

Spatial distribution of local density of states in vicinity of impurity on semiconductor surface

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Submitted 6 May 2009

We present the results of detailed theoretical investigations of changes in local density of total electronic surface states in 2D anisotropic atomic semiconductor lattice in vicinity of impurity atom for a wide range of applied bias voltage. We have found that taking into account changes in density of continuous spectrum states leads to the formation of a downfall at the particular value of applied voltage when we are interested in the density of states above the impurity atom or even to a series of downfalls for the fixed value of the distance from the impurity. The behaviour of local density of states with increasing of the distance from impurity along the chain differs from behaviour in the direction perpendicular to the chain.

PACS: 71.55.-i

1. Introduction. Influence of different impurities on the semiconductor local density of surface states was widely studied experimentally and theoretically. Most of the experiments were carried out with the help of scanning tunneling microscopy/spectroscopy technique [1–3]. Theoretical investigations of single impurities and clusters influence on density of surface states deals with Green's functions formalism [4, 5] or based on the total-energy density-functional calculations using first-principle pseudo-potential [6]. Numerical calculations based on the tight-binding model are also carried out [7].

Most of the theoretical calculations don't take into account modification of local density of continuous spectrum states due to the influence of impurity atom on semiconductor surface which we consider to play an important role in the formation of peculiarities in the local density of total surface states. So in the present work we suggest a simple model of anisotropic atomic lattice with impurity atom and we pay special attention to the changes of local density of continuous spectrum states. This model suits well for theoretical investigation of π -bonded chains on the reconstructed Ge or Si surfaces [8]. It can be also used for investigation of the sublattices on the cleaved planes of $A_{III}B_V$ semiconductors. We have found that the view of local density of surface states (amount of downfalls and their shape) strongly differs depending on the value of the distance from the impurity atom position and from the direction of observation (along the atomic chain or perpendicular to the atomic chain). It will be shown that downfall in the resonance when we are interested in the density of states

above the impurity atom can transform to a series of downfalls or even to a peak for different values of the distance from the impurity.

2. The suggested model and main results. We shall analyze 2D anisotropic atomic lattice formed by the similar atoms with energy levels ε_1 and similar tunneling transfer amplitudes between the atoms t along the atomic chain. The interaction between atomic chains is described by tunneling amplitude T , which has the same value for all the similar atoms in the chain (Fig.1). Distance between the atoms in the atomic chain is equal

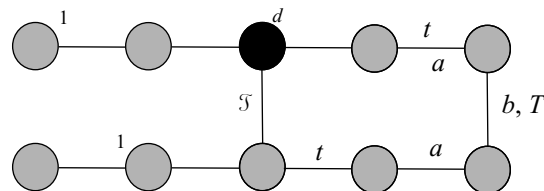


Fig.1 Schematic diagram of 2D atomic lattice with impurity atom

to a , distance between the atoms in the neighboring chains is equal to b . Atomic lattice includes impurity atom with energy level ε_d , tunneling transfer amplitude from impurity atom to the nearest atoms in the atomic chain τ and to the nearest atoms in the neighbor chains \mathfrak{S} .

The model system can be described by the Hamiltonian: \hat{H} :

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{imp}} + \hat{H}_{\text{tun}},$$

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$$\begin{aligned}
\hat{H}_0 &= \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} t c_i^\dagger c_j + \sum_{\langle k,l \rangle} T c_k^\dagger c_l + \text{h.c.}, \\
\hat{H}_{\text{tun}} &= \sum_{i,d} \tau c_i^\dagger c_d + \sum_{k,d} \mathfrak{S} c_k^\dagger c_d + \text{h.c.}, \\
\hat{H}_{\text{imp}} &= \sum_d \varepsilon_d c_d^\dagger c_d.
\end{aligned} \quad (1)$$

\hat{H}_0 is a typical Hamiltonian for atomic lattice with hoppings without any impurities. \hat{H}_{tun} describes transitions between impurity atom and neighboring atoms of the atomic lattice. \hat{H}_{imp} corresponds to the electrons in the localized state formed by the impurity atom in the atomic chain.

Indexes i, j correspond to the direction along the chain; indexes k, l correspond to the direction perpendicular to the chain.

We shall use diagram technique in our investigation of atomic chain local density of states.

