A comparative scanning tunneling spectroscopy investigation of the (12110)-surface of decagonal Al–Ni–Co and the (100)-surface of its approximant Y–Al–Ni–Co

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**Abstract.** We present a low-temperature scanning tunneling spectroscopy study of the local density of states (LDOS) on the (12110)-surface of the decagonal quasicrystal d–Al–Ni–Co and the (100)-surface of its structurally closely related approximant Y–Al–Ni–Co in the range of ±1 eV around the Fermi energy. The LDOS of both surfaces are dominated by a large parabolic pseudogap centered at the Fermi energy, which can be attributed to the Hume–Rothery stabilization mechanism or to an orbital hybridization. Superimposed on this large pseudogap, a spatially varying fine structure is revealed, whose spatial distribution correlates with the structures of both of the surfaces. This fine structure shows narrow peaks and pseudogaps exhibiting typical energy widths between 50 and 150 meV. The spatial extent of these localized states is of the order of the width of the topographic features, which is about 0.45 nm. Our findings show that specific electronic states are localized on equivalent topographic features regardless of the presence of periodic or quasiperiodic long-range order. We interpret this result as an indication that the...
fine structure in the LDOS is dominated much more by the complex short-range order than by the presence of the quasiperiodic long-range order.

1. Introduction

Quasicrystals (QC) are intermetallic compounds exhibiting rotational symmetries that are incompatible with translational periodicity, showing quasiperiodic atomic order [1] instead. Along with their quasiperiodic crystal structures, QC are well known to exhibit some physical properties markedly different from those of their constituent elements. They show high electrical resistivities, low thermal conductivities, low friction coefficients and low surface energies [2]. One of the most challenging questions is: to what extent are these particular physical properties a result of the quasiperiodic long-range order? In this regard, the decagonal quasicrystals (d-QCs) are of special interest because they are structurally built up by a periodic stack of quasiperiodic planes [3]. d-QCs therefore combine quasiperiodic (Q) and periodic (P) atomic order within one material. This allows the comparison of specific physical properties, such as electrical resistivity along the Q and P directions of one and the same crystal. Furthermore, comparative investigations can be undertaken using related approximants. QCs and their approximants possess similar chemical composition and local atomic structure. One specially adequate pair for comparative studies is the Y–Al–Ni–Co approximant [4] (with 32 atoms per unit cell) and the d–Al–Ni–Co QC [5]. d–Al–Ni–Co exhibits remarkable anisotropy between the Q and P directions for many physical properties. For instance, the electrical resistivity [6, 7] is larger by a factor of 10 along the Q direction compared to the perpendicular [00001] P direction at 4.2 K. On the other hand, the friction coefficient measured on the twofold d–Al–Ni–Co surface is reduced by a factor of 8 for the Q direction as compared to the P one [8]. Y–Al–Ni–Co also reveals significant directional anisotropy in electric properties [9]–[11], which, however, is not as pronounced as for d–Al–Ni–Co.

These recent findings [9]–[11] indicate that the long-range quasiperiodic order might influence the physical properties to a less extent than does the complex local atomic structure. As most of these exceptional physical properties are directly related to the electronic density of states (DOS), it is of great interest to reveal the DOS structure in correlation with the local atomic structure of QCs and their approximants.

