Low Temperature Physics/Fizika Nizkikh Temperatur, 2015, v. 41, No. 5, pp. 501–507

Electronic spectrum of atomic chain with Fano-Anderson impurities

Yuriy V. Skrypnyk

G.V. Kurdyumov Institute for Metal Physics, National Academy of Sciences of Ukraine
Academician Vernadsky Blvd. 36, UA-03680 Kyiv-142, Ukraine
E-mail: yuriy.v.skrypnyk@gmail.com

Received February 4, 2015, published online March 23, 2015

Electronic spectrum of one-dimensional system with a low concentration of weakly bound Fano-Anderson impurities is considered. It is assumed that the energy of the impurity resonance is located in a vicinity of the band center of the host system. It is demonstrated that with increasing the impurity concentration the dispersion of states with the low damping undergoes a transformation. This transformation passes in a threshold manner and results in the reproduction of some characteristic features inherent in the cross-type spectrum rearrangement. At that, the density of states at the energy of the impurity resonance manifests a steady growth.

PACS: **73.22.–f** Electronic structure of nanoscale materials and related systems;
71.23.–k Electronic structure of disordered solids;
71.55.–i Impurity and defect levels.

Keywords: disordered system, low-dimensional system, impurity, spectrum rearrangement, electronic spectrum.

1. Introduction

For more than two decades there was a constant interest in nanocrystalline and polycrystalline diamond-like thin films and diamondlike carbon. In this respect, the C(111) 2X1 surface remains to be an intriguing object of investigation [1–5]. Still, electronic properties of this surface are not fully understood. There is a good agreement between the experimental data and the results of the first-principles calculations for the analogous surfaces: Si(111) 2X1 and Ge(111) 2X1. It is commonly accepted that the reconstruction of all these surfaces leads to the formation of the so-called Pandey chains [6]. In the case of the Si and Ge the atoms belonging to the Pandey chains are dimerized. In contrast, it is generally agreed that the Pandey chains on the clean C(111) surface stay undimerized. *Ab initio* calculations produce the band gap in the surface states that is substantially narrower than the experimentally observed [7–9]. Usually, the reconstruction of the C(111) surface is achieved by its annealing after the cleavage. This suggests that it can remain contaminated by impurities. Numerical calculations evidently demonstrate that Pandey chains on the C(111) surface are dimerized, when ten percent or so of their atoms are passivated by hydrogen [10]. Such dimerization can help to widen the gap in the surface states, but this effect does not work for the lower impurity concentration.

At this point it is possible to ask whether or not other impurity effects can be responsible for the formation of a gap at the band center of a one-dimensional system. Below we will try to address this question in general, without taking into account specifics of Pandey chains on the diamond surface.

It is well known that electronic spectra in tree-dimensional systems can undergo a rearrangement of the cross type with increasing the amount of impurities [11–13]. When the critical concentration of impurities is exceeded, the renormalized dispersion of electrons looks like a result of the conventional hybridization between the host dispersion branch and the dispersionless branch that is located at the impurity resonance energy. It is essential that the rearranged spectrum of a disordered system features two overlapping branches of itinerant states. As a consequence, two different energies of electrons correspond to some wave vectors. These dispersion branches are separated by a true gap, which is gradually broadening with increasing the impurity concentration. As a rule, this type of the spectrum rearrangement is realized when the damping of the single-impurity resonance is much less than the interval between the impurity resonance energy and the nearest van Hove singularity in the spectrum. This condition insures the sufficient sharpness of the impurity resonance.

Cross-type spectrum rearrangement can occur in low-dimensional systems too (in particular, in one-dimensional

systems). In this case, the impurity should be weakly bound [14]. That is, the hybridization parameter for the impurity level should satisfy a certain condition, which is quite restrictive for one-dimensional systems. Again, this condition arises from the demand that the impurity resonance is to be sufficiently sharp. In addition, it is not correct to talk of itinerant states in one-dimensional disordered systems at a finite concentration of impurities.

However, all previous studies on the passage of the spectrum rearrangement in low-dimensional disordered systems were confined to the case, when the impurity resonance energy is located close to the band edge of the host system. Below we are going to consider a qualitatively different case. We will place the impurity resonance energy close to the band center of the host system, and examine transformations of the electronic spectrum, which develop with increasing the impurity concentration. The attention will be mostly focused on the close vicinity of the band center. In accordance with previous studies, we will assume that impurities are weakly bound, and will analyze the existence of possibilities for the gap formation in such a system.

