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Electronic structure and conductivity in a model approximant of the icosahedral quasicrystal Al-Cu-Fe

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We present the calculated self-consistent electronic structure and conductivity in a hypothetical model [1/1] approximant of the icosahedral phases Al-Cu-Fe. Two main features characterize the density of states. First, a well-pronounced pseudogap, commonly attributed to electron scattering by the lattice structure (the Hume-Rothery phenomenon), is found in the vicinity of the Fermi level. That pseudogap stabilizes the quasicrystalline structure but does not have a strong effect on the transport properties. Its width is about 0.035 Ry. Second, the density of states consists of a set of very fine spiked peaks. The width of each peak is about 0.001 Ry. The origin of this structure is the strong hybridization between atomic orbitals, due to the high local symmetry of quasicrystalline structure, and the variation in the height and width of the spikes is accentuated by the presence of the *d* states of the transition metals. Such a fine structure has little effect on the energetic stability but is crucial for the transport properties, both for their absolute values at 0 K and for their temperature dependence.

I. INTRODUCTION

Since the discovery of the qusicrystal in 1984 by Schechtman *et al.*,[1] the structural, thermodynamic, and transport properties of quasicrystals have been investigated thoroughly. The stability mechanism and quasicrystal growth are two of the most important subjects. Electronic structures and transport properties in quasicrystals are also another important subject for analysis.[2] Recent discoveries of stable quasicrystals of highly ordered structure has permitted experimental determination of the main aspects of the abnormal transport properties in the icosahedral phases of Al-Mn-Si,[3] Al-Cu-Fe,[4] Al-Cu-Ru,[5] Al-Pd-Mn,[6] and Al-Pd-Re,[7] and decagonal phases of Al-Cu-Co and Al-Ni-Co.[3,8,9] One of the most surprising properties is the very low conductivity at low temperature near the Mott minimum metallic value, or even much lower in Al-Pd-Re,[7] together with a weak density of states at the Fermi level and a small number of carriers.[4,10] Moreover, in the icosahedral case, the conductivity increases with temperature and structural disorder. This temperature dependence may be described at low temperatures by quantum interference effects.[11] The existence of critical states,[12,13] neither extended nor localized, may have a crucial influence on transport. In this scheme, a recent qualitative explanation of the temperature and randomness dependence of the abnormal conductivity was proposed in terms of interband transition processes.[14,15]

Recent experimental measurements[16,17] show the remarkable role of transition metals in the transport properties of quasicrystals, but in spite of several theoretical investigations[13,18–20] the effect of transition metals is not clearly understood.

Many stable quasicrystals are closely related to crystalline approximants with similar composition.[21,22] Moreover, the transport properties of some approximants, e.g., Al-Mn-Si and Al-Cu-Fe, are also similar to those of the corresponding quasicrystals. Thus theoretical investigations on approximant crystals can give interesting information on the properties of quasicrystals themselves.

In this paper, we will present the results of *ab initio* calculations of electronic structure and electronic conductivity in a crystalline model approximant of icosahedral Al-Cu-Fe. After comparison of these results with other approximants studied previously, we will try to discuss several aspects of electronic structure, stability, and transport properties which are characteristic of stable quasicrystalline alloys containing transition metals.

II. STRUCTURE AND COMPUTATIONAL DETAILS

The self-consistent electronic structure is calculated in a hypothetical model [1/1] approximant, corresponding to the approximate rational number 1/1 for the golden ratio, of the icosahedral quasicrystal Al-Cu-Fe, provided by Cokayne *et al.*[23] This structural model was constructed by simulated annealing to partition types of atoms among the distinct sites, and relaxation of the position of the atoms, using pair potentials.

This model approximant contains 128 atoms in a simple cubic cell ($P2_13$), its lattice parameter is 12.30 Å and its composition $Al_{80}Cu_{32}Fe_{15}$ The building block of this structure is the Bergman cluster (33 atoms) consisting of a central atom of Cu surrounded by a distorted icosahedral shell of nine Al and three Fe atoms and a distorted dodecahedral shell of 13 Cu and seven Al atoms. Each cluster is joined to six other clusters through a shared pair of Cu atoms. Each unit cell contains four clusters and 20 glue atoms: 16 Al and four Fe.

The electronic structure is calculated self-consistently by using the linear muffin-tin orbital method in the atomic sphere approximation (LMTO-ASA).[24] Orbitals up to angular momentum $l=2$ are used and the valence states are Al $3s,3p,3d$, Cu $4s,4p,3d$, and Fe $4s,4p,3d$. The distribution of atoms is homogeneous and the structure is compact so that no empty spheres are necessary to fill up the space within the atomic sphere approximation. The

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radius of atomic spheres are chosen to have the overlap between two atomic spheres less than 35% of the atomic sphere radius and the charge transfer in each atomic sphere is less than 0.2 electrons per atom. For the total density of states (DOS) calculation the energy mesh is 0.0001 Ry and for local DOS calculations 0.001 Ry. 35 **k** points in the irreducible zone are included during the self-consistent procedure. Further increase of the number of **k** points does not change the electronic structure significantly, especially the sharp peaks of the DOS.