Photoelectron emission spectroscopy (PES) is a well-established tool to investigate the valence electronic structure of materials. It has been successfully applied to show the existence of the pseudogap in a large set of QCs and their approximants [12]–[14] and to reveal band folding in d–Al–Ni–Co [15, 16]. However, PES lacks sufficient spatial resolution to reveal LDOS variations on the sub-nanometer level, which is in the range of the characteristic...
length scale of atomic structure motifs in QCs and their approximants. By high-resolution scanning tunneling spectroscopy (STS) the LDOS can be explored while scanning the surface by scanning tunneling microscopy (STM). Recently, Widmer et al [17, 18] showed the presence of sharp 30–50 meV and spatially localized (typical extent of 0.5 nm) electronic states by STS investigations on twofold and fivefold i-AlPdMn surfaces [17, 18]. Localized states have been predicted by theoretical studies of QCs and termed ‘spiky DOS’ [19, 20]. This localization of states has been related to a large effective mass of valence electrons and the experimentally observed low electrical conductivity of QCs [20–22]. In the STS investigation of twofold and fivefold i-AlPdMn surfaces [17, 18], the spiky spectral features could not be assigned to specific topographic features due to the complex surface structures. In this respect the (12110)-surface of d–Al–Ni–Co [23] has the advantage of possessing a structurally less complex surface as it is spanned by a quasiperiodic and a periodic direction. Therefore, it is a very promising candidate to study the influence of the quasiperiodic structure compared to a periodic atomic arrangement on the LDOS. The LDOS on the (100)-surface of the Y–Al–Ni–Co approximant [24] can be investigated comparatively in the absence of quasiperiodicity but in the presence of similar structural motifs.

In this paper, we focus our discussion on the spatial variability of the LDOS measured by STS along the quasiperiodic and the periodic axis of the (12110)-surface of d–Al–Ni–Co, which we then compare to the corresponding directions of the Y–Al–Ni–Co (100)-surface.

2. Experimental details

In this study, we have investigated the (12110)-surface with twofold point symmetry of d-Al\textsubscript{72.9}Ni\textsubscript{10.4}Co\textsubscript{16.7}, which has been grown by means of the self-flux technique [25, 26], and the (100)-surface of a Y-Al\textsubscript{75.8}Ni\textsubscript{2.1}Co\textsubscript{22.1} single crystal grown by the Czochralski method. Both surfaces were oriented using Laue diffraction and cut to expose the desired crystallographic surface. The surfaces were then mechanically polished to mirror finish with diamond paste down to a grain size of 0.1 \(\mu\)m. UHV preparation (base pressure below \(10^{-10}\) mbar) was carried out by repeated sputter–annealing cycles. For both samples the cycles consisted of Ar\textsuperscript{+} ion bombardment at 1.5 kV at 30\degree grazing angle for 30 min, followed by annealing at 1080 K for 1 h. The temperature was measured by an optical pyrometer Raytek MA2B with the emissivity set to \(\varepsilon = 0.35\). This procedure was repeated 6–8 times. The as-prepared surfaces showed sharp LEED patterns from 15 to 170 eV kinetic electron energy. STM imaging and STS measurements using the lock-in technique were performed with an Omicron low-temperature scanning tunneling microscope at 5 K using mechanically cut Pt\textsubscript{80}/Ir\textsubscript{20} tips. The typical parameters for the lock-in STS measurements were 10–20 mV rms amplitude of the ac-voltage signal at a frequency of 860 Hz. Large sets (>500) of \(dI/dV\) spectra have been recorded by acquiring single spectra on equidistant grid positions during a topography scan. During the measurement of STS grid data, the thermal drift is below 0.5 nm h\textsuperscript{-1}, which allows for a faithful alignment of the STS measurements with the STM topography and serves as the basis to evaluate the spatial variability in the LDOS. In this paper, the STS spectra are mostly presented as spatially resolved \(dI/dV\) intensity maps: the vertical axis represents the sample bias and the horizontal axis the position along a chosen line cut in the corresponding topography image. For a clearer identification of the fine structure in the STS spectra, they have been background subtracted. This background subtraction has been performed by taking the difference between each single spectrum and the averaged spectrum of the whole grid, which was then divided by the averaged spectrum and
multiplied by 100%. The background-subtracted spectra represent the magnitude (given in %) of the deviation between the single $dI/dV$ spectra and the averaged spectrum.