2. Impurity model

Let's consider the electron spectrum in a one-dimensional system with impurities. One can usually assume that the Hamiltonian of a disordered system decomposes into a translation-invariant host part and an impurity part:

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{imp}}, \tag{1}$$

where $\hat{H}_0$ is the host Hamiltonian, and $\hat{H}_{\text{imp}}$ is the impurity perturbation. We will describe the host system by means of the tight-binding approximation, taking into account only hoppings between nearest-neighbors in a linear chain of atoms. The resulting Hamiltonian reads:

$$\hat{H}_0 = -t\sum_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n), \quad t > 0, \tag{2}$$

where n enumerates lattice sites, $c_n^\dagger$ and c_n are the creation and annihilation Fermi operators at the corresponding lattice site, and $t > 0$ is the transfer integral. The negative sign before the right-hand part of the equation appears because the transfer integral between the carbon p-orbitals in a Pandey chain is negative. Indeed, this choice of the sign does not diminish the degree of generality of the problem. It is supposed that impurities are represented by adsorbed atoms of some kind, and that these atoms are distributed absolutely at random along the chain. Besides, it is assumed that each adatom is coupled only to a single host lattice site, and can be described by the Fano-Anderson model:

$$\hat{H}_{\text{imp}} = \sum_n \eta_n (E_{\text{imp}} d_n^\dagger d_n + t_{\text{imp}} c_n^\dagger d_n + t_{\text{imp}}^* d_n^\dagger c_n), \tag{3}$$

where t_{imp} is the transfer integral between the orbital, which is added to the system by an impurity, and the orbital of the adjacent host atom from the chain, E_{imp} is the bare energy of the impurity level, $d_n^\dagger$ and d_n are the creation and annihilation operators at this level, the variable η_n takes the value of 1 with the probability c or the value of 0 with the probability $1 - c$, and c is the impurity concentration. The problem can be reduced to a more simple form by eliminating wave-function amplitudes at adatoms from the stationary Shrödinger equation for the Hamiltonian $\hat{H}$. Then, the impurity perturbation takes the form:

$$\hat{H}_{\text{imp}} = V(E)\sum_n \eta_n \; c_n^\dagger c_n \;, \quad V(E) = \frac{|\, t_{\text{imp}}\,|^2}{E - E_{\text{imp}}}. \tag{4}$$

It is trivial to obtain the dispersion relation for electrons in the host system (the band width equals $4t$):

$$E(\mathbf{k}_d) = -t\,(\mathrm{e}^{ik_d a} + \mathrm{e}^{-ik_d a}) = -2t\cos(k_d a), \tag{5}$$

where a is the lattice constant, and k_d is the wave vector. Correspondingly, the diagonal element of the host Green's function

$$\hat{g}^d(E) = (E\hat{I} - \hat{H}_0)^{-1} \tag{6}$$

reads:

$$g_{00}^d(E) = \frac{1}{N}\sum_{\mathbf{k}_d} \frac{1}{E - E(\mathbf{k}_d)} = -\frac{i}{\sqrt{(2t)^2 - E^2}}, \quad |\,E\,| < 2t, \tag{7}$$

where N is the number of atoms in the chain, and $\hat{I}$ is the identity matrix. It is convenient to pass to dimensionless variables:

$$\varepsilon = \frac{E}{2t}, \quad k = k_d a\,. \tag{8}$$

Then, the dispersion relation becomes:

$$\varepsilon(\mathbf{k}) = -\cos(k), \tag{9}$$

and the dimensionless diagonal element of the host Green's function takes the form:

$$g_{00}(\varepsilon) = -\frac{i}{\sqrt{1-\varepsilon^2}}, \quad |\,\varepsilon\,| < 1. \tag{10}$$

Accordingly, it is helpful to introduce following dimensionless variables:

$$\gamma = \frac{t_{\text{imp}}}{2t}, \quad \varepsilon_{\text{imp}} = \frac{E_{\text{imp}}}{2t}, \quad v = \frac{V(E)}{2t}, \tag{11}$$

so that the on-site impurity perturbation reads:

$$v = \frac{|\,\gamma\,|^2}{\varepsilon - \varepsilon_{\text{imp}}}\,. \tag{12}$$

We are going to study possible scenarios of the gap formation in a spectral region around $\varepsilon = 0$. The impurity scattering, which is responsible for the gap formation in the ordinary course of events, is the strongest at the energy of the impurity level ε_{imp}. Consequently, the energy of the impurity level should be located nearby the zero energy. On the other hand, the density of states in the one dimensional system under consideration is nearly flat close to the band center. Because of that, subsequent results will not significantly change, when ε_{imp} is varied to a certain extent around the zero energy. Then, it is possible, for the sake of simplicity, to put everywhere below $\varepsilon_{\text{imp}} = 0$:

$$v = \frac{|\gamma|^2}{\varepsilon}, \tag{13}$$

without any considerable loss of generality.

