Electron Localization and Conduction Mechanism of Icosahedral Quasicrystal Al-Pd-Ru

Y.Sekiyama and I.Kanazawa

Department of Physics, Tokyo Gakugei University, Tokyo 184-8501, Japan

Kanazawa@u-gakugei.ac.jp

Abstract. We have argued the temperature dependence of conductivities of the icosahedral Al-Pd-Ru quasicrystals from the standpoint of the quasicrystal-like system with sp-d hybridization, using the thermal Green's function technique.

1. Introduction

A variety of Al-based quasicrystals shows unusual electronic properties which seem to be different from those of metals and semiconductors.

One of the most anomalous properties of Al-based quasicrystals is a very low electrical conductivity close to the metal-insulator transition [1,2]. However, there is no evidence for a gap as in semiconductors, and the structure is highly ordered, although it is nonperiodic. These are unlike Anderson insulators, where disorder is the reason for a localization of electronic wave function.

It has been suggested that the anomalous conductivity of Al-based quasicrystals is due to the combination of a Hume-Rothery pseudogap and the presence of localized states at the Fermi level [3].

It has been proposed that the unusual transport properties of Al-based quasicrystals might be much related to hopping processes between wave functions localized inside atomic clusters [4,5].

Especially Trambly de Laissardiere et al. [5] argued the creation of virtual bond states due to an icosahedral cluster of transition metal (TM) atoms and an icosahedral cluster of the TM clusters. In addition, in views of the ab initio calculations [6,7], Tamura et al. [8] have suggested strongly the creation of the virtual bond states or confinement of electrons, in the icosahedral clusters of TM atoms.

Kanazawa and coworkers [9-16] have considered the transport property in the randomly distributed system of the cluster composed of correlated N number of configurations such as the prolate and oblate rhombohedra, in which the nearest distance between each configuration is $\sim 2\pi/2k_F$ (the quasicrystal-like state). The quasicrystal-like state is regarded as the system composed of the Gaussian correlated distribution of the icosahedral cluster such as the Bergman type and the Mackay type, which include $2k_F$-phase shift scattering.

Taking into account the mean free path 15~20Å of electrons in quasicrystals, it looks like that the anomalous transport properties of quasicrystals are not directly related to quasicrystal structure in the longer range than the mean free path 15~20Å. Thus the transport property in the quasicrystal-like system might be closely analogous to one in the quasicrystal.

Tamura et al. [17] have measured the temperature dependence of the resistivity of the icosahedral Al-Pd-Ru quasicrystals, and 1/0 and 2/1 cubic approximant phases.

In this study, we have analyzed the temperature dependence of the conductivities of the icosahedral Al-Pd-Ru quasicrystals from the standpoint of the quasicrystal-like system, using the thermal Green's function technique, and taking into account the sp-d hybridization.

2. A model system and electrical conductivities in Al-Pd-Ru quasicrystals

In the quasicrystal-like system, we shall consider the effect of the $2k_F$-phase shift scattering by the randomly distributed icosahedral cluster composed of correlated N number of configuration such as the prolate and oblate rhombohedra, in which the nearest distance between each configuration is $\sim 2\pi/2k_F$, in the Feynman graph with thermal Green's function technique.

It has been proposed that the sp-d hybridization plays an important role in the transport property of quasicrystals [18,19].

The $2k_F$-phase shift scattering induces a strong density wave of sp electrons with wavelength $\sim 2\pi/2k_F$.

When the high density region of the standing wave of sp electrons is located on the transition metal atoms, the sp electrons hybrize more strongly the d orbitals of transition metal atoms. Thus $2k_F$-phase shift scattering and the sp-d hybridization are much correlated to each other. In this case, the value γ, which is defined as $1/[2\pi\rho\tau]$, becomes large. Note that $\gamma \propto n_i N |V_{d,sp}|^2$. Here ρ is the density of state per spin at the Fermi energy and τ is the life time of the sp electron wave due to the sp-d hybridization et al. The matrix element $V_{d,sp}$ represents the sp-d hybridization, and n_i is the density of the icosahedral cluster, which is composed of N number of configurations such as the prolate and oblate rhombohedra, connection by distance $\sim 2\pi/2k_F$. This icosahedral cluster might be identified with one such as Bergman type and the Mackay type [20-22]. N depends on the kind of materials. When many defects are introduced in the system, the icosahedral cluster, which is composed of correlated N number of configurations connected with the distance $\sim 2\pi/2k_F$, is broken. As a result, the value of γ will decrease remarkable and the resistivity of the system decreases.

Performing an average over the position of the icosahedral cluster, we assume the potential of the icosahedral cluster as a random quantity having a Gaussian δ-correlated distribution,

$$\langle V(r)V(r')\rangle = \frac{n_i N |V_{d,sp}|^2}{2\pi\rho}\delta(r-r')$$

Where $V(r)$ is the effective potential of the clusters, and ρ is the state density per spin at the Fermi energy. The propagator $\Gamma(q,\omega_l)$ of the $2k_F$-phase shift scattering with the sp-d hybridization can be introduced as

$$\Gamma(q,\omega_l) \sim \frac{\gamma}{1-\gamma\Pi(q,\omega_l)}\ , \tag{1}$$

where, ω_l is $2\pi lT$. l is an integer. $\gamma = \frac{n_i N |V_{d,sp}|^2}{V_s}$. V_s is volume of the system.