3. Results

Figure 1(a) shows a representative STM image of the $d$–Al–Ni–Co (12110)-surface. The surface structure consists of characteristic 0.4 nm periodic columns along the [00001] (periodic) direction; in-between regions of complex structural order are found. The positions of these columnar features are indicated by black arrows. Their sequence follows a section of the quasiperiodic Fibonacci chain, which is illustrated by colored boxes and labeled with the Fibonacci segments $S'$ and $L'$, with $L' = 1.48$ nm and $S' = L'/\tau$, where $\tau$ denotes the golden mean ratio $1.61803 \ldots$. The fast-Fourier transform (FFT) of the STM topography image (inset of figure 1(a)) reveals along the [00001] direction the smallest bulk model periodicity of 0.4 nm but also the presence of 0.8 nm periodic arrangements. For a more detailed surface characterization, we refer the reader to [23].

The STM image in figure 1(b) shows the so-called A-termination of the Y–Al–Ni–Co (100)-surface [24] with the $c$-axis ($c = 0.74910(9)$ nm in the bulk model [4]) horizontally and the $b$-axis ($b = 0.40993(6)$ nm in the bulk model) vertically oriented. The surface structure of the A-termination recorded at $-1.28$ V reveals columnar features along the $b$-axis with a few local defects. The A-termination has been identified as a $(2 \times 1)$ reconstruction [24]. The inset in the upper right corner of figure 1(b) shows the corresponding FFT pattern, where the doubling of the bulk model periodicity along the $b$-axis to 0.8 nm is clearly demonstrated. For a more detailed description of the Y–Al–Ni–Co (100)-surface, we refer the reader to [24].

The comparison of the STM topography images of the $d$–Al–Ni–Co (12110)-surface and the Y–Al–Ni–Co (100)-surface in figure 1 reveals obvious differences. Nevertheless, similarities can also be found, such as the appearance of columnar structures along [00001] and the $b$-axis, respectively, and, for the same directions, the doubling of the characteristic 0.4 nm periodicity to 0.8 nm. Beyond that, the observed surface reconstructions in both cases can be related to the bulk structure model [23, 24]. Finally, bear in mind that both systems show an almost identical ratio of Al to transition metal atoms.

Figure 2 summarizes the results of STS line scan measurements taken along the quasiperiodic and the pseudo-quasiperiodic ($c$-axis) direction of the $d$–Al–Ni–Co (12110)-surface and the Y–Al–Ni–Co (100) surface, respectively. For the $d$–Al–Ni–Co surface, two $dI/dV$ scans (at $+1$ and $-1$ V set point voltage) have been recorded equally spaced (spacing: 0.27 nm) along a single scan line of the STM image shown in figure 2(a). In the case of the Y–Al–Ni–Co surface, the $dI/dV$ map is recorded with 0.1 nm spacing and a set point of $-1$ V along a single line scan of the STM image shown in figure 2(e). The averaged spectra of both $dI/dV$ scans (shown as dashed curves in figures 2(d) and (g), respectively) reveal a common feature, which is the convex parabolic shape of the spectrum with a pronounced minimum at 0 V bias. This particular shape is attributed either to the reduced DOS at the Fermi energy ($E_F$) due to the Hume–Rothery stabilization mechanism, in analogy to the case of $i$-AlPdMn [17], or to an orbital hybridization [27].