III. DENSITY OF STATES

The total DOS and the integrated DOS are presented in Fig. 1. The tail of the band at low energy (less than -0.5 Ry) is mainly the nearly free electron s band of Al. At higher energy, three main peaks, named A, B, and C in Fig. 1, are distinguished. The peaks A and C are mainly from d electrons of Cu and Fe, respectively, and the peak B is mainly from p electrons of Al. The self-consistent Fermi level E_F is located just above the d peak of Fe at the energy -0.077 Ry. A pseudogap is observed in the vicinity of E_F; the width is about 0.035 Ry and the DOS at its minimum is 1.57 states/(Ry atom), i.e., about 30% of the pure aluminum value. This pseudogap, called the Hume-Rothery pseudogap,[25] originates from the strong diffraction of valence electrons by the lattice. Moreover, the DOS is very sharply peaked, and the width of one narrow peak is about 0.001 Ry. The sharp-peaked structure in the DOS is observed from -0.42 Ry to 0.04 Ry, which corresponds to the energy range where the d local DOS of copper and iron is large.

The general aspect of this DOS is similar to the DOS's of other icosahedral approximants previously studied: α-Al-Mn-Si,[26] R-Al-Cu-Li, and $Al_{13}Fe_4$.[27] In the case of the decagonal aproximant Al-Cu-Co,[28] the Hume-Rothery pseudogap is also found near the Fermi level, but the presence of a periodic direction smears out the sharp peaks of the DOS in quasiperiodic planes.

The model structure of $Al_{80}Cu_{32}Fe_{16}$ contains 14 inequivalent classes of atoms. Furthermore, some of these inequivalent atoms have similar atomic environment and local density of states. Thus we group them into several almost equivalent classes of atoms as follows: three kinds of almost equivalent aluminum atoms, 46 Al(i), 30 Al(d), and 16 Al(g) per unit cell, corresopnding to the Al in the icosahedral shell, the dodecahedral shell, and glue atoms, respectively; one kind of almost equivalent copper atoms, 32 Cu per unit cell; and two kinds of almost equivalent iron atoms, 12 Fe(i) in the icosahedral shell and four Fe(g) glue atoms per unit cell. The average partial s, p, and d local DOS's on almost equivalent atoms are presented in Figs. 2, 3, and 4, respectively.

If we do not take into account the sharp structure of the DOS, the s band at very low energy (less than -0.5 Ry) is the parabolic band of free electrons. Secondly, a very wide valley in the DOS is observed from -0.4 Ry to -0.04 Ry in the partial s DOS. The right-hand part of this valley, above E_F, is clearly due to the Hume-Rothery phenomenon of electron diffraction by the lattice, but the valley below E_F, which is not observed in p and d bands, results from a strong resonance effect between s states of Al and d states of Cu and Fe. This effect pushes down the s states of Al to lower energy, and then stabilizes the structure energetically. The Cu atoms, which have the d peak located at lower energy than the Fe atoms, have the predominant stabilizing effect. This may be related to the fact that the most stable highly ordered quasicrystals always contain Cu atoms. A similar resonance effect was also found in the crystalline phase ω-Al_7Cu_2Fe.[29] Experi-

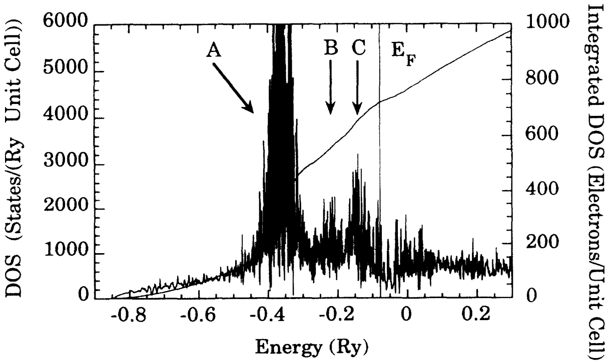

FIG. 1. Total density of states (DOS) and integrated density of states in the [1/1] icosahedral approximant $Al_{80}Cu_{32}Fe_{16}$. (For the DOS calculation the energy mesh is 0.0001 Ry.) The peaks A and C are mainly from d states of Cu and Fe, respectively, and the peak B is mainly from Al p states.

