Electronic structure and transport in a model approximant of the decagonal quasicrystal Al-Cu-Co

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The electronic structure and conductivity in a model approximant $Al_{66}Cu_{30}Co_{14}$ of decagonal quasicrystals Al-Cu-Co is presented theoretically. As in most quasicrystals and approximants, the density of states exhibits a well pronounced pseudogap at the Fermi level, commonly attributed to the Hume-Rothery phenomenon. From the local density of states and band dispersion, wave functions of eigenstates at the Fermi level are analyzed. They are very flat bands, located on a specific group of atoms, and of p-d symmetry. This suggests the importance of hybridization between transition metals and aluminum in quasicrystals. The intraband electronic conductivity at $T = 0$ K, calculated in Boltzmann theory, agrees quantitatively with experimental values. Its temperature dependence is also discussed. The strong anisotropy of decagonal phases has a crucial effect on all aspects of the electronic structure and then on transport properties and stability.

I. INTRODUCTION

The decagonal (d) quasicrystals form a new class of anisotropic materials with a crystalline axis perpendicular to a quasiperiodic plane with fivefold symmetry. This phase includes metastable (Al-Mn, Al-Fe, Al-Pd) and stable (Al-Cu-Co, Al-Ni-Co, Al-Pd-Mn) decagonal systems. Since the discovery of the first stable decagonal phase in Al-Cu-Co system[1] many experimental investigations have been performed to understand their structures. Now, several structural models have been proposed (for a review of models of d phase, see, for instance, Ref. 2), but the real atomic positions are not completely established.

Many quasicrystals are closely related to crystalline approximants with similar composition. For instance, the d-phase $Al_{70}Cu_{15}Co_{20}$ is stable at high temperatures and at reduced temperatures it transforms to microcrystalline structure composed of one or more approximants of large unit cells.[3,4] Local orders in quasicrystals are expected to be similar with those in their crystalline approximants.[5] This is the case for the d-phase Al-Cu-Co and the crystalline phases η-$Al_{13}Co_4$ (Ref. 6) and Al_5Co_2. Then the study of crystalline approximants can give useful results to understand the quasicrystalline properties in itself.

The origin of quasicrystalline stability, as well as the importance of phasons and other defects in it, is still an open question. Nevertheless real aluminum based quasicrystals are commonly considered as Hume-Rothery alloys.[7] They are stabilized when the number of conduction electrons per atom is such that the Fermi sphere touches the pseudo-Jones zone constructed by several principal peaks of diffraction pattern. Consequently, the density of states (DOS) exhibits a well pronounced valley, called pseudogap, in the vicinity of the Fermi energy E_F.[8–11] This pseudogap was observed experimentally.[12] The width of the pseudogap is 0.03–0.08 Ry.[10,11] Moreover, the electronic structure of icosahedral (i) approximants consists of a set of very spiky peaks of a width

of ≈ 0.001 Ry, called "*spiky structure*" which originates from long-range correlated cluster packing and the high symmetry of clusters.[10,11] This fine structure of the DOS, characteristic of quasicrystals, seems less important in stability but should be crucial for transport properties.[13]

The electrical transport properties have been studied intensively. For review articles, see Refs. 14 and 15. Very low conductivity, increasing conductivity with temperature, strong composition dependence of transport coefficients, anomalous Hall conductivity, thermoelectric power, diamagnetic susceptibility, and optical conductivity have been observed in the stable i phases Al-Mn-Si,[14] Al-Cu-Fe,[16] Al-Cu-Ru,[17] and Al-Pd-Mn.[18] Recently, a very low conductivity at low temperatures, much smaller than the minimum metallic Mott value, was reported in a stable i-Al-Pd-Re.[19] In particular, in the case of the d phase, transport properties of metastable Al-Mn (Ref. 20) are similar to those of the amorphous phase, and anisotropic transport has been measured in several stable phases. For d-Al-Ni-Co and d-Al-Cu-Co,[14,21,22] the ratio of the electrical conductivity along periodic and quasiperiodic directions ranges from 4 to 12. The conductivity along quasicrystalline directions increases with temperature as in the stable i phase. But the temperature dependence along the crystalline direction depends on the composition. Anisotropic behaviors are also found in thermal conductivity,[23] Hall conductivity,[24] and thermoelectric power[25] measurements.