3. Local density of states

To start with, we will examine the behavior of the local density of states at the impurity site, when the system under consideration contains a single impurity. Usually, this characteristic appears to be rather informative regarding possible modifications of the spectrum, which develop with increasing the impurity concentration. To be more specific, we will assume that a single adatom is occupying the zeroth site. The corresponding diagonal element of the Green's function

$$\hat{G}(\varepsilon) = (\varepsilon\hat{I} - \hat{H})^{-1}, \tag{14}$$

which yields the local density of states at the host atom, can be expressed as follows:

$$G_{00}(\varepsilon) = g_{00}(\varepsilon) + g_{00}(\varepsilon)\frac{|\gamma|^2}{\varepsilon - |\gamma|^2 g_{00}(\varepsilon)} g_{00}(\varepsilon). \tag{15}$$

In a vicinity of the band center $(\varepsilon = 0)$ the host Green's function is nearly constant:

$$g_{00}(\varepsilon) \approx -i, \quad |\varepsilon| \ll 1. \tag{16}$$

As a result, we have

$$G_{00}(\varepsilon) \approx -i - \frac{|\gamma|^2}{\varepsilon + i|\gamma|^2} = -i\frac{\varepsilon}{\varepsilon + i|\gamma|^2}. \tag{17}$$

Thus, the local density of states at the host atom

$$\rho^h_{loc}(\varepsilon) = -\frac{1}{\pi}\operatorname{Im} G_{00}(\varepsilon) \approx \frac{1}{\pi}\frac{\varepsilon^2}{\varepsilon^2 + |\gamma|^4} \tag{18}$$

features the Fano antiresonance at the energy of the impurity level (i.e., at the band center). Moreover, this local density of states recedes at this energy to the exact zero (see Fig. 1). The half-width of the antiresonance is $|\gamma|^2$. Therefore, the more impurities is present in the system, the more the total density of states of host atoms is depleted at the band center. However, this effect, as it will be evident later, is not that much pronounced at a small concentration of impurities.

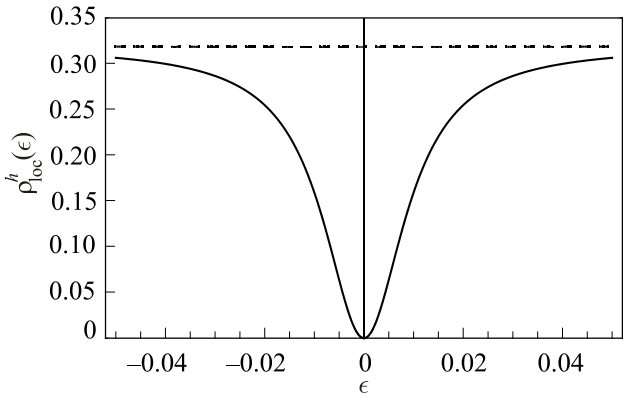

Fig. 1. Local density of states at the host atom occupied by the impurity (solid line) compared to the local density of states at an atom from the unperturbed chain (dashed line), $\gamma = 0.1$

We expect to get certain qualitative transformations in the spectrum. Consequently, different portions of the spectrum should change in a different manner under an increase in the impurity concentration. This task can be fulfilled only when the Fano antiresonance is rather sharp:

$$|\gamma|^2 \ll 1. \tag{19}$$

It is worth mentioning that the other partial local density of states at the impurity site, namely the local density of states at the adatom reads:

$$\rho^i_{\text{loc}}(\varepsilon) = -\frac{1}{\pi}\operatorname{Im} G^i_{00}(\varepsilon) = -\frac{1}{\pi}\operatorname{Im}\frac{1}{\varepsilon - |\gamma|^2 g_{00}(\varepsilon)} \approx$$

$$\approx -\frac{1}{\pi}\operatorname{Im}\frac{1}{\varepsilon + i|\gamma|^2} = \frac{1}{\pi}\frac{|\gamma|^2}{\varepsilon^2 + |\gamma|^4}. \tag{20}$$

In other words, the local density of states at the adatom shows a sharp, well defined resonance at the energy of the impurity level, provided that the inequality (19) is satisfied.