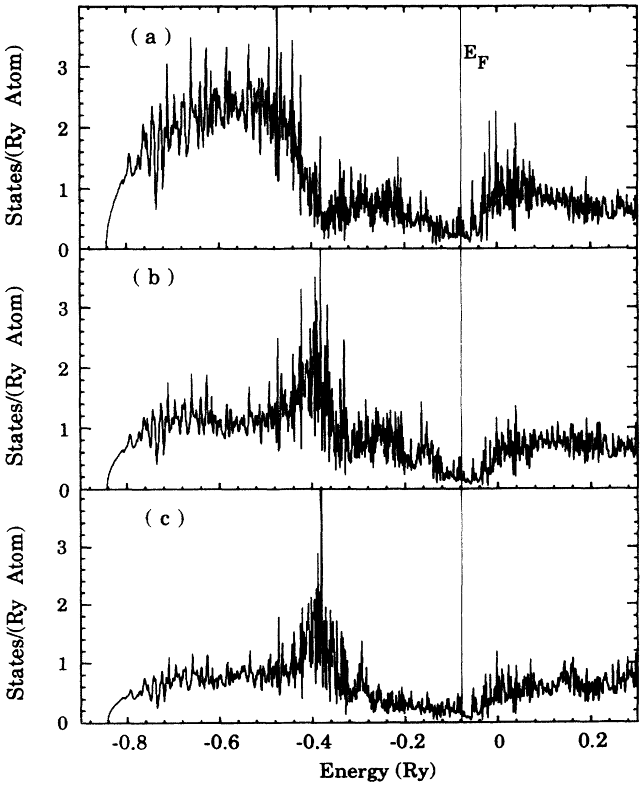

FIG. 2. Average partial s local density of states in the atomic spheres of (a) Al, (b) Cu, and (c) Fe sites. (For the DOS calculation the energy mesh is 0.001 Ry.)

mentally, the large pseudogap in the Al *s* band was observed by soft x-ray and photoelectron spectroscopic measurements in *i*-$Al_{63}Cu_{25}Fe_{12}$ and ω-Al_7Cu_2Fe.[30] Experimental results show that the resonance is more pronounced in quasicrystals than in crystals.

In the case of *p* bands (Fig. 3) we distinguish the three kinds of Al atoms mentioned above. The *p* peaks of Al(*i*) and Al(*d*) are located at about -0.23 Ry, and the *p* peak of Al(*g*), which is strongly hybridized with the *d* peak of Fe(*g*) [Fig. 4(d)], at about -0.16 Ry.

The *d* local DOS of Al [Fig. 4(a)] is not negligible. Nevertheless, the *d* band, from low energy to the vicinity of E_F, is not actually the 3*d* electrons of Al, but corresponds to the tail of the *d* band of Cu and Fe near neighbors of the Al.[31]

The two inequivalent iron atoms, Fe(*i*) and Fe(*g*), have very different *d* local DOS's [Figs. 4(c) and 4(d)]. That is correlated with their very different chemical environment. The nearest neighbor atoms of Fe(*i*) are four Cu and two Al; and the nearest neighbor atoms of Fe(*g*) are seven Al(*d*). As Fe(*i*) has few Al near neighbors, the Fe(*i*) *d* states are not strongly hybridized with Al states; nevertheless a small coupling is found with Al(*i*) *p* and also with Cu *p* local DOS's. The *d* band of Fe(*g*) has two main peaks: peaks 1 and 2 located at about -0.22 Ry and -0.16 Ry, respectively. The position of peak 2 is similar to the position of the Fe(*i*) peak and corresponds to the atomic level of Fe. This peak is observed in the Al(*g*) *p* band. The peak 1, which is easily found in the Al(*d*) *p* band, seems to come from a chemical bonding between Fe(*g*) *d* and Al(*d*) *p* states. Such a chemical bond does not exist in the Fe(*i*) electronic structure. This suggests the stabilizing effect of glue atoms, mainly Fe atoms. Such a stabilization effect of glue atoms has been observed al-