The origin of the abnormal behaviors of perfectly ordered icosahedral and decagonal quasicrystals is still not clear. Experimentally, temperature and magnetic-field dependence of conductivity at low temperatures in i quasicrystals seems to be well described by quantum interference effects.[16,26,27] In the two-dimensional quasiperiodic lattice[28] the competition between localization and delocalization due to nonperiodicity and self-similarity of the lattice seems to lead to a new kind of wave functions, called critical states, as in a one-dimensional Fibonacci

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lattice.[29] Recently, Mayou *et al.*[30] proposed a new explanation of the temperature dependence of transport properties in terms of interband transitions. Theoretical calculations of transport properties[13] based on the calculated band structure show that the spiky structure of the density of states is very essential for absolute value of transport and its abnormal temperature and randomness dependence.

Despite several theoretical investigations,[8,31-33] the contribution and the importance of transition metals (TM's) in quasicrystalline properties are not completely understood. New experimental measurements[34,35] show the remarkable role of TM ions in quasicrystals in electrical conductivity and Hall effects. In *i*-Al-Cu-Fe and *i*-Al-Mn, it is known from soft-x-ray and photoelectron spectroscopic measurements[12] that d states of TM's are present at the Fermi level and are strongly hybridized with the sp states of Al. The Hume-Rothery pseudogap of the conduction band is also observed in d band. This is in good agreement with *ab initio* calculations performed in crystalline approximants[10,11] and Hume-Rothery alloys[32] containing TM's.

In this paper we present the calculated electronic structure and conductivity in a hypothetical approximant of d-Al-Cu-Co: $Al_{66}Cu_{30}Co_{14}$. Electronic structure of this approximant is calculated self-consistently by the linear-muffin-tin-orbital method in an atomic sphere approximation (LMTO-ASA).[36] Crystalline structure and the density of states of the studied approximant are presented in Secs. II and III. Then, from these results, we analyze the nature of the wave functions (Sec. IV) and the effect of anisotropy (Sec. V) in the decagonal quasicrystal. In Sec. VI, former considerations are used to discuss transport coefficients in approximant and decagonal phases.

II. STRUCTURE AND COMPUTATIONAL DETAILS

We study a hypothetical approximant $Al_{66}Cu_{30}Co_{14}$ of decagonal phase Al-Cu-Co. This crystal is an approximant[37] of the quasicrystalline structure proposed by Burkov for decagonal Al-TM's,[38] which was constructed on the basis of x-ray-diffraction and high-resolution electron-microscopy data.[6,39] The structure, shown in Fig. 1, can be viewed as a periodic approximant of a binary tiling decorated by large and small clusters centered on the odd and even vertices, respectively, of the binary tilling. In the original model by Burkov, the Cu atoms are treated as TM atoms, but during calculation Cu and Co sites have to be distinguished to get a stable self-consistent electronic structure (see Sec. III B). The space group of the approximate crystal is the face-centered-orthorhombic $Cc2m$. The centered face contains two pseudoquasiperiodic axes and is perpendicular to the pseudoperiodic axis. In the following, to simplify the notation, the pseudoquasiperiodic axes and pseudoperiodic axis will be respectively referred to as "quasiperiodic" axes and "periodic" axis. Each unit cell contains 110 atoms distributed among two equivalent layers perpendicular to the periodic axis. Lattice parameters of
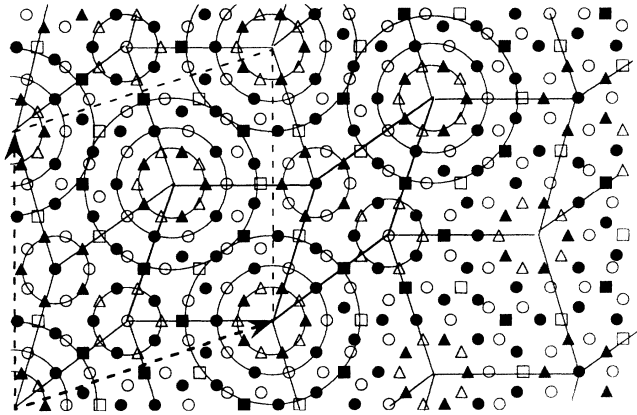