At this point, it seems instructive to consider the dispersion of electrons in the case, when all atoms in the chain are occupied by impurities. It is obvious that the on-site potential in this case is given by the impurity perturbation v. Thus, the new dispersion relation is a solution of the equation:

$$\tilde{\varepsilon}(k) - \frac{|\gamma|^2}{\tilde{\varepsilon}(k)} + \cos(k) = 0. \tag{21}$$

This quadratic yields:

$$\tilde{\varepsilon}_{1,2}(k) = \frac{1}{2}\left(-\cos(k) \pm \sqrt{\cos^2(k) + 4|\gamma|^2}\right). \tag{22}$$

It is not difficult to see that the width of the gap is equal to $2|\gamma|^2$ for a small hybridization parameter:

$$\tilde{\varepsilon}_1(0) = \frac{1}{2}\,(-1+\sqrt{1+4|\gamma|^2}) \approx |\gamma|^2,$$

$$\tilde{\varepsilon}_2(\pi) = \frac{1}{2}\,(1-\sqrt{1+4|\gamma|^2}) \approx -|\gamma|^2, \quad |\gamma|^2 \ll 1. \qquad (23)$$

Therefore, the condition $|\gamma|^2 \ll 1$, provides both for the narrow transport gap (as compared to the band width) and for the sharp (well-defined) impurity resonance (antiresonance).

4. Critical impurity concentration

With increasing the impurity concentration, the spectrum of a disordered system can change noticeably. Renormalized approaches, such as the coherent potential approximation and the modified propagator method, prove to be most effective in describing states inside the continuous spectrum of the system. Averaging over all possible impurity distributions restores the translational invariance of the single-electron Greens function:

$$\hat{\mathcal{G}}(\varepsilon) = \langle \hat{G}(\varepsilon) \rangle \approx \hat{g}(\varepsilon - \sigma(\varepsilon)), \qquad (24)$$

where $\sigma(\varepsilon)$ is the self-energy. Since the modified propagator method, the coherent potential approximation, and the average T-matrix approximation are all of the single-site type, the self-energy $\sigma(\varepsilon)$ within their frameworks does not depend on the wave vector. For example, according to the modified propagator method,

$$\sigma(\varepsilon) = \frac{c\,v}{1 - v g_{00}(\varepsilon - \sigma(\varepsilon))} = \frac{c|\gamma|^2}{\varepsilon + \dfrac{i|\gamma|^2}{\sqrt{1-\tilde{\varepsilon}(\varepsilon)^2}}}, \qquad (25)$$

where

$$\tilde{\varepsilon}(\varepsilon) = \varepsilon - \sigma(\varepsilon) \qquad (26)$$

is the renormalized energy. The quantity $|\tilde{\varepsilon}|$ will always remain small (much less than unity) below. Therefore, the expression for the self energy can be simplified even more:

$$\sigma(\varepsilon) \approx \frac{c|\gamma|^2}{\varepsilon + i|\gamma|^2}. \qquad (27)$$

At this stage, it becomes clear that it is insignificant whether the approximation with the renormalized propagator, such as the coherent potential approximation and the modified propagator method, or with the unrenormalized propagator, such as the average T-matrix approximation, is used. The new (renormalized) dispersion relation $\tilde{\varepsilon}(k)$ is defined by the equation:

$$\mathrm{Re}\,\tilde{\varepsilon}(\tilde{\varepsilon}(k)) = -\cos(k). \qquad (28)$$

Since the function $\cos(k)$ varies linearly with wave vector at the band center, the attention should be paid to the behavior of the dependence $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon)$. At low impurity concentrations, the equation $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon) = 0$ has only one real root, namely $\varepsilon = 0$. At that, the point $\varepsilon = 0$ is also an inflection point of the graph of $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon)$. With increasing the impurity concentration, the convex and concave parts are gradually developing on the $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon)$ curve. Finally, starting from the certain impurity concentration, the equation $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon) = 0$ has three distinct real roots instead of one. Let's take a closer look at this equation:

$$\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon) = \varepsilon - \mathrm{Re}\,\sigma(\varepsilon) \approx \varepsilon - \frac{c|\gamma|^2\,\varepsilon}{\varepsilon + |\gamma|^4} = 0. \qquad (29)$$

It is easy to see that the root $\varepsilon = 0$ is always present. The other two are

$$\varepsilon_{1,2} = \pm|\gamma|\sqrt{c - |\gamma|^2}. \qquad (30)$$

Both these roots are real if the condition

$$c > |\gamma|^2 = c_{cr} \qquad (31)$$

is met. Thus, the concentration c_{cr} is the critical concentration for the spectrum transformation. Indeed, this critical concentration should be small $c_{\mathrm{cr}} \ll 1$ in order to be consistent with the approximations adopted above. This condition translates to the inequality $|\gamma|^2 \ll 1$, which already appeared earlier as the criterion for the antiresonance sharpness and for the narrowness of the transport gap in a system fully covered by impurities.