The dependence of local density of states on the distance along the atomic chain and in the direction perpendicular to the atomic chain in the presence of impurity atom is described by the equation:

$$\rho(\omega, \mathbf{r}) = \frac{-1}{\pi} \text{Sp} \left(\text{Im} \sum_{\kappa, \kappa_1} \hat{G}^R(\kappa, \kappa_1, \omega) e^{i\kappa \mathbf{r}} e^{i\kappa_1 \mathbf{r}} \right). \quad (2)$$

Where $\mathbf{r} = (x, y)$, $\kappa = (\kappa_x, \kappa_y)$ and $\kappa_1 = (\kappa_{x1}, \kappa_{y1})$. Green function $\hat{G}^R(\kappa, \kappa_1, \omega)$ corresponds to the electron transition from the impurity to the semiconductor continuum states and can be found from the system of equations:

$$\begin{aligned}
G_{\kappa_x 0 dd}^R(\omega) &= G_{\kappa_x 0 \kappa_x 0}^{0R}(\omega) \tau G_{dd}^R(\omega) + \\
&+ G_{\kappa_x 0 \kappa_x 0}^{0R}(\omega) T \sum_{k_y} G_{\kappa_x \kappa_y dd}^R(\omega), \\
G_{0 \kappa_y dd}^R(\omega) &= G_{0 \kappa_y 0 \kappa_y}^{0R}(\omega) \mathfrak{S} G_{dd}^R(\omega) + \\
&+ G_{0 \kappa_y 0 \kappa_y}^{0R}(\omega) t \sum_{k_x} G_{\kappa_x \kappa_y dd}^R(\omega), \\
G_{dd}^R(\omega) &= G_{dd}^{0R}(\omega) + G_{dd}^{0R}(\omega) \tau \sum_{k_x} G_{\kappa_x 0 dd}^R(\omega) + \\
&+ G_{dd}^{0R}(\omega) \mathfrak{S} \sum_{k_y} G_{0 \kappa_y dd}^R(\omega), \\
G_{\kappa dd}^R(\omega) &= G_{\kappa \kappa}^{0R}(\omega) \tau G_{\kappa_x 0 dd}^R(\omega) + G_{\kappa \kappa}^{0R}(\omega) \mathfrak{S} G_{0 \kappa_y dd}^R(\omega), \\
G_{\kappa \kappa_1}^R(\omega) &= G_{\kappa \kappa}^{0R}(\omega) + \\
&+ G_{\kappa \kappa}^{0R}(\omega) \tau G_{dd \kappa_1}^R(\omega) + G_{\kappa \kappa}^{0R}(\omega) \mathfrak{S} G_{dd \kappa_1}^R(\omega).
\end{aligned}$$

Where zero Green function is evaluated for the 2D atomic lattice without any impurities and has the form:

$$G_{\kappa_x \kappa_y}^{0R}(\omega) = \frac{1}{\omega - \varepsilon_1 - 2t \cdot \cos(k_x a) - 2T \cdot \cos(k_y b)}. \quad (3)$$

Substituting the expression for Green function $\hat{G}^R(\kappa, \kappa_1, \omega)$ obtained from system into equation (2) and performing summarization over wave vectors k_x

and k_{x1} (k_y and k_{y1}) we get the final expression for the local density of continuous spectrum states along (perpendicular) the atomic chain $\rho_{\text{vol}}(x)$ ($\rho_{\text{vol}}(y)$):

$$\begin{aligned}
\rho_{\text{vol}}(\omega, x) &= \rho_0(\omega) \cdot \frac{(\omega - \varepsilon_d)^2 + \gamma^2 \cdot (1 - f(2k_x(\omega)x))}{(\omega - \varepsilon_d)^2 + \gamma^2}, \\
\rho_{\text{vol}}(\omega, y) &= \rho_0(\omega) \cdot \frac{(\omega - \varepsilon_d)^2 + \gamma^2 \cdot (1 - f(2k_y(\omega)y))}{(\omega - \varepsilon_d)^2 + \gamma^2}.
\end{aligned} \quad (4)$$