Figure 2(b) shows the spatially resolved background-subtracted $dI/dV$ intensity maps of the $d$–Al–Ni–Co (12110)-surface at $-1$ V set point voltage. Clear asymmetry between the occupied (negative bias) and the unoccupied (positive bias) LDOS is visible. The occupied part of the LDOS is characterized by a variety of fine structures, which are spatially and energetically
Figure 1. Topography of the twofold d–Al–Ni–Co (a) and Y–Al–Ni–Co (b) surfaces. (a) High-resolution STM image of the twofold d–Al–Ni–Co; window size: 25 × 25 nm², \( \Delta z = 268 \) pm, \( V_T = -0.5 \) V, \( I_T = 70 \) pA, recorded at 5 K. The prominent columnar structures are indicated by black arrows. Their quasiperiodic order is illustrated by colored boxes and labeled by Fibonacci segments. (b) High-resolution STM image of the Y–Al–Ni–Co (100)-surface; window size: 25 × 25 nm², \( \Delta z = 30 \) pm, \( V_T = -1.28 \) V, \( I_T = 1 \) nA, recorded at 5.2 K. The upper right insets present the FFT of the corresponding STM images.
Figure 2. Variation in the differential conductance spectra along the quasiperiodic direction of the d–Al–Ni–Co (12110)-surface (left panel) and along the pseudo-quasiperiodic direction (c-axis) of the (100) A-termination of the Y–Al–Ni–Co surface (right panel). (a) 18.7 $\times$ 2.27 nm$^2$ STM image of the twofold d–Al–Ni–Co (12110)-surface recorded at 5.4 K, $\Delta z = 0.11$ nm, sample bias ($U_S$) = 1 V, $I_T = 0.9$ nA. (e) 9.7 $\times$ 2.0 nm$^2$ STM image of the Y–Al–Ni–Co (100)-surface recorded at 5.7 K, $\Delta z = 42$ pm, $U_S = 1$ V, $I_T = 0.2$ nA. The spatially resolved maps of the background-subtracted differential conductance (b, c, f) are taken along the quasiperiodic direction or c-axis, respectively. The set point of (b) and (f) was $-1$ V, 0.9 nA and 0.2 nA, respectively, whereas for (c), +1 V, 0.9 nA. The color scale represents the difference between single and averaged spectra in %. (d, g) The averaged differential conductance spectra recorded on and between columns, as well as the total averaged spectrum, are shown.

localized. We found the spatial and energetic extent of this fine structure to be of the order of 0.5 nm and 0.18 V, respectively.

The large-intensity modulation along the quasiperiodic structure of the d$I$/d$V$ intensity maps correlates with the positions of the characteristic columnar surface structures in the
corresponding STM image (figure 2(a)). The dashed vertical lines indicate regions on the columns (A) and between the columns (B). For +1.0 V set point voltage, the high intensity is between the columns and the low intensity is on the columns. To analyze the magnitude of the dI/dV intensity modulation along the quasiperiodic direction, we have averaged the non-background-subtracted dI/dV spectra with +1 V set point: for dI/dV spectra recorded on and between the columnar surface structures. The respective areas between the columns are indicated by gray boxes at the bottom of figure 2(c). Figure 2(d) displays the averaged dI/dV spectrum on the columns (pink) and between the columns (gray), as well as the total averaged spectrum (blue) for comparison. All three dI/dV spectra almost coincide in the unoccupied DOS. This can be attributed to the constant current mode, which imposes that the integral of the spectra from 0 V to the set point voltage, which is +1.0 V here, must be constant. On the other hand, the integral over the occupied DOS of the dI/dV spectra exhibits a reduction of 31% for the averaged spectrum on the columns as compared to the one between the columns. This behavior shows that there is a systematic asymmetry in the shape of the parabolic pseudogap. This asymmetry resides in a higher relative occupied DOS between the columns as compared to on the columns.

When the sample bias is chosen to be −1.0 V, the integral over the occupied part of the dI/dV spectrum is constant. This leads to the contrast inversion observed between figures 2(b) and (c). For a −1.0 V sample bias, the unoccupied LDOS shows now the dominant intensity modulation along the quasiperiodic direction. Please note that in figure 2(b) a measurement artifact is present in the range of +0.8 to +1 V due to a signal overload of the lock-in amplifier input channel.

In comparison, figure 2(f) shows the local variation in the normalized dI/dV spectra along the c-axis (pseudo-quasiperiodic axis) of the A-termination of the Y–Al–Ni–Co (100)-surface. The very distinct dI/dV intensity modulation of the unoccupied states along the horizontal axis (c-axis) and the fine structure in the occupied DOS are again obvious. For the same bias set point (−1 V), a similar qualitative picture is observed to that in figure 2(b). But, in contrast to the d–Al–Ni–Co (12110)-surface, the high intensity in the unoccupied DOS is now located between the columnar structures, as indicated by the dashed lines A and B. The spatial modulation of the unoccupied DOS in the dI/dV spectra of about 24% extends slightly into the occupied DOS up to −0.25 V. Compared to the d–Al–Ni–Co surface, the fine structure features (from −0.25 to −1 V in figure 2(f)) show a similar spatial extent, but seem to be broadened in energy to typically 0.25 eV.