The thermal Green's function $D(k,\varepsilon_n)$ ($\varepsilon_n = (2n+1)\pi T, T$ is the temperature) is given by

$$D(k,\varepsilon_n) = \left[i\varepsilon_n - \xi_k + \frac{i}{2\tau}\mathrm{sgn}\varepsilon_n\right]^{-1}\ , \tag{2}$$

$$\frac{1}{\tau} \sim 2\pi\rho\gamma$$

where $\xi_k = k^2/2m - E_F$.

$\prod(q,\omega_l)$ is represented as

$$\prod(q,\omega_l) = \sum_k D(k+q-2k_F, \varepsilon_n+\omega_l)D(k,\varepsilon_n)$$

$$\sim \rho\int_{-\infty}^{\infty} d\xi \int d\,\Omega \left[i\varepsilon_n + i\omega_l - \xi - vq + \frac{i}{2\tau}\mathrm{sgn}(\varepsilon_n+\omega_l)\right]^{-1}$$

$$\times \left[i\varepsilon_n - \xi + \frac{i}{2\tau}\mathrm{sgn}(\varepsilon_n) \right]^{-1} , \tag{3}$$

where $\xi_{-k} = \xi_k$ and $v \equiv k/m$, and k_F is the vector of the Fermi momentum.

The integration over $d\Omega$ is over angle of v. If $\varepsilon_n(\varepsilon_n + \omega_l) < 0$, $\Pi(q, \omega_l)$ is evaluated for small q and ω_l as

$$\prod(q, \omega_l) \sim 2\pi\rho\tau[1 - Dq^2\tau - |\omega_l|\tau] , \tag{4}$$

where $D = v_F^2\tau/d$ is the diffusion constant. v_F and d are Fermi velocity and dimensions of system, respectively. Thus, $\Gamma(q, \omega_l)$ is represented as

$$\Gamma(q, \omega_l) = \frac{1}{2\pi\rho\tau^2[Dq^2 + |\omega_l|]} . \tag{5}$$

By using $\Gamma(q, \omega_l)$, the replacement $\omega_l \to i\omega$, and the Green's functions $D_\pm(k)$ we can estimate the conductivity approximately in $d = 3$,

$$\Delta\sigma(\omega) = \frac{e^2}{\pi} \sum_k \sum_{k'} (\hbar/m)^2 k_x k'_x \, D_+(k) D_-(k) D_+(k') D_-(k') \Gamma(k + k' = q, -i\omega) . \tag{6}$$

$$\propto \frac{e^2}{\hbar^2} \sqrt{\frac{\Gamma}{D}} T. \tag{7}$$

This shows T-liner effect for the conductivity.

We shall analyze the conductivity of Al-Pd-Ru quasicrystals of Tamura et al. [17] in order to discuss the effect of the electron localization in the quasicrystal-like system.