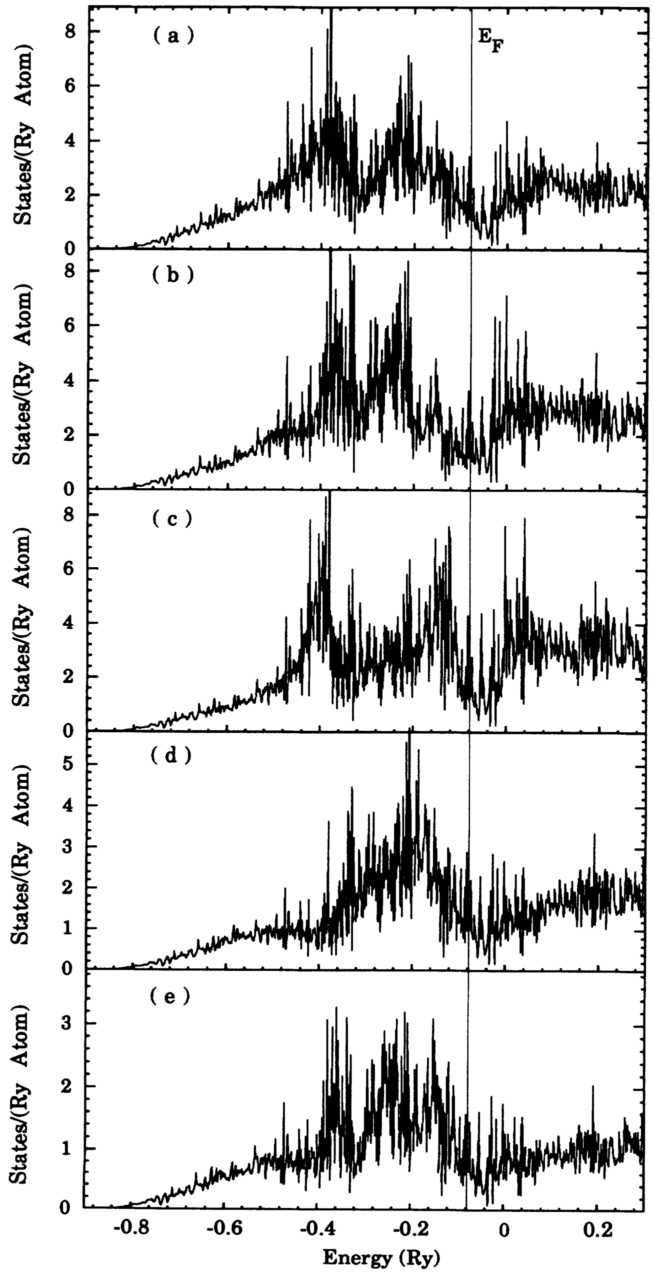

FIG. 3. Average partial *p* local density of states in the atomic spheres of (a) Al(*i*), (b) Al(*d*), (c) Al(*g*), (d) Cu, and (e) Fe sites. (For the DOS calculation the energy mesh is 0.001 Ry.)

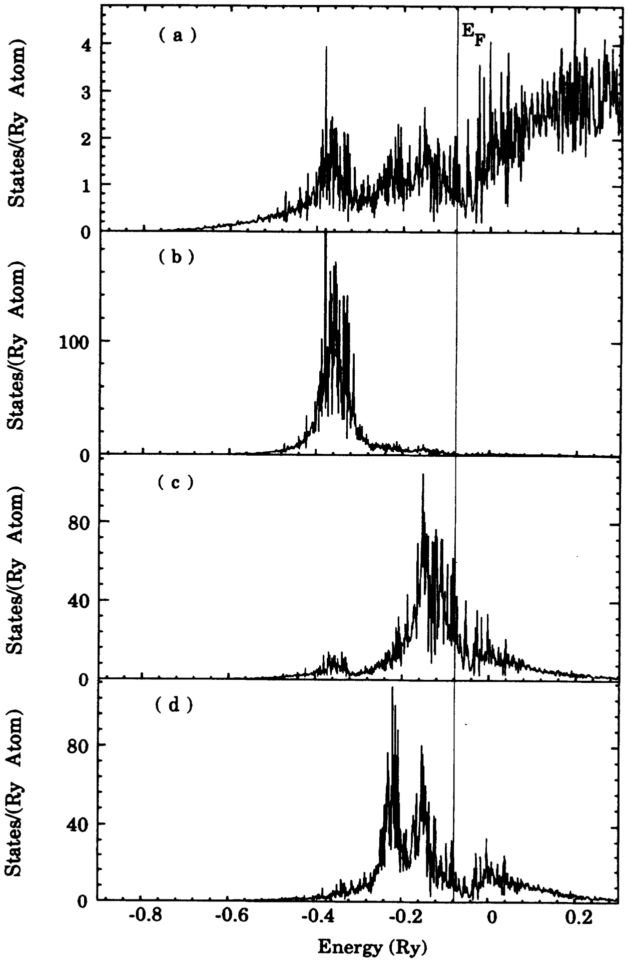

FIG. 4. Average partial *d* local density of states in the atomic spheres of (a) Al, (b) Cu, (c) Fe(*i*), and (d) Fe(*g*) sites. (For the DOS calculation the energy mesh is 0.001 Ry.)

ready in the approximants of icosahedral Al-Mn-Si (Ref. 26) and decagonal Al-Cu-Co (Ref. 28) quasicrystals. The values of the d local DOS of Fe(i) and Fe(g) at E_F are 20 states/(Ry atom) and 7.8 states/(Ry atom), respectively. The high value of the d local DOS on Fe located in the icosahedral shell suggests a possible local instability of Fe atoms at these positions in the present hypothetical approximant.