Where parameter $\gamma = (\tau^2 + \mathfrak{S}^2) \cdot \rho_0(\omega)$ corresponds to relaxation rate of electron distribution at the localized state formed by impurity atom, $\rho_0(\omega)$ is a local density of states for the atomic chain without any impurities. Functions $f(2k_x(\omega)x)$ and $f(2k_y(\omega)y)$ are periodical and have the property: $f(2k_x(\omega)x) = 1$ if $x = 0$ and $f(2k_y(\omega)y) = 1$ if $y = 0$. If both directions are equivalent $f(2k_x(\omega)) = f(2k_y(\omega)y) = J_0(2k_x(\omega))$. Expression for $k_x(\omega)$ or $k_y(\omega)$ can be found from the dispersion law of the 2D atomic lattice which has the form.

$$\omega(k_x, k_y) = 2t \cdot \cos(k_x a) + 2T \cdot \cos(k_y b). \quad (5)$$

Impurity atom density of states has lorentzian form line shape and can be evaluated as:

$$\rho_{\text{imp}}(\omega) = -\frac{1}{\pi} \cdot \text{Im} \sum_d G_{dd}^R(\omega) = \frac{\gamma^2}{(\omega - \varepsilon_d)^2 + \gamma^2}. \quad (6)$$

Local density of total surface states $\rho(\omega)$ is the result of summarization between local density of continuous spectrum states and impurity atom density of states.

$$\rho(\omega) = \rho_{\text{vol}}(\omega) + \rho_{\text{imp}}(\omega). \quad (7)$$

Let's start from the 1D case of the atomic chain. In this case it is necessary to put in the Hamiltonian: $b = 0$, $T = 0$ and $\mathfrak{S} = 0$. Final expression for the local density of continuous spectrum states ρ_{vol} will have the form:

$$\rho_{\text{vol}}(\omega) = \rho_0(\omega) \cdot \frac{(\omega - \varepsilon_d)^2 + \gamma^2 \cdot (1 - \cos(2k(\omega)r))}{(\omega - \varepsilon_d)^2 + \gamma^2}. \quad (8)$$

Expression for $k(\omega)$ can be found from the dispersion law of the 1D atomic chain.

Typical numerical results for local density of total surface states and local density of continuous spectrum states calculated above the impurity atom in 1D case (distance value is equal to zero ($r = 0$)) are shown on (Fig.2a,b). For the local density of continuous spectrum states (Fig.2a) a downfall exists in the resonance when energy is equal to the impurity atom energy level deposition ($\omega = \varepsilon_d$). Width of the downfall depends on the parameters of the atomic chain, such as relaxation rate