FIG. 1. Atomic structure of the model approximant $Al_{66}Cu_{30}Co_{14}$. The periodic axis is perpendicular to the figure. The dashed lines show the unit cell, two arrows show the vectors $(a+b)/2$ and $(a-b)/2$, where a and b are the basis vectors of the Bravais lattice (see text in Sec. II). In a unit cell, 110 atoms are distributed on two pseudoquasiperiodic layers: white atoms on $z = 0$, and black atoms on $z = c/2$. Circles are aluminum sites, triangles copper sites, and squares cobalt sites. The binary tiling is shown with lines. Larges clusters (three shells) and small clusters (one shell) are centered, respectively, at odd and even vertices of the tiling.

the orthorhombic lattice are $a = 31.8848$ Å, $b = 23.1656$ Å, and $c = 4.12328$ Å. There are two equivalent large clusters, two equivalent small clusters in a unit cell, and no glue atoms. A large cluster contains 40 atoms distributed on three shells: 10 Co atoms on the inner shell, 10 Al atoms on the middle shell, and 20 Al plus 14 Co atoms on the outer shell. A small cluster is a single shell of five Al and five Co atoms, centered by one Al atom.

Self-consistent calculations are performed using 45 **k** points in a 1/8 reduced Brillouin zone. The number of **k** points in the reduced Brillouin-Zone is chosen so that its increase does not change significantly the resulting electronic structure. For all kinds of atoms, Al, Cu, and Co, s, p, and d states are included during the self-consistent procedure. In a unit cell, there are two large vacancies V, located at the center of the large clusters. Only s and p states of these vacancies are included in the calculation. The radius of the overlapping atomic sphere is chosen to have a small charge transfer (less than 0.25 electrons per atomic sphere) and only small overlap between two spheres. For the calculation the radius Cu, Co, and V spheres are 1.40 Å, 1.35 Å, and 1.68 Å, respectively. The radius of most of the Al spheres is 1.55 Å, but we adopt atomic spheres of 1.40-Å radius for 10 Al atoms in a unit cell, which have one first neighbor atom of a distance shorter than the others.

III. DENSITY OF STATES

A. Total density of states

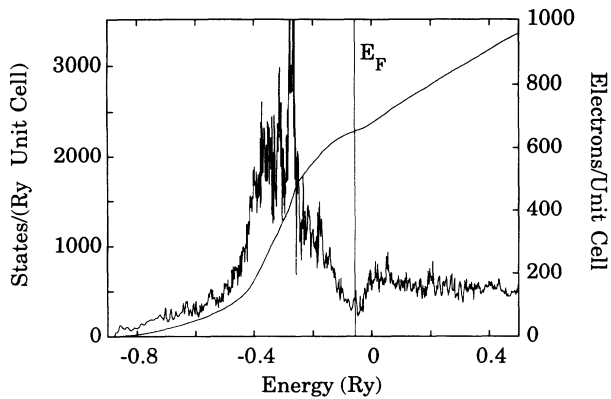The DOS in $Al_{66}Cu_{30}Co_{14}$ is shown in Fig. 2. At low energies (less than -0.5 Ry) the DOS is of the free elec-

FIG. 2. Total density of states (DOS) and integrated DOS in $Al_{66}Cu_{30}Co_{14}$. The Fermi energy E_F is indicated by a vertical line.

tron s band of Al. This is also confirmed from the energy dispersion curves $E(\mathbf{k})$. The main peak in DOS is a d peak of Cu and its right shoulder is a d peak of Co. The self-consistent Fermi energy E_F is -0.057 Ry, the d peak of Cu is located between -0.40 Ry and -0.23 Ry, and the d peak of Co between -0.25 Ry and -0.13 Ry. A large pseudogap is formed near the Fermi level. This pseudogap, commonly observed in several quasicrystals,[31] is due to the electron scattering by the Bragg planes of a pseudo-Jones zone constructed by the principal peaks of diffraction pattern.[40] This phenomenon, known as Hume-Rothery mechanism, stabilizes the quasicrystalline structure (see Sec. I).