IV. BAND DISPERSION AND TRANSPORT PROPERTIES

The enlarged self-consistent bands [$E(\mathbf{k})$ curves] of the approximant $Al_{80}Cu_{32}Fe_{16}$ in the vicinity of E_F are shown in Fig. 5. Details of these bands as well as the exact position of the Fermi level depend strongly on the atomic structure and the chemical order, and may not be exactly the actual ones in real approximants. Moreover, the notion of $E(\mathbf{k})$ curves in quasicrystals, without translation periodicity, is meaningless. Meanwhile, several general aspects of the $E(\mathbf{k})$ curves in icosahedral approximants can be discussed from the present results. These aspects are similar to those found in the approximant α-Al-Mn.[32] As several approximants have transport properties comparable to high quality quasicrystals, we expected that the general aspects of $E(\mathbf{k})$ will give significant information on one-electron spectra in quasicrystals themselves.

The dispersion of $E(\mathbf{k})$ curves is very small, typically about 0.01 Ry or even less. That originates mainly from the large number of atoms in a unit cell and the strong hybridization between atomic orbitals discussed in the previous section. From analysis of the components of the wave functions, each band results from a strong coupling between atomic orbiatls, chiefly Fe d and Al p orbitals. As a consequence of this flatness of bands, the Fermi level crosses only a very small number of bands. Another important remark is that some bands are very close to each together at some specific $\mathbf{k}$ points or symmetric lines. The energy difference between the two nearest bands is often about 2 mRy ($\approx$300 K) at the same $\mathbf{k}$ point or even less bewteen different $\mathbf{k}$ points. That argues for the existence and importance of interband transitions in the transport properties of realistic quasicrystals.[14,15]

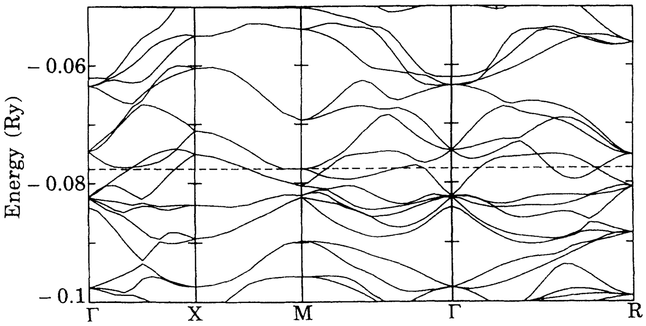

FIG. 5. Self-consistent band dispersion in $Al_{80}Cu_{32}Fe_{16}$ crystalline approximant. The horizontal dashed line shows the position of the self-consistent Fermi level E_F. The number of calculated $\mathbf{k}$ points along ΓX, XM, $M\Gamma$, and ΓR symmetric lines is 13, 7, 18, and 22, respectively. Full lines connecting these points are chosen by numbering band energies, at every $\mathbf{k}$ point, from the lowest to the highest band. Like this, some band crossings may be missed. But considering the present $E(\mathbf{k})$ curves, the number of undetermined crossings is rather small and does not change significantly the general aspect of the $E(\mathbf{k})$ curves.

The dc conductivity can be decomposed into intraband and interband conductivity as

$$\sigma=\sigma_{\text{intra}}+\sigma_{\text{inter}} . \tag{1}$$

These two terms have completely different absolute values ($T=0$ K), temperature dependence, and structural quality dependence.

At zero temperature, a transition between two bands should be very small. Using the self-consistent electronic structure and the Boltzmann theory the intraband contribution at $T=0$ K, σ^0_{intra}, is calculated. Computational details are given in Ref. 15. In these calculations an important term is the effective (n/m^*), where n is the effective number of electrons per unit cell at the Fermi energy and m^* the effective mass. The quantity (n/m^*), which is a function of the Fermi energy, is determined directly from the LMTO self-consistent calculation. The enlarged total DOS and the factor (n/m^*) are presented in Fig. 6. In the Boltzmann theory, the intraband dc conductivity at $T=0$ K is