In the following, the variation of the dI/dV spectra along the periodic direction of the twofold d–Al–Ni–Co (12110)-surface is investigated. Figure 3(a) displays an STM image of the twofold d–Al–Ni–Co (12110)-surface, where the periodic direction is horizontally oriented. On this surface area, a grid of 2500 individual dI/dV spectra with a spacing of 0.075 nm along the periodic direction and 0.3 nm along the quasiperiodic direction has been recorded. Four lines, which are offset along the quasiperiodic direction, have been chosen to discuss the correlation of spectral features with topography. The arrow e in figure 3(a) indicates a column of 0.4 nm periodicity. At a vertical distance of L’S/L’, the same type of column labeled by the arrow d is found again. As discussed in [23], columns with a 0.8 nm periodicity are also present. Two such columns are indicated by the arrows c and b, again spaced by the L’S/L’ distance.

The spatially resolved background-subtracted dI/dV intensity maps taken along the 0.8 nm periodic columns are displayed in figures 3(b) and (c). The most apparent characteristic is the 0.8 nm modulation of the dI/dV intensity along the periodic (x-) axis within the full sample bias.
Figure 3. Correlation of peaks and pseudogaps of the differential conductance with topography. (a) 7.5 × 7.5 nm² STM image of the twofold d–Al–Ni–Co (12110)-surface recorded at 5.4 K, Δz = 0.10 nm, $U_S = -0.5$ V, $I_T = 0.1$ nA. Please note that the periodic direction of the surface lies along the horizontal and the quasiperiodic direction along the vertical direction. Two distinct types of columns are indicated: full line arrows, the columns with a 0.4 nm dominant bulk periodicity; and dashed line arrows, the 0.8 nm periodic columns. Both types are separated by an $L'S'L' = 3.95$ nm Fibonacci segment. Spatially resolved background-subtracted $dI/dV$ intensity maps along a 0.8 nm periodic (b and c) and a 0.4 nm periodic (d and e) columnar structure are presented. The location of the $dI/dV$ maps is indicated by arrows in the STM image in (a).

range. The $dI/dV$ map of figure 3(c) shows that the high intensity features in the positive sample bias range (unoccupied DOS) are in registry with topographic protrusions. On the other hand, within the negative sample bias range (occupied DOS), peaks at $-0.2$ and $-0.45$ V are shifted by 0.4 nm and appear at topographic depressions. The $dI/dV$ map recorded at the structurally equivalent line (b) shows a similar structure. Some differences are nevertheless present due to structural imperfections, which can be seen in the topographic image along line (b). The characteristic extent of the spectral features is about 0.1 eV in energy and the confinement along the periodic axis is about 0.45 nm, and therefore smaller than the 0.8 nm periodicity.

The comparison of the two 0.8 nm periodic lines indicates that equivalent columns, with regard to topography and position (characteristic spacing of L’S’L’), yield equivalent spectroscopic features in the LDOS. By comparing the differential conductance maps along the 0.4 nm periodic columns in figures 3(d) and (e), this observation is corroborated. The modulation of the $dI/dV$ intensity along the periodic axis shows now the same striped pattern, but exhibiting a periodicity of 0.4 nm. A characteristic confinement of spectral features in energy is about 50 meV and the spatial extent is of the order of 0.25 nm.

In the following, we extend our investigation of the connection of LDOS as measured by STS and topography to the related Y–Al–Ni–Co (100)-surface. We map the LDOS along the b-axis in order to allow a comparison with the measurements along the periodic axis of the d–Al–Ni–Co (12110)-surface.

