer for first gap and up to 0.1 for second gap) localized modes exist. This is opposite to Au/V nanostructure with thin vanadium capping layer case. Then for thickness of vanadium capping layer (up to 0.5 of internal layer) acoustic localized modes not exist [11].

4. Conclusions

In the paper the conditions of generation of localized acoustic modes in case of higher acoustic impedance of capping layer in multilayer structure were considered. Determination of excitation conditions for localized vibration modes and control of their placement in frequency gap, which corresponds to energetic levels of impurities of semiconductors is very important due to possibility of application in nanophononic devices. Nanolayers also can be used as high frequency acoustic filters.

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