5. Parameters of the transformed spectrum

The portion of the renormalized dispersion curve with the negative (anomalous) dispersion, which passes through the zero energy at $k = \pi/2$, is not valid because of the high damping, caused by impurity scatterings. For the same reason, one cannot speak about the formation of the real gap in the spectrum with increasing the impurity concentration. At the same time, a transport gap does develop in the spectrum when the critical concentration c_{cr} is exceeded. According to (30), the "apparent" (or "perceived") width of the gap between dispersion branches at $k = \pi/2$ is

$$\Delta_a = 2|\gamma|\sqrt{c - c_{\mathrm{cr}}} \approx 2|\gamma|\sqrt{c}, \quad c \gg c_{\mathrm{cr}}. \qquad (32)$$

However, the width of the actual transport gap is significantly smaller. It is not difficult to find extrema of the function $\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon)$. They are determined by the following equation:

$$\frac{d\,\mathrm{Re}\,\tilde{\varepsilon}(\varepsilon)}{d\varepsilon} = 1 - \frac{c|\gamma|^2\,(|\gamma|^4 - \varepsilon^2)}{(\varepsilon^2 + |\gamma|^4)^2} = 0. \qquad (33)$$

This comes to the quadratic:

$$x^2+|\gamma|^2\,(2|\gamma|^2+c)x+|\gamma|^6\,(|\gamma|^2-c)=0,\quad x=\varepsilon^2. \quad (34)$$

Its roots are:

$$x_{1,2}=\frac{1}{2}\left[-|\gamma|^2\,(2|\gamma|^2+c)\pm c|\gamma|^2\sqrt{1+8\frac{|\gamma|^2}{c}}\right]. \quad (35)$$

The second root is negative, and, therefore, should be omitted. Expanding the expression for the first one at $c\gg c_{\rm cr}$, we get:

$$\varepsilon_{1,2}\approx\pm|\gamma|^2\,. \quad (36)$$

Thus, the distance between extrema on the energy axis at $c>c_{\rm cr}$ is nearly equal to the width of the gap in the system with full coverage of the chain by impurities. This result can be obtained much faster. At $c\gg c_{\rm cr}$, the renormalization of the energy is significant. Therefore:

$$\frac{d\,{\rm Re}\tilde{\varepsilon}(\varepsilon)}{d\varepsilon}\approx-\frac{d\,{\rm Re}(\varepsilon)}{d\varepsilon}\approx-\frac{c|\gamma|^2\,(|\gamma|^4-\varepsilon^2)}{(\varepsilon^2+|\gamma|^4)^2}=0, \quad (37)$$

which immediately yields (36). Correspondingly, at the extrema points we have:

$${\rm Re}\tilde{\varepsilon}(\varepsilon_{1,2})\approx{\rm Re}\tilde{\varepsilon}(\pm|\gamma|^2)\approx\mp\frac{c}{2}. \quad (38)$$

Thus, the relative size of the distorted region on the dispersion curve is small. The effective damping of an electronic state at some energy ε is given by the imaginary part of the self energy

$$\Gamma(\varepsilon)=-{\rm Im}\,\sigma(\varepsilon)\approx\frac{c|\gamma|^4}{\varepsilon^2+|\gamma|^4}. \quad (39)$$

It reaches its maximum at $\varepsilon=0$ ($\Gamma(0)=c$). At the extrema points the damping amounts to $c/2$, which is in good correspondence with (38). Since the damping magnitude near the band center is around $c>c_{\rm cr}=|\gamma|^2$, the broadening of the portion of the dispersion curve with the anomalous dispersion is larger than the width of the gap between two portions of the dispersion curve with the positive dispersion ($2|\gamma|\sqrt{c}$). Thus, the presence of the negative dispersion in the spectrum is not justified, and the respective portion of the dispersion curve is smeared out by impurity scatterings. In addition, that means that no real gap should be seen in the density of states.

It is not correct to speak about mobility edges in a one-dimensional system with impurities. However, heuristically it is possible to separate electronic states with high and low damping. Edges $\pm\varepsilon_{\rm th}$ between them at $c>c_{\rm cr}$ will limit those portions of the dispersion curve, which have the positive dispersion. One can demand that the distance between portions of the dispersion curve with positive and negative dispersion should be less than the concentration broadening of the dispersion curve. In the first approximation, the portion of the dispersion curve with the negative dispersion can be considered as a dispersionless. Then, the aforementioned distance is approximately equal to $|\varepsilon|$. The resulting condition reads:

$$|\varepsilon|>\varepsilon_{\rm th}=-{\rm Im}\,\sigma(\varepsilon_{\rm th})\approx\frac{c|\gamma|^4}{\varepsilon_{\rm th}^2+|\gamma|^4}. \quad (40)$$