B. Local density of states

The 110 atoms in a unit cell of the approximant are classified into 29 inequivalent types. These atomic types can be grouped into several kinds of *almost-equivalent* atoms, which have similar local DOS (LDOS). In the large clusters we find 2 vacancies V, 20 copper atoms Cu(L), 54 aluminum atoms Al(L), 14 cobalt atoms, 6 Co(La)atoms located between two large clusters, and 8 Co(Lb) atoms near small clusters, per unit cell. In the small clusters we find 12 aluminum atoms Al(S) and 10 copper atoms Cu(S) per unit cell. The LDOS's are rather different in large and small clusters, as presented in Ref. 40. Indeed, atomic orbitals are more strongly hybridized with each other in the large clusters than in the small clusters. The origin of this mixing is the high local symmetry or contacting arrangement in large clusters. Strong hybridizations could also exist between some Al(S) sp bands and Co(L) d bands or Cu(S) d bands. On the other hand, the main peak of LDOS in small clusters is located at lower energy than the main peak in LDOS in large clusters. These two points claim to consider small clusters as a kind of "glue clusters" stabilizing the network of large clusters.

Another important point is the crucial effect of transition metals (Co) on the DOS,[40] which makes us choose the present set of positions of Cu and Co atoms. Oth-

erwise, the system would be energetically unstable. In the present calculation of $Al_{66}Cu_{30}Co_{14}$ approximant we can easily distinguish two kinds of almost-equivalent Co, Co(La), and Co(Lb), with very different LDOS. That can be understood qualitatively with a simple model[32] developed to study nearly free electrons coupled with d impurity. The main result of this model is that both effects of sp electrons scattered by the lattice and sp-d hybridization lead to DOS depending on TM positions. In approximants of quasicrystal—and then in quasicrystals—containing transition metals, whereas the scattering of sp-electrons by the Bragg planes is important, such DOS and stability dependence on TM atomic position should be crucial.

IV. NATURE OF WAVE FUNCTIONS

In this section, we discuss in great detail the nature of the wave functions at the energies near the Fermi level. As we focus on the energy range in the vicinity of the Fermi level, s states of aluminum have no strong effects.

A. Strong p-d hybridization

The partial LDOS around E_F on different kinds of atoms in percentage of the total DOS are shown in Fig. 3. The LDOS on Al sites have essentially p symmetry and LDOS on Co sites have d symmetry. Furthermore, the rather large value of d LDOS on Al sites should be stressed. Al d LDOS at low energies and in the vicinity of E_F is not actually Al $3d$ electrons, but the d-symmetric tail of Al neighbors with overlapping atomic spheres. More details about the role of Al d states are given elsewhere.[41] Total DOS at the Fermi level is mainly $p(Al)$ 30%, $d(Co)$ 24% and $d(Al)$ 16%. Analysis of components of the wave functions around E_F shows that most of the wave functions are similar and result from strong hybridization between atomic orbitals in similar proportion of $p(Al)$, $d(Co)$, and $d(Al)$ to the total DOS. Together with this strongly hybridized character, the dis-
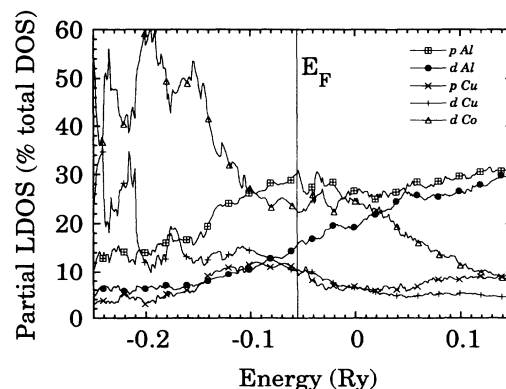

FIG. 3. Partial average local density of states (LDOS) on Al, Cu, and Co sites. Partial LDOS are given in percentage of the total DOS.
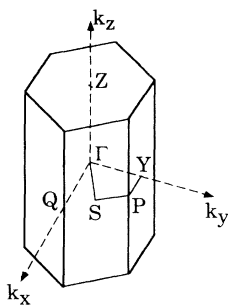
FIG. 4. First Brillouin zone of the $Al_{66}Cu_{30}Co_{14}$ structure. Periodic direction is k_z and quasiperiodic layers are parallel to the (k_x, k_y) plane.

tribution of the wave functions is extended only on several atomic sites; typically, 50% of a charge density of an eigenstate is located on about 25 atoms (Al and/or Co) in a unit cell, or even less atoms for a few states. Then the wave function in the vicinity of the Fermi level in $Al_{66}Cu_{30}Co_{14}$ is located on a specific group of atoms, with a p-d symmetry.