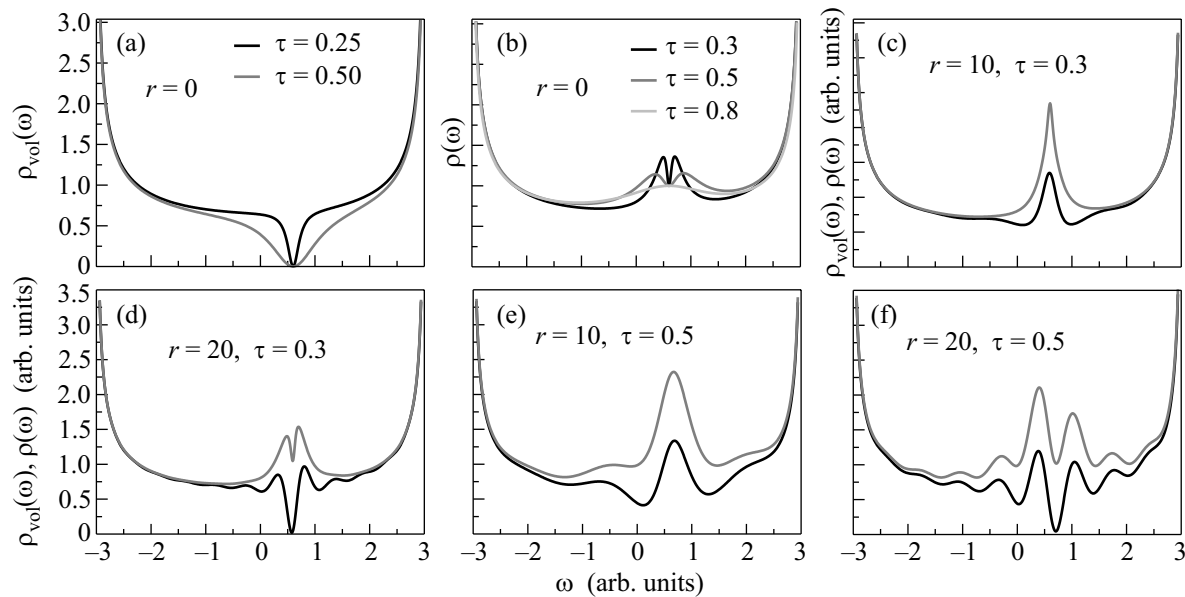


Fig.2. (a) Local density ρ_{vol} in the case of the distance from the impurity atom along the atomic chain equal to zero. (b) Local density ρ in the case of the distance from the impurity atom along the atomic chain equal to zero. (c)–(f) Local densities ρ_{vol} (black line) and ρ (grey line) for the different values of the distance from the impurity atom along the atomic chain. For all the figures values of the parameters are the same: $a = 1$, $t = 1.5$, $\varepsilon_d = 0.6$

or tunneling transfer amplitude, it rises with the increasing of tunneling transfer amplitude from impurity atom to the neighbor atoms of the atomic chain. Local density of surface states (Fig.2b) has lorentzian form with a downfall in the resonance. With the increasing of relaxation rate (increasing of τ) the downfall depth at the top of the peak decreases, resonance peak shape spreads and it's amplitude falls down.

Now let's start to analyze the dependence of local density of continuous spectrum states and local density of surface states at the fixed value of the distance r along the atomic chain from the impurity atom position (Fig.2c-f). We shall again start from the local density of continuous spectrum states (black lines on Fig.2c-f).

When the value of a distance is not equal to zero a series of downfalls in the local density of continuous spectrum exists. Amount of downfalls increases with the increasing of distance value and downfalls amplitude decreases when energy aspire to the edges of the band. The most significant amplitude of the downfalls corresponds to the vicinity of the resonance region. It is clearly evident that positions of the downfalls on the energy scale can be found from the equation $2\pi n = 2k(\omega)r$ where n is an integer number. This means that numerator of the Eq. (8) is equal to zero. When the distance is not equal to zero not only a downfall in the resonance (Fig.2d,f) but also a peak (Fig.2c,e) can exist in the local density of continuous spectrum states. At the fixed parameters

of the atomic chain existence of a downfall or a peak in the resonance is determined by the value of the distance.

Local density of surface states is shown by the grey line on Fig.2c-f. Comparison between local density of surface states and local density of continuous spectrum states for the fixed value of r make it clearly evident that impurity atom density of states can drastically influence on the local density of continuous spectrum states. Result depends on the value of tunneling transfer amplitude from impurity atom to the nearest atoms of the chain. We have found that the most significant influence corresponds to the situation when tunneling transfer amplitude between the atoms in the chain t significantly exceeds tunneling transfer amplitude from impurity atom to the atoms of the chain τ . In this case downfall in the resonance becomes a peak with a small downfall on the top of the peak (Fig.2e). So only one significant downfall exists in the resonance region and there are no downfalls at the energies different from the resonance value (Fig.2c) in the local density of surface states, while in the continuous spectrum density of states a series of downfalls exists. With increasing of τ local density of surface states differs from the local density of continuous spectrum states only by the amplitude of the downfalls (Fig.2e,f). In this case number of downfalls is the same in comparison with the continuous spectrum density of states, downfalls don't change their shape or position on the energy scale and contribution to the local density of