Let's assume that $|\varepsilon_{\rm th}|\gg|\gamma|^2$. Then, we have

$$|\varepsilon_{\rm th}|^3\approx c|\gamma|^4=\frac{c}{c_{\rm cr}}|\gamma|^6, \quad (41)$$

or

$$|\varepsilon|>\left(\frac{c}{c_{\rm cr}}\right)^{1/3}|\gamma|^2\,. \quad (42)$$

The opposite assumption ($|\varepsilon_{\rm th}|<|\gamma|^2$) leads to the contradiction:

$$|\gamma|^2>|\varepsilon_{\rm th}|\approx c>c_{\rm cr}=|\gamma|^2\,. \quad (43)$$

Thus, the threshold magnitude of energy $\varepsilon_{\rm th}$ is larger than the distance from the extremum on the renormalized dispersion curve to the zero energy $|\gamma|^2$ due to the factor $(c/c_{\rm cr})^{1/3}$. At the same time, $\varepsilon_{\rm th}$ is smaller than the half distance between dispersion branches Δ_a at $k=\pi/2$ (see (32)). Thus, branches of states with low damping overlap with each other.

6. Density of states and spectral function

The density of states of host atoms in the impure chain is given by the expression:

$$\rho^h(\varepsilon)=-\frac{1}{\pi}{\rm Im}\,\mathcal{G}_{00}(\varepsilon)\approx-\frac{1}{\pi}{\rm Im}\,g_{00}(\varepsilon-\sigma(\varepsilon))\,. \quad (44)$$

Close to the band center we have:

$$\rho^h(\varepsilon)\approx-\frac{1}{\pi}{\rm Im}\,\frac{-i}{\sqrt{1-\left(\varepsilon-\dfrac{c|\gamma|^2}{\varepsilon+i|\gamma|^2}\right)^2}}\approx\frac{1}{\pi},\qquad|\varepsilon|\ll1. \quad (45)$$

Thus, the density of states of host atoms does not significantly deviate from the unperturbed one (see Fig. 2). In this figure the density of states of host atoms is shown at the impurity concentration $c=0.05$. In this and following figures we take the hybridization parameter $\gamma=0.1$. The corresponding critical concentration $c_{\rm cr}$ is equal to 0.01. Therefore, even at $c\gg c_{\rm cr}$ the expected reduction of the density of states of host atoms is negligibly small at the band center. It is not difficult to check that with a considerable further increase in the impurity concentration the deviation will remain barely discernible.

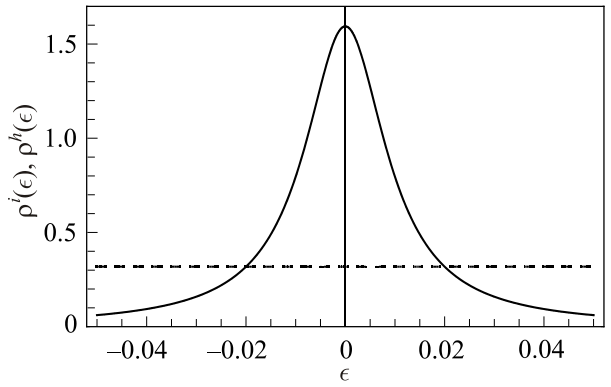

Fig. 2. The density of states of adatoms (solid line) compared to the density of states of host atoms (dashed line) at $c = 0.05$ and $\gamma = 0.1$.

The density of states of adatoms reads:

$$\rho^i(\varepsilon) = -\frac{1}{\pi}\operatorname{Im}\mathcal{G}^i_{00}(\varepsilon) \approx -\frac{1}{\pi}\operatorname{Im}\frac{c}{\varepsilon - |\gamma|^2\, g_{00}(\varepsilon - \sigma(\varepsilon))}. \quad (46)$$

Close to the band center this expression can be simplified:

$$\rho^i(\varepsilon) \approx -\frac{1}{\pi}\operatorname{Im}\frac{c}{\varepsilon + i|\gamma|^2} = \frac{1}{\pi}\frac{c|\gamma|^2}{\varepsilon^2 + |\gamma|^4}, \qquad |\varepsilon| \ll 1. \quad (47)$$

Thus, the density of states of adatoms does not remarkably differ from the corresponding local density of states weighted with the impurity concentration. The density of states of adatoms unambiguously dominates in this domain by a good margin at $c \gg c_{\rm cr}$ (see Fig. 2), and peaks at the zero energy. Indeed, there is no gap in the total density of states.