B. Band dispersion

Band dispersion along three symmetric lines of the first Brillouin zone (Fig. 4) of $Al_{66}Cu_{30}Co_{14}$ is presented in Fig. 5. Free-electron-band dispersion along the periodic direction in the same structure is also drawn for comparison [Fig. 5(c)]. The strong anisotropy between periodic (ΓZ) and quasiperiodic (ΓS and SP) directions will be discussed later, but we focus first on the nature of wave functions.

The parabolic free-electron bands [Fig. 5(c)] can be

grouped into three classes of bands, as shown in the figure. The bands of class A are associated with the reciprocal lattice points on the layer perpendicular to the periodic axis ΓZ and containing the Γ point. The bands of classes B and C are associated with layers perpendicular to the ΓZ axis containing the points Z (001) and (00$\bar{1}$), respectively.

In the LMTO band dispersion, the numbers of calculating k points are 6, 5, and 46 along the symmetric lines ΓS, SP [Fig. 5(a)], and ΓZ [Fig. 5(b)], respectively. The full lines, connecting calculated $(E(k), k)$ values, are chosen by numerating the bands, at every k point, from the lowest-energy band to the highest one, without considering the symmetry. It is possible to recognize on Fig. 5(b) some bands as one of three-band classes originated from free-electron bands. For instance, the points m_i delimit three examples of approximately parabolic bands that should correspond to nearly-free-electron bands as follows: A band (m_1, m_2), B band (m_2, m_3), and C band (m_4, m_5). These A-, B-, and C-self-consistent bands are free- (or nearly-free-) electron-like. However, they have a p-d symmetry, as we saw previously, and, furthermore, both in periodic and quasiperiodic directions, the width of the energy dispersion of A-, B-, and C-self-consistent bands is smaller than that of A-, B-, and C-free-electron bands. For example, an effective mass of A-self-consistent bands along the crystalline axis is more than twice that of the free-electron mass. Such a difference comes from the d-character of the self-consistent bands.

Considering the strong hybridization characterizing the wave functions near the Fermi level, we should say that most of the A-, B-, and C-like bands are hybridized with each other and split themselves into very flat bands. As a consequence, the band dispersion curves are very flat and hardly identified with A-, B-, and C-free- (or nearly-free-) electron-band types.
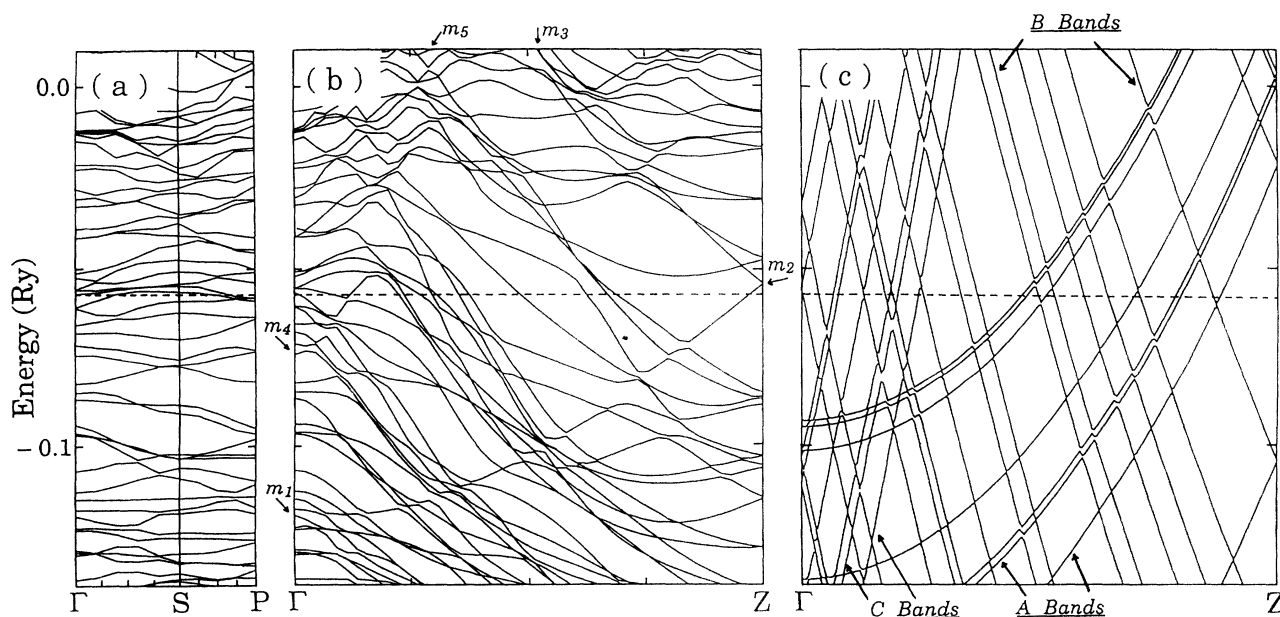