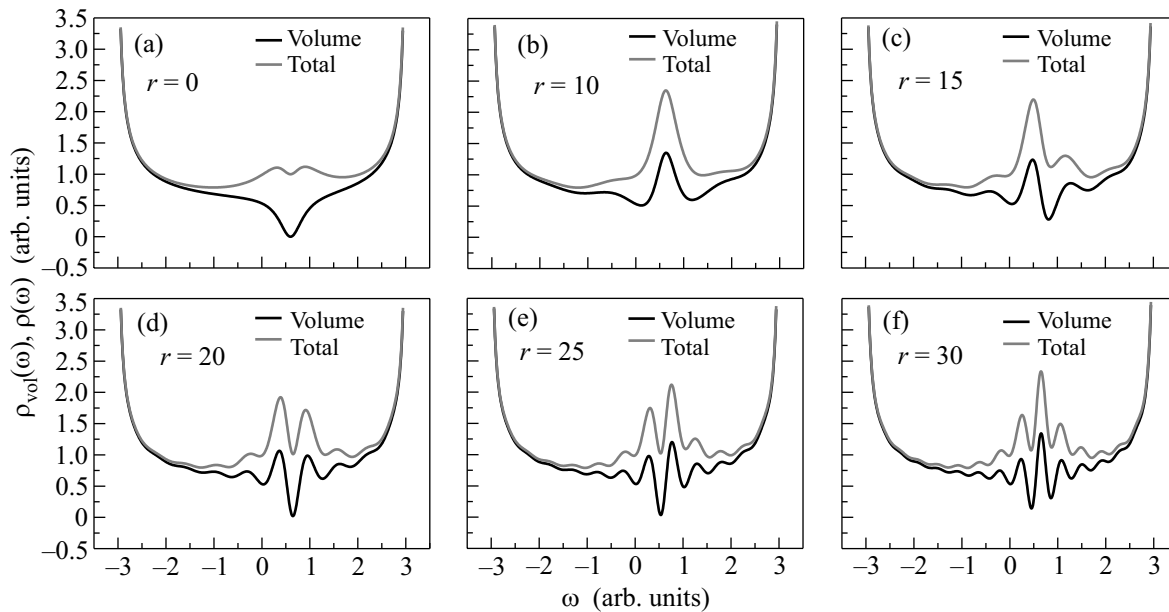


Fig. 3. (a) Local densities ρ_{vol} (black line) and ρ (grey line) for the different values of the distance from the impurity atom along the atomic chain. For all the figures values of the parameters are the same: $a = 1$, $b = 2$, $t = 1.5$, $T = 1.2$, $\tau = 0.6$, $\mathfrak{S} = 0.3$, $\varepsilon_d = 0.6$

surface states from the impurity atom can be considered to be a background. This effect can be qualitatively understood by the following way: with increasing of transfer amplitude from impurity atom to the atom of the chain increases relaxation rate and lorentzian form peak of impurity atom density of states spreads and it's amplitude decreases.

Now let's start to analyze 2D atomic lattice. Numerical results for local density of total surface states and local density of continuous spectrum states calculated above the impurity atom in perpendicular directions (along the atomic chain and perpendicular to the atomic chain) are shown on Fig.3a, Fig.4a. It's clear that in this case all the results are equal for both directions and downfall in the continuous spectrum density of states or a peak in the local density of surface states poses just the same properties as in the case of 1D atomic chain.

Let's analyze the situation when the value of the distances from the impurity atom position along the atomic chain (Fig.3b-f) and perpendicular to the atomic chain (Fig.4b-f) are not equal to zero. We shall start from the local density of continuous spectrum states (black lines on Fig.3, 4).

In this case number of downfalls, their shape and position on the energy scale in each of the perpendicular directions can be found from the dispersion law just in the same way as for 1D atomic chain. When the distance is not equal to zero not only a downfall in the resonance

(Fig.3d,e; Fig.4e,f) but also a peak (Fig.3c,f; Fig.4c,d) can exist in the local density of continuous spectrum states.

We have found distance interval for both directions (along the atomic chain and perpendicular to the atomic chain) where exists replacement of a peak by a downfall (Fig.3c-f; Fig.4c-f) in local density of continuous spectrum states (and also in the local density of surface states). Moreover peak in one direction can correspond to a downfall in the another direction. Let's analyze this interval carefully. We shall start from the distance value when peaks in the resonance in local density of continuous spectrum states for both directions can be seen ($x(y) = 15 \cdot a$) (Fig.3c, Fig.4c). With increasing of the distance value ($x(y) = 20 \cdot a$) a resonance peak in the direction perpendicular to the atomic chain still exists (Fig.4d) and in the direction along the atomic chain a downfall appears (Fig.3d). Further increasing of the distance value ($x(y) = 25 \cdot a$) shows that in the direction along the atomic chain a downfall still exists (Fig.3e) and in the perpendicular direction a downfall substitutes peak (Fig.4e). Finally when the value of distances in both directions becomes equal to $x(y) = 30 \cdot a$ in the perpendicular direction a downfall still exists (Fig.4f) and in the direction along the atomic chain a resonance peak can be seen (Fig.3f).