The spectral function for host atoms is of the form:

$$A(\varepsilon, k) = -\frac{1}{\pi}\operatorname{Im}\mathcal{G}(\varepsilon, k) = -\frac{1}{\pi}\operatorname{Im}\frac{1}{\varepsilon - \sigma(\varepsilon) - \varepsilon(k)}. \quad (48)$$

This spectral function is shown for $c = c_{\rm cr}$ and $c = 5c_{\rm cr}$ in Figs. 3 and 4, respectively. In both plots the range of the energy axis is limited to a small neighborhood of the band center. It is clear from these figures that the distorted portion of the spectrum is confined to a close vicinity of the zero energy. Gradual formation of the transport gap with increasing the impurity concentration is evident from the comparison of these figures. It should be mentioned that the overall shape of the spectrum possesses some characteristic features of the cross-type spectrum rearrangement. However, it is symmetric about the energy of the Fano antiresonance. Such symmetry was not inherent in the known types of the cross spectrum rearrangement.

The spectral function for adatoms reads:

$$A^i(\varepsilon, k) = -\frac{1}{\pi}\operatorname{Im}\mathcal{G}^i(\varepsilon, k) = -\frac{1}{\pi}\operatorname{Im}\frac{\sigma(\varepsilon)(\varepsilon - \varepsilon(k))}{|\gamma|^2\,(\varepsilon - \sigma(\varepsilon) - \varepsilon(k))}. \quad (49)$$

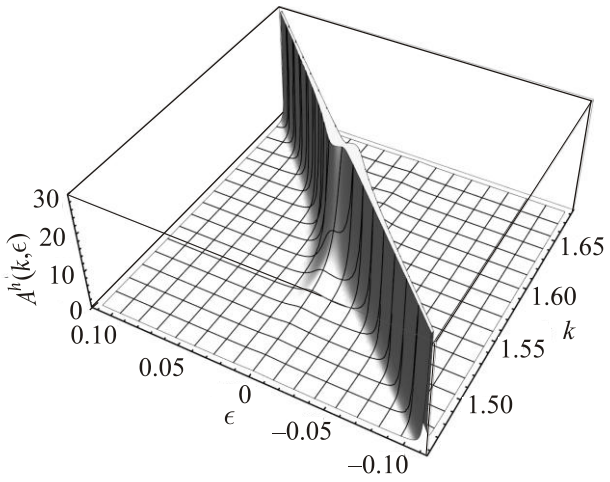

Fig. 3. Spectral function for host atoms at $c = 0.01$, $\gamma = 0.1$.

This spectral function is shown in Fig. 5 at the impurity concentration $c = 5c_{\rm cr}$. The range of the z-axis is the same as the one that is used in Figs. 3 and 4. It is apparent that the height of spectral function for adatoms is nearly negligible compared with the height of the spectral function for host atoms.

7. Conclusion

To summarize, the local density of states at the host atom manifests a sharp Fano antiresonance, when the corresponding host atom is occupied by a weakly bound impurity. The energy, at which the Fano antiresonance is located, coincides with the energy of the impurity level. Despite the antiresonance, the density of states of host atoms does not express any substantial reduction at the energy of the Fano antiresonance under an increase in the impurity concentration, provided that the impurity concentration remains small $(c \ll 1)$. In the case of a single weakly bound impurity, the local density of states at the adatom features a

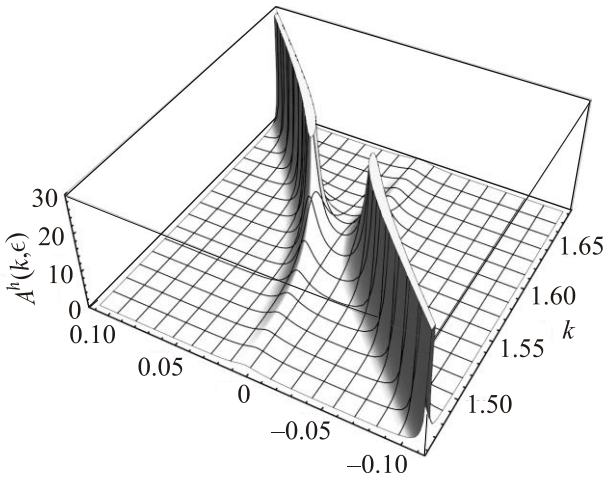

Fig. 4. Spectral function for host atoms at $c = 0.05$, $\gamma = 0.1$.