$$\sigma^0_{\text{intra}}=(n/m^*)\Omega\tau^{-1} , \tag{2}$$

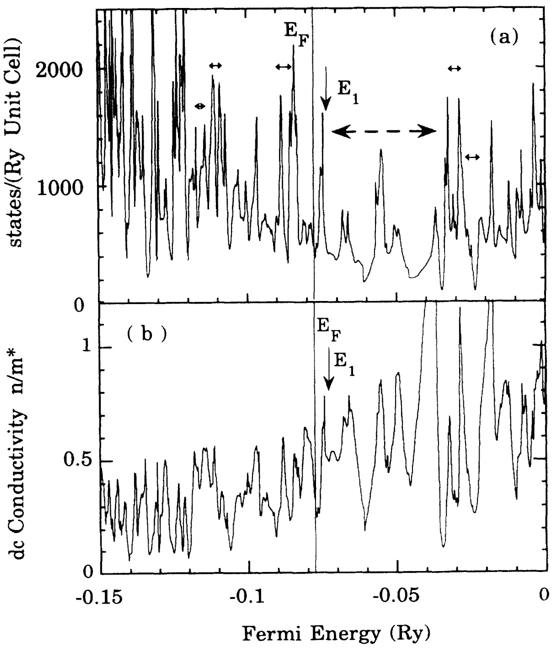

FIG. 6. (a) Total DOS in the vicinity of self-consistent Fermi energy E_F. The widths, indicated by a dashed horizontal double arrow and small horizontal double arrows, show approximately the position of the Hume-Rothery pseudogap and several small pseudogaps originating from the sharp-peaked structure, respectively. (For the DOS calculation the energy mesh is 0.0001 Ry.) (b) dc conductivity, actually the value (n/m^*) at $T=0$ K.

where Ω is the unit cell size of $Al_{80}Cu_{32}Co_{16}$, $\Omega = 1866.09$ Å^3, and τ is the average intraband scattering time. The parameter (n/m^*) as a function of Fermi energy fluctuates very rapidly between 0.2 and 0.6. Though the notion of scattering time in quasicrystals is not clear, it can be defined in quasicrystalline approximants. The exact value of the scattering time is still unknown but a reasonable value may be between 10^{-15} s (amorphous case) and 10^{-13} s.[11] Assuming a value of $\tau = 10^{-14}$ s, the intraband conductivity fluctuates between 300 and 1000 $\Omega^{-1}\,cm^{-1}$, without any simple correlation with the fluctuating DOS. For instance, the DOS's at E_F and E_1 (indicated in Fig. 6) are almost the same, but the conductivities are very different, $0.30(n/m^*)$ and $0.52(n/m^*)$, respectively. The reason for the small intraband conductivity is the small number density of electrons at the Fermi energy and the large value of the effective mass originating from the flatness of the bands.

In a rigid band scheme, a very small variation of atomic composition of the alloys may shift the position of the Fermi energy (from stability arguments the Fermi energy cannot be located on top of a sharp peak), and cause a strong deviation of the conductivity even if the density of states does not change significantly. Typically, the difference of the number of electrons between two nearest valleys in the DOS is of the order of one electron (for instance, the Fermi level shifts from E_F to E_1 by an addition of three electrons in a unit cell) and corresponds rougly to a variation of the atomic composition of the order of several percent or less.

At finite temperatures, both intraband $\sigma_{\mathrm{intra}}(T)$ and interband $\sigma_{\mathrm{inter}}(T)$ transitions are possible. In the case of crystals, especially crystals with a small unit cell, the interband transition is neglected at low temperatures. Nevertheless, in quasicrystals or approximants of large unit cells, the distance between two bands in reciprocal space (Fig. 5) is often very small and interband transitions are possible even at very low temperature. Thus, $\sigma_{\mathrm{inter}}(T)$ should dominate the temperature dependence and the structural quality dependence of the transport properties.[14,15] As a consequence, the sharp-peaked structure should smear out and the conductivity increase with increase of temperature or structural disorder.

It should be mentioned that the nonsmooth abnormal DOS could be the limit, in infinite periodicity, of the sharp-peaked structure of the DOS in crystalline approximants. Actually, if the approximant structure is chemically disordered, the electronic bands would be folded infinite times and still the crossed bands would be repulsively separated due to hybridization effects, forming flat and dispersionless bands. As already discussed in previous papers[15,28] the extent of the eigenfunctions near the Fermi energy is not homogeneous but selectivity chooses specific atomic sites, which may be a generalization of the critical wave function in low-dimensional cases. Therefore we expect that the infinitesimally small conductivity may be generic in chemically ordered perfect quasicrystals. As a matter of fact, both the crystalline approximants and actual quasicrystals contain several kinds of disorder, e.g., random phason and chemical disorder. Our understanding above is not complete, and even in the finite crystalline approximants the scattering time should be clarified more from a basic viewpoint.