FIG. 5. Self-consistent band dispersion in $Al_{66}Cu_{30}Co_{14}$, $E(k)$ curves, along (a) the quasiperiodic directions ΓS and SP, and (b) along a periodic direction ΓZ. (c) shows the free electron bands in the same structure along the periodic direction ΓZ.

To summarize, considering $E(\mathbf{k})$ curves and partial DOS, a large number of eigenstates consists of a linear combination of A, B, and C bands. These eigenstates have p-d symmetry together with a small dispersion and are located on specific groups of atoms (about 25 atoms in the case of $Al_{66}Cu_{30}Co_{14}$).

C. Fermi surface

It is very interesting how the Fermi surface is in quasicrystals. Upon the Hume-Rothery point of view, the electrons near Fermi energy are strongly scattered by the Bragg planes of the pseudo-Jones zone. Stability is achieved when the Fermi surface touchs the pseudo-Jones zone. The resulting Fermi surface is very spherical with a hole at the center of the facet of the pseudo-Jones zone.[8] Experimental investigations from Hall effect measurements[24] seem to agree with this analysis.

From a self-consistent band structure we draw a section of the reduced Fermi surface in the first Brillouin zone of $Al_{66}Cu_{30}Co_{14}$ in Fig. 6. As for $E(\mathbf{k})$ curves, the points of the Fermi surface are actually calculated but curves linking them are just guided by eye. In the free electron case [see Fig. 5(c)], the equivalent figure consists of a set of arcs of circle with the same radius. Such arcs of circle can be found in the LMTO Fermi surface, for instance those drawn by full lines in Fig. 6. Many bands seem to be parallel to the k_x-k_y plane, but some points of the LMTO Fermi surface cannot be fitted by an arc of circle. This leads us to conclude that a number of bands are not free- (or nearly-free-) electron-like, such as the proposed ones drawn with a dashed line. A future study should be to investigate the shape of the Fermi surface of quasicrystals.

V. EFFECTS OF ANISOTROPY

The strong anisotropy of the decagonal structure has an important effect on electronic properties. This anisotropy is easily seen in the $E(\mathbf{k})$ curves (Fig. 5). Indeed, bands in the quasiperiodic directions (ΓS and
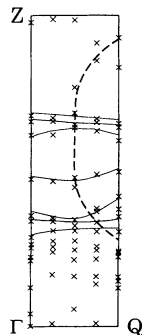

FIG. 6. Section of the Fermi surface of $Al_{66}Cu_{30}Co_{14}$, calculated from LMTO $E(\mathbf{k})$ curves, in the layers (Γ, Q, Z). Points are the calculated ones of the Fermi surface, and lines are guided by eye (see the text).

SP) have a very small dispersion compared to those in the periodic directions (ΓZ). In fact, the bands in the quasiperiodic direction are very much dispersionless and similar to those found in a two-dimensional Penrose lattice.[28] In the two-dimensional case, the very small band dispersion leads to a very spiky DOS. Furthermore, in an infinite periodic limit, the quasiperiodic lattice causes exotic energy spectrum and wave functions. But in the present case this spikiness of the DOS, which should result from the two dimensional quasiperiodic layer, is strongly attenuated or smeared by the effect of the periodic direction. Indeed, in periodic direction (ΓZ) the dispersion is very large as compared with the quasiperiodic directions (ΓS and SP), and the number of bands at the same energy is larger in quasiperiodic directions than in periodic direction. For instance, the Fermi level crosses over one band along the directions ΓS and SP, whereas it crosses over about 12 bands along ΓZ.