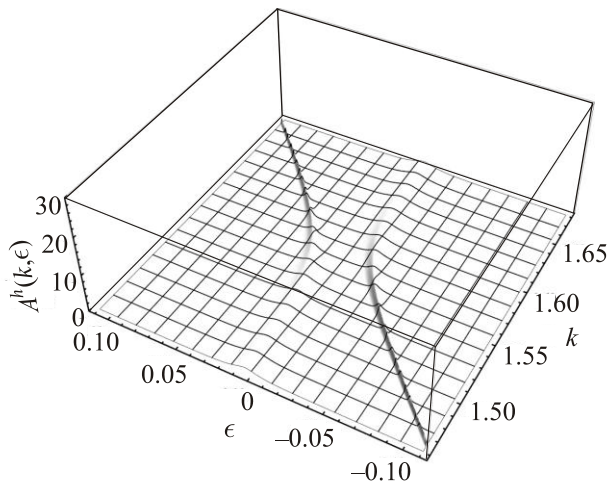

Fig. 5. Spectral function for adatoms at $c = 0.05$, $\gamma = 0.1$.

strong resonance positioned at the energy of the impurity level. With increasing the impurity concentration, the density of states of adatoms does not significantly deviate from the simple sum of the individual local densities of states at adatoms, which are treated as single impurities. When the impurity concentration exceeds a certain critical one (c_{cr}), the density of states of adatoms becomes larger than the density of states of the host atoms near the energy of the impurity resonance. The critical concentration depends only on the hybridization parameter of the impurity level ($|\gamma|$).

At the same critical concentration the dispersion relation of the disordered system under consideration undergoes a noteworthy transformation, which is reflected in the shape of the spectral function of the system. However, the scope of this transformation is limited to the close vicinity of the impurity resonance energy. The dispersion curve splits into the two branches with the positive dispersion. These branches are showing a saturation-type behavior when approaching to the domain of the impurity resonance broadening ($\sim|\gamma|^2$). Threshold energies for the states with the low damping are situated somewhat farther from the zero energy than the above margins. Overall, the shape of the transformed spectrum reminds the result of the cross-type spectrum rearrangement. In contrast to the known examples of the cross-type spectrum rearrangement, there is no real gap filled with the states that are strongly localized on pairs and larger clusters of impurities. In addition, the branches of the states with the low damping are symmetrical about the point $[k = \pi/2, \varepsilon = 0]$. Between these branches there is a transport gap, which width is increasing with an increase in the impurity concentration.

As regards the application of the above results to the Pandey chains on the diamond surface, the main challenge is to find impurity atoms or molecules that can be considered as a weakly bound.

Author is grateful to Prof. Olivia Pulci for fruitful discussions and inspiring comments. This work was supported by the European FP7 program Grant No. 246937 (SIMTECH).

1. F.J. Himpsel, D.E. Eastman, P. Heimann, and J.F. van der Veen, *Phys. Rev. B* **24**, 7270 (1981).
2. C. Noguez and Sergio E. Ulloa, *Phys. Rev. B* **53**, 13138 (1996).
3. A. Scholze, W.G. Schmidt, and F. Bechstedt, *Phys. Rev. B* **53**, 13725 (1996).
4. R. Graupner, M. Hollering, A. Ziegler, J. Ristein, L. Ley, and A. Stampfl, *Phys. Rev. B* **55**, 10841 (1997).
5. A.V. Petukhov, D. Passerone, F. Ercolessi, E. Tosatti, and A. Fasolino, *Phys. Rev. B* **61**, R10590 (2000).
6. K.C. Pandey, *Phys. Rev. Lett*. **47**, 1913 (1981).
7. M. Marsili, O. Pulci, F. Bechstedt, and R. Del Sole, *Phys. Rev. B* **72**, 115415 (2005).
8. M. Marsili, O. Pulci, F. Bechstedt, and R. Del Sole, *Phys. Rev. B* **78**, 205414 (2008).
9. M. Marsili and O. Pulci, *J. Phys. D* **43**, 374016 (2010).
10. A.I. Shkrebtii, M. Marsili, E. Heritage, O. Pulci, R. Del Sole, and F. Bechstedt, *Phys. Status Solidi A* **209**, 669 (2012).
11. M.A. Ivanov, *Sov. Phys. Solid State* **12**, 1508 (1971).
12. I.M. Lifshitz, S.A. Gredeskul, and L.A. Pastur, *Introduction to the Theory of Disordered Systems*, Wiley, N. Y. (1988).
13. M.A. Ivanov, V.M. Loktev and Yu.G. Pogorelov, *Phys. Rep*. **153**, 209 (1987).
14. M.A. Ivanov and Yu.V. Skripnik, *Sov. Phys. Solid State* **34**, 342 (1992).