V. DISCUSSION AND CONCLUSION

The total density of states of the studied approximant is similar to those calculated previously (α-Al-Mn, Al-Li-Cu, Al-Fe) and is characterized by two main features: a Hume-Rothery pseudogap and a sharp-peaked structure, associated respectively with two very different kinds of valleys in the DOS. The well-pronounced Hume-Rothery pseudogap is commonly attributed to strong conduction electron scattering by the lattice structure.[18,27,33] Its width is about 0.05 Ry, and the DOS at the minimum of this pseudogap can go down to 30% of the pure aluminum value. Hume-Rothery alloys are alloys with small differences of electronegativities and radii between constituents, and thus the band energy has a crucial effect on their stability. In these alloys, the electronic energy is minimized when the Fermi surface just touches a pseudo-Jones-zone constructed by the Bragg planes created by the main peaks of the diffraction pattern. This correlation between the atomic structure and the conduction electron density is summarized by the equation

$$k_F \simeq K_p/2 \ , \tag{3}$$

where k_F is the Fermi momentum and K_p the reciprocal vector of the main peaks in the diffraction pattern. On the DOS curve, the Fermi level is thus located in the vicinity of the minimum of the Hume-Rothery pseudogap. In a simple rigid band model, a small variation of the electron per atom ratio (e/a) shifts the position of E_F in the Hume-Rothery pseudogap, the DOS at the Fermi level, and the electrical conductivity at $T = 0$ K. This results in a simple correlation between conductivity at $T = 0$ K and the factor (e/a). This phenomenon has often been observed experimentally, for instance, in the case of Al-Mg-Zn and Ga-Mg-Zn alloys,[34] but it is not observed in a small composition range in *i*-Al-Cu-Fe quasicrystals.[17] Finally, the effect of the Hume-Rothery pseudogap on the temperature-dependent conductivity should be rather small, because the temperature characteristic of the pseudogap is very large (several thousand kelvin).

The other important feature of the DOS is the very fine sharp-peaked structure. Its energy range is about 0.001 Ry. This structure is associated with a large number of nondegenerate flatbands in quasicrystals. Flatbands were also observed numerically in several approximants of icosahedral and decagonal quasicrystals. They originate from the strong hybridization between atomic orbitals, due to the long-range correlated cluster packing and the high local symmetry of the quasicrystalline structure. Moreover, the presence of transition metal atoms, which increases the density of the bands, accentuates the structure of the DOS. The energy associated with the sharp-peaked structure is difficult to evaluate but it should be rather small compared to other energetically significant effects such as the Hume-Rothery phenomenon and resonance between the *s* states of Al and the *d* states of Cu and Co. The presence of the sharp-peaked structure can explain the very low intraband conductivity (at $T=0$ K). When this structure is important, namely, in icosahedral quasicrystals containing transition metals, its effect on transport properties should be stronger than the effect of the Hume-Rothery pseudogap and little simple correlation between the conductivity and the structural factor (e/a) is expected, as was observed in *i*-Al-Cu-Fe.[17] Moreover, by considering interband transitions at finite temperature, the temperature and structural quality dependence of the conductivity can be described qualitatively.

Finally, it is important to stress the crucial role of Cu and transition metals (Fe in the present case) on electronic structure. Several effects of Cu and transition metals are observed on stability. First, a strong resonance between the *d* bands of Cu and Fe and the *s* band of Al pushes down the Al *s* band and stabilizes the structure. This phenomenon does not depend directly on the position of Cu and transition metal atoms. On the other hand, the DOS at the Fermi level is mainly the *d* local DOS of transition metals. For instance, the *d* local DOS's of the transition metal in $Al_{80}Cu_{32}Fe_{16}$, α-Al-Mn, and $Al_{66}Cu_{30}Co_{14}$ are 51%, 50%, and 24% of the total DOS, respectively. Moreover, the shape of the transition metal *d* local DOS, especially the shape of the sharp-peaked structure, depends strongly on the positions of the transition metal atoms. As a consequence, some local instability may occur (becuase of the high *d* local DOS of the transition metal at E_F) and transport properties should depend strongly on the position of the transition metal stoms.

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[1] D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 2477 (1984).

[2] S. J. Poon, Adv. Phys. **41**, 303 (1992).

[3] K. Kimura and S. Takeuchi, in *Quasicrystal: The State of the Art*, edited by D. P. DiVincenzo and P. J. Steinhardt (World Scientific, Singapore, 1991), p. 313.

[4] T. Klein, C. Berger, D. Mayou, and F. Cyrot-Lackmann, Phys. Rev. Lett. **66**, 2907 (1991).

[5] B. D. Biggs, S. J. Poon, and N. R. Munirathnam, Phys. Rev. Lett. **65**, 2700 (1990).

[6] P. Lanco, T. Klein, C. Berger, F. Cryot-Lackmann, G. Fourcaudot, and A. Sulpice, Europhys. Lett. **18**, 227 (1992).