Usually decagonal quasicrystals Al-Cu-Co and Al-Ni-Co have two quasiperiodic layers in a periodic unit along the periodic axis, the c axis.[2] Then, the periodicity along c axis is about 4 Å. In other decagonal phases,[2] c periodicity can be 8 Å (d-Al-Co and d-Al-Ni), 12 Å (d-Al-Mn and d-Al-Pd-Mn), 16 Å (d-Al-Pd and d-Al-Cu-Fe), 24 Å and 36 Å, corresponding, respectively, to 4, 6, 8, 12, and 18 layers. Here it should be mentioned that icosahedral quasicrystals can be regarded as a special case of infinitely long c period. The most anisotropic case is two layers. In d-Al-Cu-Co and d-Al-Ni-Co, two layers seems necessary to be more stabilized to some extent. A possible preliminary explanation from the $E(\mathbf{k})$ curves of the approximant in d-Al-Cu-Co is as follows. Considering free-electron bands [Fig. 5(c)] along the periodic direction (for instance, along ΓZ, but it is also true along other periodic directions), bands of the C class are located in the vicinity of the quasiperiodic axis enclosing the Γ point near the Fermi level. So the density of bands is not uniform along periodic direction (for instance ΓZ). That comes directly from the presence of only two layers. In the cases of four layers or more, the C bands spread more uniformly along periodic directions because the number of C bands is proportional to the number of quasiperiodic layers in the periodic unit. The bands located near the Γ point at E_F contribute less to the DOS. As consequence of the nonuniform density of bands along the periodic direction in the two-layer case, compared with four or more-layer cases, a Hume-Rothery pseudogap near Z should be more easily open in the two-layer case than in other cases. Then, for some specific composition and structures, it seems possible for decagonal phases to be more stable with two layers in periodic direction than with four or more layers. This seems to be the case in d-Al-Cu-Co and d-Al-Ni-Co.

VI. TRANSPORT

A. Resistivity at $T = 0$ K

The transport coefficients are calculated in the Boltzmann theory from the LMTO self-consistent band struc-
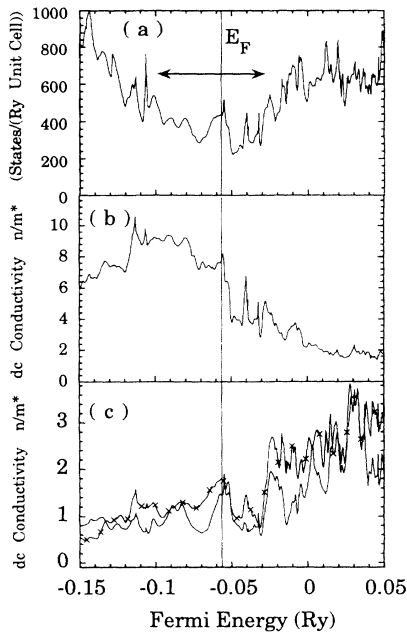
FIG. 7. (a) Total DOS in the vicinity of E_F. Resistivity [actually the value of (n/m^*)] at $T = 0$ K, calculated in Boltzmann theory from LMTO electronic structure; (b) shows resistivity ρ_p along periodic, and (c) shows resistivity ρ_{qp} along two quasiperiodic directions ΓQ ($\times$) and ΓY (no marks).

ture as in the previous work.[13] Figure 7 shows conductivity calculated in periodic and quasiperiodic directions as a function of the Fermi energy in a rigid-band scheme. In this figure the self-consistent Fermi level is shown by the vertical line. A small variation of atomic composition can shift the Fermi energy E_F and then sensitively the absolute values of transport coefficients. Unit of conductivity here is the effective (n/m^*), where n is the effective number of electrons per unit cell and m^* the effective mass. The intraband conductivity can be calculated by the formula, $\sigma = (n/m^*)\Omega\tau^{-1}$, where (n/m^*) is directly deduced from the self-consistent band structure (Fig. 7), Ω is the unit cell size of $Al_{66}Cu_{30}Co_{14}$, $\Omega = (abc)/2 = 1522.80$ Å^3, and τ is the scattering time. In quasicrystals, the notion of scattering time is not very clear. We do not claim to solve this question here but in the case of an approximant—especially the case of a relatively small approximant—the scattering time can be defined. Scattering time of pure crystalline Al is 6.5×10^{-14} s (at 77 K), a typical value for amorphous is 10^{-15} s, and analysis of conductivity at low temperatures in quasicrystals in terms of the quantum interference effect[27] gives a scattering time of 10^{-13} s in several icosahedral quasicrystals. For the approximant $Al_{66}Cu_{30}Co_{14}$ one can expect a scattering time between 10^{-15} and 10^{-13} s. Considering a scattering time of 10^{-14} s, the resistivity $(\rho = \sigma^{-1})$ along the periodic direction ρ_p and quasiperiodic directions ρ_{qp} are $\rho_p = 69$ $\mu\Omega$ cm and $\rho_{qp} = 340$ $\mu\Omega$ cm. These absolute values are comparable with experimental results.[14,21,22] For instance, Martin et al.[21] found, in d-$Al_{65}Cu_{15}Co_{20}$ phase, $\rho_p = 32$ $\mu\Omega$ cm and $\rho_{qp} = 341$ $\mu\Omega$ cm at very low