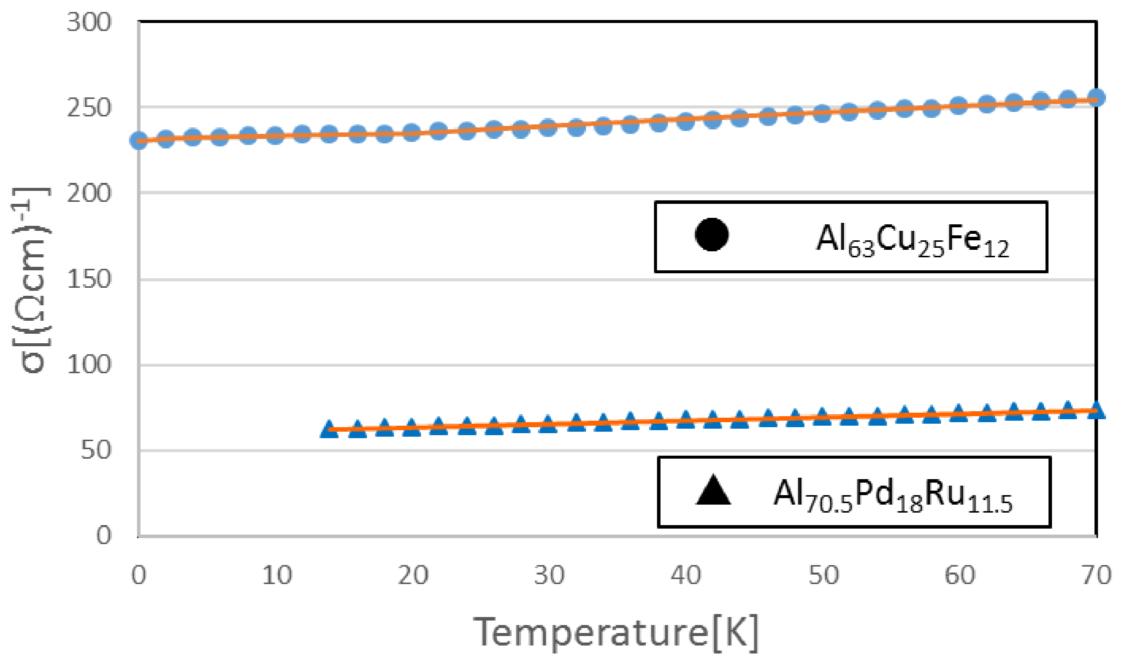

Figure 1. Solid triangles represent data of conductivities of $Al_{70.5}Pd_{18}Ru_{11.5}$ quasicrystal [17]. Solid circles represent data of conductivities of $Al_{63}Cu_{25}Fe_{12}$ quasicrystal [23]. Solid lines show fitted ones.

Figure 1 shows the conductivity for the $Al_{70.5}Pd_{18}Ru_{11.5}$ quasicrystal.

Each data point is represented by the solid triangle [17]. The solid line shows the fit. For comparison, experimental data and fitting of the $Al_{63}Cu_{25}Fe_{12}$ quasicrystal [15,23] are also shown in Fig.1.

As the inelastic scattering length L_{int} (T) decreases when temperature increases, samples can leave from the metallic regime at low T into the critical regime at enough high T. Taking into account the analysis by scaling of the conductivity in quasicrystals [24], we think that the Al-Pd-Ru quasicrystal in Fig.1 is on the metallic side, where the condition, L_{int} (T) > the electron mean free path is satisfied below ~70K. That is, it is inadequate that the temperature curves for the conductivity σ of the Al-Pd-Ru quasicrystal in the temperature region above ~70K are analyzed by the weak localization theory or the present theoretical formula. A solid line for Al-Pd-Ru quasicrystal in Fig.1 shows the temperature curve for σ described by a power law $\sigma(T) = a + bT$. This relation is consistent with T-liner effect in eq.(7) for the conductivity, which is derived theoretically from the quasicrystal-like system. A solid line for Al-Cu-Fe quasicrystal was fitted by a power law $\sigma(T) = c + dT^{3/4}$ from 20 to 70K [15]. $T^{3/4}$ dependence is introduced from higher-order perturbation effect of conducting mechanism in the quasicrystal-like system.

In addition, we stress strongly that the present conducting mechanism can explain evidently the reduction of the resistivity due to introducing many defects in quasicrystals.

3. Conclusion

The T-liner power law fits well conductivity of Al-Pd-Ru quasicrystal below 70K.

It is suggested strongly that the anomalous transport properties are much related to localization effect in the quasicrystal-like system.

.

References

[1] Poon S J, 1992 *Adv. Phys*. **41**, 303
[2] Klein T et al. 1991 *Phys. Rev. Lett*. **66**, 2907
[3] Berger C, in LECTURES ON QUASICRYSTALS (Eds. D.Gratias Les Editions de physique Les Ulis, 1994) p 463
[4] Mayou D et al. 1993 *Phys. Rev. Lett*. **70**, 3915
[5] Trambly G de Laissardiere and Mayou D, 1997 *Phys. Rev*. **B55**, 2890
[6] Fujiwara T and Yokokawa T, 1991 *Phys. Rev. Lett*. **66**, 333
[7] Hafner J and Crajci M, 1992 *Phys. Rev. Lett*. **68**, 2321
[8] Tamura R et al. 2001 *Phys. Rev. Lett*. **68**, 3104
[9] Kanazawa I, 2000 *Physica B* **284-288**, 1161
[10] Kanazawa I, 2002 *J.Alloys Compounds* **342**, 381
[11] Kanazawa I, 2003 *Physica B* **328**, 111
[12] Kanazawa I, 2003 *Mod. Phys. Lett.* **B 17** 841
[13] Kanazawa I, 2003 *Physica E* **18**, 306
[14] Akiyama K, Takagiwa Y, Kanazawa I, 2006 *Philo. Mag*. **86**, 747
[15] Kanazawa I, Kitahata H, Sekiyama Y, 2008 *Z.Kristallog.* **223**, 813
[16] Yamada K et al. 2012 *Physica Procedia* **35**, 51
[17] Tamura R et al. 1999 *J.Phys:Condens. Matter* **11**, 10343
[18] Trambly G de Laissardiere et al. 1993 *Europhys. Lett*. **21**, 319
[19] Takeuchi T et al. 1998 *Phys. Rev*. **B58**, 11345
[20] Janot C and Boissien M, 1994 *Phys. Rev. Lett*. **72**, 1674
[21] Janot C, 1996 *Phys. Rev*. **B58**, 181
[22] Katz A and Gratias D, 1994 *J.Non-Cryst. Solids* **153-154,** 184
[23] Klein T et al. 1992 *Phys. Rev*. **B45**, 2046
[24] Delahaye J and Berger C, 2001 *Phys. Rev*. **B64**, 094203