[7] H. Akiyama, Y. Honda, T. Hashimoto, K. Edagawa, and S. Takeuchi, Jpn. J. Appl. Phys. **32**, L1003 (1993); F. S. Pierce, S. J. Poen, and Q. Cuo, Science **261**, 737 (1993); C. Berger, T. Grenet, P. Lindqvist, P. Lanco, J. C. Grieco, G. Fourcaudot, and F. Cyrot-Lackmann, Solid State Commun. **87**, 977 (1993).

[8] S. Martin, A. F. Hebard, A. R. Kortan, and F. A. Thiel, Phys. Rev. Lett. **67**, 719 (1991).

[9] W. Yun-ping and Z. Dian-lin (unpublished; W. Yun-ping, L. Li, and Z. Dian-lin, J. Non-Cryst. Solids **153&154**, 361 (1993).

[10] E. Belin and A. Traverse, J. Phys. Condens. Matter. **3**, 2157 (1991); M. Mori, S. Matsuo, T, Ishimasa, T. Matsuura, K. Kamiya, H. Inokuchi, and T. Matsukawa, *ibid.* **3**, 767 (1991).

[11] T. Klein, H. Rakoto, C. Berger, G. Fourcaudot, and F. Cyrot-Lackmann, Phys. Rev. B **45**, 2049 (1992); A. Sahnoune, J. O. Ström-Olsen, and A. Zaluska, *ibid.* **46**, 10 629 (1992).

[12] H. Tsunetsugu, T. Fujiwara, K. Ueda, and T. Tokihiro, J. Phys. Soc. Jpn. **55**, 1420 (1986).

[13] T. Fujiwara and H. Tsunetsugu, in *Quasicrystal: The State of the Art* (Ref. 3), p. 343.

[14] D. Mayou, C. Berger, F. Cyrot-Lackmann, T. Klein, and P. Lanco, Phys. Rev. Lett. **70**, 3915 (1993).

[15] T. Fujiwara, S. Yamamoto, and G. Tambly de Laissardière, Phys. Rev. Lett. **71**, 4166 (1993).

[16] F. S. Pierce, P. A. Bancel, B. D. Biggs, Q. Guo, and S. J. Poon, Phys. Rev. B **47**, 5670 (1993).

[17] P. Lindqvist, C. Berger, T. Klein, P. Lanco, and F. Cyrot-Lackmann, Phys. Rev. B **48**, 630 (1993).

[18] J. Friedel, Helv. Phys. Acta **61**, 538 (1988).

[19] G. Trambly de Laissardière, D. Mayou, and D. Nguyen Manh, Europhys. Lett. **21**, 25 (1993); D. Mayou, F. Cyrot-Lackmann, G. Trambly de Laissardière, and T. Klein, J. Non-Cryst. Solids **153&154**, 412 (1993).

[20] L. Do Phuong, D. Nguyen Manh, and A. Pasturel, Phy. Rev. Lett. **71**, 372 (1993).

[21] F. Spaepen, L. C. Chen, S. Ebalard, and W. Ohashi, in *Proceedings of the Anniversary Adriatico Research Conference on Quasicrsytals*, edited by M. V. Jarić and S. Lundqvist (World Scientific, 1989), p. 1.

[22] P. Launois, M. Audier, F. Dénoyer, C. Dong, J. M. Dubois, and M. Lambert, Europhys. Lett. B **13**, 629 (1990); K. Hiraga, W. Sun, F. J. Lincoln, M. Kaneko, and Y. Matsuo, Jpn. J. Appl. Phys. **30**, 2028 (1991).

[23] E. Cokayne, R. Phillips, X. B. Kan, S. C. Moss, J. L. Robertson, T. Ishimasa, and M. Mori, J. Non-Cryst. Solids **153&154**, 140 (1993).

[24] O. K. Andersen, Phys. Rev. B **12**, 3060 (1975).

[25] W. Hume-Rothery and G. V. Raynor, *The Structure of Metals and Alloys* (Institute of Metals, London, 1954).

[26] T. Fujiwara, Phys. Rev. B **40**, 942 (1989).

[27] T. Fujiwara and T. Yokokawa, Phys. Rev. Lett. **66**, 333 (1991).

[28] G. Trambly de Laissardière and T. Fujiwara (unpublished).

[29] G. Trambly de Laissardière, D. Nguyen Manh, and D. Mayou (unpublished).

[30] E. Belin and D. Mayou, Phys. Scr. **T49**, 356 (1993).
[31] T. Fujiwara, G. Trambly de Laissardière, and S. Yamamoto, Mater. Sci. Eng. A **179/180**, 118 (1994).
[32] T. Fujiwara (unpublished).
[33] A. P. Smith and N. W. Ashcroft, Phys. Rev. Lett. **59**, 1365 (1987).
[34] J. L. Wagner, B. D. Biggs, and S. J. Poon, Phys. Rev. Lett. **65**, 203 (1990).