temperature. The theoretical ratio ρ_{qp}/ρ_p is 5, whereas experimental ratios fluctuated from 4 to 10 with composition and structural quality. The large difference between ρ_p and ρ_{qp} is mainly due to the small energy dispersions along the quasiperiodic directions compared with the periodic direction (see Sec. V).

It is interesting to remark how the shape of resistivity as a function of the Fermi energy can be understood by the analysis of the $E(\mathbf{k})$ curves (Fig. 5). Above -0.06 Ry, ρ_p decreases with the Fermi energy because bands along the periodic direction become more flat. Below -0.1 Ry, bands along the periodic direction are also more flat compared with bands around -0.06 Ry, and then ρ_p increases with Fermi energy. On the other hand, the increase of ρ_{qp} above -0.04 Ry is due to an increase of the number of bands, whereas their flatness does not change significantly. Below -0.04 Ry, ρ_{qp} is almost constant. Another important remark is the fact that the Hume-Rothery pseudogap (Sec. III A), shown with an arrow in Fig. 7, has no direct effect on conductivity along quasiperiodic and periodic directions.

B. Temperature-dependence of resistivity

Experimentally,[14,21,22] a large anisotropy has been found in temperature-dependent transport in decagonal quasicrystals. Along the periodic axis the resistivity ρ_p is metallic and increases with temperature over the entire temperature range. The behavior of ρ_p is qualitatively accounted for by the semiclassical Bloch-Gruneisen theory electron-phonon scattering in d-Al-Cu-Co and d-Al-Cu-Ni.[21] On the other hand, in most experimental results, the resistivity in quasiperiodic planes ρ_{qp} decreases with temperature, sometimes with a saturation at low temperature, and in few results ρ_{qp} increases with temperature. This behavior was interpreted in terms of phonon-assigned tunneling,[21] or in terms of multiphonon scattering.[22]

The energy difference between bands at the Fermi level is about 0.001 Ry along the ΓS and SP directions. Therefore, the temperature increase can easily smear out several different bands and electron transport on the quasiperiodic plane can be enhanced so this mechanism can be assisted by electron-electron inelastic scattering.

VII. CONCLUSION

In this paper, we presented the self-consistent electronic structure in an approximant of decagonal quasicrystals $Al_{66}Cu_{30}Co_{14}$. The atomic structure was proposed by Burkov for decagonal Al transition metal, and we have to distinguish Co and Cu sites to get a stable electronic structure.

The resulting electronic structure is characterized by two principal aspects. First a Hume-Rothery pseudogap, due to the diffraction of conduction electrons by the lattice, is created near the Fermi level. The correlation between atomic structure and electron valency per atom

stabilizes the alloys, but does not have an important effect on electrical conductivity. Second, wave functions of eigenstates at the Fermi energy result essentially from a strong mixing of Al p- and Co d-atomic orbitals. They have very flat energy dispersion and are located on a specific group of atoms. Such an unusual character of wave functions is essential to understand the abnormal transport properties observed in quasicrystals at $T = 0$ K and at finite temperatures.

Based upon the self-consistent band structure in $Al_{66}Cu_{30}Co_{14}$ and Boltzmann theory, the calculated intraband conductivity at $T = 0$ K is in good agreement with experiments. At finite temperatures, interband transition between flat bands separated by a few mRy should dominate the conductivity.

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