The spectra shown in figure 4(b) have been recorded along the blue line in figure 3(a) with 0.1 nm lateral resolution and are displayed with background subtraction. As shown in figure 1(b), the surface structure of the A-termination is (2 × 1) reconstructed, which leads to

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Figure 4. Correlation of peaks and pseudogaps of the differential conductance with topography. (a) $4.7 \times 4.7$ nm$^2$ STM image of the A-termination of the Y–Al–Ni–Co (100)-surface recorded at 5.7 K, $\Delta z = 29.1$ pm, $U_S = -1$ V, $I_T = 0.2$ nA. The red rectangle indicates the unit cell of the $(2 \times 1)$ reconstruction, whereas in this representation the $b$-axis lies horizontally and the $c$-axis vertically. (b) Spatially resolved background-subtracted $dI/dV$ intensity map recorded along the blue line indicated in (a).

a 0.8 nm periodicity along the $b$-axis. The same 0.8 nm periodicity is observed in the $dI/dV$ intensity modulation in the occupied DOS, which is indicated by blue vertical lines. Here, a characteristic confinement of spectral features in energy is about 150 meV and the spatial extent is of the order of 0.45 nm. At three different energies (sample biases), we observe a modulation in agreement with topographic protrusions at $-0.17$, $-0.39$ and $-1$ V and one in agreement with topographic depressions at $-0.65$ V. Nevertheless, in comparison to the $dI/dV$ intensity maps recorded along the periodic direction of the twofold d–Al–Ni–Co (12110)-surface, the A-termination of the Y–Al–Ni–Co (100)-surface shows the 0.8 nm modulated $dI/dV$ intensity only in the occupied part of the DOS. In the unoccupied part of the DOS, we observe hardly any correlation to the 0.8 nm periodic topography features.
4. Discussion and conclusion

Although the structures of the d–Al–Ni–Co (12110)-surface and of the A-termination of the Y–Al–Ni–Co (100)-surface are different, some similarities are observed, such as the 0.4 or 0.8 nm periodicities, or the presence of characteristic columnar features along the periodic or \( b \)-axis [23, 24]. Likewise, the LDOS investigated by STS of these two surfaces reveals similar properties. The main feature of the \( dI/dV \) spectra for both surfaces is a pronounced pseudogap (see figures 2(d) and (g)). The appearance of this parabolic pseudogap is attributed either to the reduction in DOS at \( E_F \), which is characteristic of the Hume–Rothery stabilization mechanism [12, 13, 28–30], or to an orbital hybridization [27].

Single point \( dI/dV \) spectra originating from very local topographic positions show a significant fine structure (composed of small peaks and pseudogaps) observed as energy-dependent modulations on top of the large pseudogap (see figures 2(b), (c) and (f), figures 2(b–e) and figure 3(b)). These spectral features of the two surfaces are confined in energy to about 50–150 meV and in space to about 0.5 nm. Thus, our STS analysis of the (12110) d–Al–Ni–Co and the A-termination of the (100) Y–Al–Ni–Co supports the results obtained on the fivefold and twofold i-AlPdMn [17] surface, where the spectral features show an energy confinement between 30 and 50 meV and a spatial extent below 1 nm. In agreement with the findings of Widmer \textit{et al} [17], we interpret these local spectral features as a signature of a spiky local DOS. Likewise, we observe, as reported by Widmer \textit{et al} [17] for the i-AlPdMn system and as suggested in [31]–[35], that much of the essential fine structure of the spiky DOS is smeared out by averaging over small surface areas of a few tens of nm\(^2\) and approaches thus a smooth total DOS. This explains the absence of a spiky DOS in experiments applying surface integrating methods, such as ultraviolet photoemission spectroscopy (consider, for instance, [36]). These findings lead to the interpretation that the \( dI/dV \) spectra are composed of two contributions: (i) a large pseudogap and (ii) a superimposed modulation consisting of small peaks and pseudogaps that depend strongly on the local position at the surface.