Local density of total surface states is shown by the grey lines on Fig.3, 4. It is clearly evident that for the studied parameters of the system taking into account

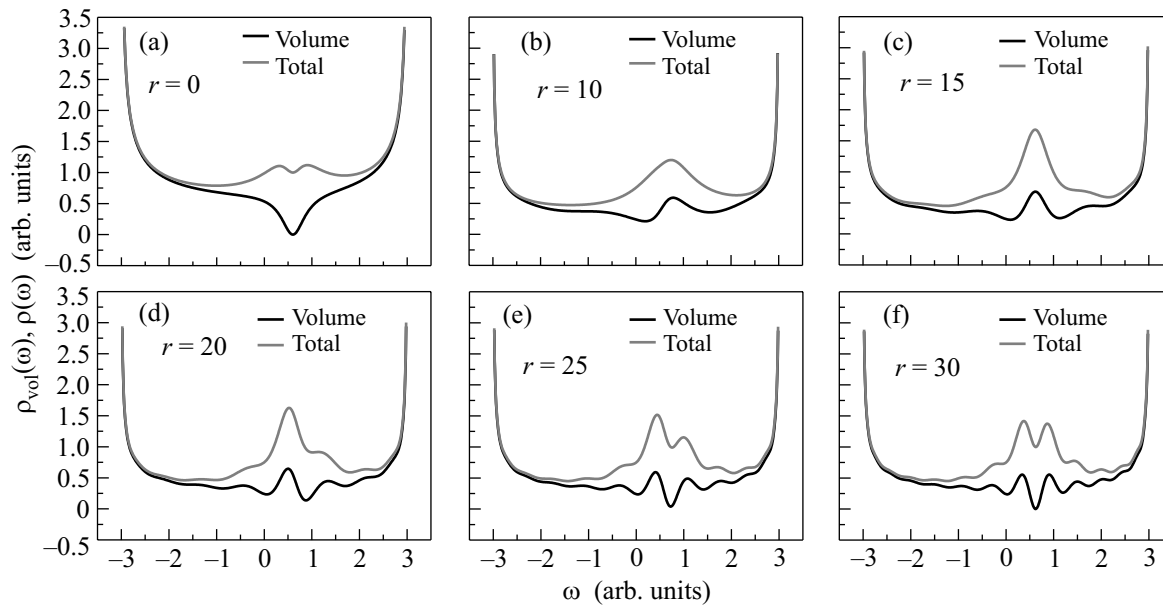


Fig.4. Local densities ρ_{vol} (black line) and ρ (grey line) for the different values of the distance from the impurity atom perpendicular to the atomic chain. For all the figures values of the parameters are the same: $a = 1$, $b = 2$, $t = 1.5$, $T = 1.2$, $\tau = 0.6$, $\Im = 0.3$, $\varepsilon_d = 0,6$

impurity atom density of states slightly changes local density of total surface states in comparison with local density of continuous spectrum states for both directions. In this case number of downfalls is the same in comparison with the continuous spectrum density of states, downfalls don't change their shape or position on the energy scale.

3. Conclusion. In this work we have shown that taking into account changes of the local density of continuous spectrum states formed by the presence of the impurity atom in the 2D anisotropic atomic lattice or even in the 1D atomic chain leads to significant modification of the total local density of surface states and consequently to the modification of STS spectra. We have found that a downfall exists in the STS spectra measured just above the impurity when impurity atom energy level is equal to the applied bias voltage. With changing of the distance from the impurity a series of downfalls is formed on the energy scale both in the local density of continuous spectrum states and in the local density of total surface states. Number of downfalls and their position are determined by the atomic lattice dispersion law. It was shown that at some values of the distance from the impurity a peak can exist in the resonance region instead of a downfall. We have found

that behaviour of local density of surface states depends on the direction of the observation. Switching on and off of impurity atom in both directions was found. This effect can be well observed experimentally with the help of STM/STS technique.

This work was supported by RFBR grants and by the National Grants for technical regulation and metrology # 01.648.12.3017 and # 154-6/259/4-08.

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