The locally resolved \( dI/dV \) spectra along the quasiperiodic direction of the d–Al–Ni–Co (12110)-surface and along the \( c \)-axis of the Y–Al–Ni–Co (100)-surface show an intensity modulation of about 30%, which is in agreement with the topographic intensity variation as imaged by STM. This variation is the result of a distinct asymmetry with respect to \( E_F \) in the LDOS of the two systems. A specific location possesses either a higher relative intensity on the occupied part as compared to the unoccupied part of the LDOS or vice versa. In the case of the d–Al–Ni–Co (12110)-surface, we observe higher intensity in the occupied LDOS between the columnar structures. For the A-termination of the Y–Al–Ni–Co (100)-surface, the situation is the opposite.

The spatially resolved \( dI/dV \) spectra along the periodic direction for the d–Al–Ni–Co (12110)-surface and along the \( b \)-axis for the Y–Al–Ni–Co (100)-surface reveal a periodic fine structure in agreement with the STM topography. The localization of spectral features is very narrow and ranges from 0.25 to 0.45 nm, depending on the size of the corresponding topography features. Whereas the spectral intensity modulation in the case of the quasiperiodic and the \( c \)-axis direction of the two systems is extended to the full energy range, it is confined to distinct energies in the periodic and the \( b \)-axis direction. This means that, in both systems, the quasiperiodic and pseudo-quasiperiodic directions can be spectroscopically distinguished from the periodic one. Although this distinction is possible, it is not yet clear how this is connected to the asymmetry in the electrical resistivity [6, 7] or the friction coefficient [8].
Our STS investigations demonstrate that similar topographic locations reveal similar features in the LDOS. Furthermore, the spatial extent of the narrow spectral features is in the same range as the extent of topographic features that possess typical widths of about 0.45 nm. These results lead to the conclusion that the local electronic fine structure (modulation on the large pseudogap) depends on the atomic configuration of the specific measured site. Our findings mimic well the situation of ‘cluster virtual bound states’ described by T de Laissardière et al [22], where clusters of transition metals can trap electrons at some specific energies. These electronic states are considered as virtual bound states at the length scale of the clusters. As a consequence, these virtual bound states lead to a spiky structure in the DOS. Experimentally, we observe both the characteristics of ‘cluster virtual bound states’ by STS: the spatial localization of electronic states and hence the spiky features in the LDOS. However, the identification of the involved three-dimensional clusters or truncated clusters is hindered in the case of the d–Al–Ni–Co (12110)-surface by the fact that no sufficiently detailed model of the atomic surface structure is available. In the case of the Y–Al–Ni–Co (100)-surface, theoretical LDOS calculation should be possible in view of the fact that the atomic structure of the investigated A-termination has been resolved [24].

In conclusion, we find that the d–Al–Ni–Co (12110)- and the A-termination of the Y–Al–Ni–Co (100)-surface possess qualitatively a very similar LDOS structure that correlates with surface structures along the periodic (b-axis) as well as along the quasiperiodic (c-axis) direction. This correlation is not due to an STM topography-related measurement artifact, but indeed shows spatial anisotropies of the LDOS. Regardless of the presence of quasiperiodicity, the LDOS and its local extent of the two investigated surfaces are comparable to each other. This analogy, and especially the fact that specific electronic states are located on topographic features, indicate that the LDOS is affected much more by the complex local atomic arrangement on the scale of nearest neighbors than by a long-range ordered quasiperiodicity. Therefore, our experiments support the concept of cluster virtual bound states as suggested by T de Laissardière et al, at least for a part of the valence electrons. In this respect, the application of STS with sub-nanometer resolution can yield important new insights into the electronic structure of complex metallic alloys. We wish to stress, however, that progress in the interpretation of STS data on these systems will require a detailed understanding of the atomic surface structure as well as comparison to the spatial variation of the LDOS as obtained from appropriate DFT calculations.

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