The Lack of Full Lattice Periodicity Strongly Renormalizes and Enhances the Electron Phonon Interaction in Quasi Crystals, with High Electrical Resistivity to Follow

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Abstract

The lack of full periodicity in quasi crystal's lattice potential and the narrow "quasi bandwidths" that follow may strongly enhance the electron phonon interaction therein. This renormalized and enhanced interaction is primarily and directly responsible than the lack of geometrical periodicity, alone, in affecting the electrical transport in quasi crystals, as can be verified through experimentally observed quasi crystal's poor electrical conducting behavior which we demonstrate.

Discussions about electrical transport in quasi crystals can be found in. [1] Theoretical studies about the electrical transport behaviors in quasi crystals have mostly been carried out using a generalized Drude's formula. [2] Much of the discussion has focused on the geometrical aspect of the problem, that a quasi crystal's potential is not fully periodic. We wish to discuss this also from a more dynamical and interactional aspect. We will start by showing that the electron phonon interaction renormalization has a direct and profound impact on the transport properties of the sample. Because of that, not only does the geometrical aspect has an immediate effect on transport as it is univerally recognized, it also has an effect, indirectly, through renormalization and enhancement of the electron phonon interaction due to the lack of full periodicity of its lattice which we demonstrate below.

The resistivity, ρ, of normal metals at below the Debye temperature, T_D, usually obeys Bloch's "fifth law," $\rho \propto T^5$, [3] without the "Umklapp corrections" included, while at even lower temperatures, quantum interference may lead to a different temperature dependency for the conductance where the transport is most likely controlled by weak localization [4] which most experimental observations from quasi crystals do not find to be primary. It is therefore reasonable to expect effects being dominated by strong electron phonon interaction or polaron (in metals?) corrections. This is consistent with the observation that the carrier density in quasi crystal is low, typically on order of $n \sim 10^{21} cm^{-3}$ which we obtain independently from observations of the Hall effect coefficient and of the specific heat coefficient, while good, crystalline metals usually have $n \sim 10^{23} cm^{-3}$. Thus the inter–carrier distance, on order of $\sim 10^{-7} cm$, is comparable to or greater than the inter–nearest atomic distance and we expect the (quasi) "bandwidth" to be narrow. The electrical transport in quasi crystals can therefore be expected to be carried by heavy carriers without, however, being fully localized. In discussions about transport, large angle scatterings, $\delta p \sim p_F$, have more significant impact. On the other hand, what makes a quasi crystal different from either a normal, crystalline metal or a metallic glass, geometrically, is at intermediate to large inter–atomic separations which corresponds to smaller δp, $\delta p \ll p_F$, effects less significant in transport. Thus we may suggest that what dominates the difference in transport between quasi crystal and normal metal is more electron phonon interaction and less those aperiodic, though static, potential scatterings. To estimate $\epsilon_F = (\hbar k_F)^2/2m$ we use $k_F \sim (3\pi^2 n)^{1/3}$ with an estimated carrier density $n \sim 10^{21} cm^{-3}$ to find $k_F \sim 3.1 \times 10^7 cm^{-1}$ and $\epsilon_F \sim$ 0.34 eV. For typical values of quasi crystal's electrical conductivity we use the result of [1] where it was observed in YMgZn icosahedral quasi crystal between 1 K to 150 K to be at around $\sigma \sim 4.5 \times 10^{15} cm^{-1}$ stat mOhm. The relaxation time τ can then be estimated to be at around $\tau \sim 1.8 \times 10^{-14}$ sec, with $\epsilon_F \tau/\hbar \sim 9.8$. Approximately a similar result can be found in quasi crystal Al $_{65}$ Vu_{20} Ru_{15}, a quasi crystal with electrical conductivity $\sigma \sim 5 \times 10^{15} cm^{-1} \hbar \gg 1$ suggest not near localization, and the temperature dependency of the conductivity also indicates that localization is not the main, dominating controlling factor for conduction in quasi crystals either. From the temperature dependency of the conductivity we conclude that *weak* localization, following which a three dimensional sample's conductivity obeys $\sigma \propto 1/\sqrt{T}$, is not a major controlling factor affecting electrical conduction in quasi crystals at low temperatures. It is useful to note that *weak* localization is a result of quantum wave coherent backscattering. This is not in contradiction with the result of [5] where strong, *Anderson* localization was observed, with localization length found to be at around $10\mathring{A}$. In addition to and independent of all these, the appearance of gap near the Fermi surface and the Hume–Rothrey rule for alloys [6] also have effects. We also note that Umklapp effect [7] has been observed leading to different temperature dependencies of the mean free path, power law at lower temperature but experimental law at higher temperatures. Both the Hall effect and the thermal power coefficient show that the transport is n type at lower temperatures but p type at higher temperatures which has been discussed theoretically which discussion, however, may well have been incomplete in failing to include the atomic form factor. The transport has also been studied in terms of 3D Penrose tiling and large angle resonant scatterings which complications also have effects.

Quasi crystals are generally known to be poor electrical conductors. [1] Indeed it has been noted that, typically, better quasi crystals are poorer electrical conductors. The room temperature conductivity of YMgZn icosahedral quasicrystal is about $4.5 \times 10^{15} cm^{-1}$ stat mOhm, to be compared with Cu, a good conductor, having its room temperature conductivity at $\sim 5 \times 10^{18} cm^{-1}$ stat mOhm, a factor of ~ 1000 difference. Much of the discussion has focused on the geometrical aspect of the problem, that a quasi crystal's lattice potential is not fully periodic, and the resulting, correspondingly narrow bandwidth Δ will imply that $\partial\Delta/\partial p$ is small, that the effective carrier mass is heavy which, by Drude's formula, $\sigma = ne^2\tau/m$, would lead to a lower conductivity. We note that, while not being fully periodic is certainly detrimental to conduction, in the case of quasi crystal that alone does not explain fully sample's poor conductivity. Geometrically, the difference between a typical quasi crystal and a typical good crystalline metal having a fully periodic potential is usually no more than a factor of two or three, and can neither immediately nor fully account for those three orders of magnitudes reductions in conductivity. In addition, that suggested mechanism does not explain the temperature dependency of the conductivity either. It is our suggestion that, independent of and in addition to these, an enhanced electron phonon interaction, enhanced by the nontrivial geometry, has a direct and far more significant impact than that geometrically not fully periodic, though static, potential aspect alone in affecting the transport properties of quasi crystals. We now outline a scenario to show that these two aspects are related, that the electron phonon interaction in quasi crystal may well have been significantly enhanced by the geometrical structure, and quasi crystal is an interesting many body system exhibiting this character. Experimentally, narrow quasi valence band in quasi crystals has been observed in AlNiCo quasi crystals [8] and in other quasi crystals. [9] We may also provide an estimate for the effective "quasi bandwidth" from the lack of full periodicity in lattice potential using a simple argument as follows. For immediate simple estimate we set the bandwidth to $\Delta \sim \hbar^2/2mb^2$, where we introduce as an "effective lattice constant" b to account for the quasi periodicity which we set to be $2a$. This may be acceptable when we recall that the inter-atom distance in a quasi crystal, while not constant as in a good metal, varies typically within no more than a factor of 2. With $a \sim 10^{-7}$ cm from $a \sim n^{-1/3}$ and $n \sim 10^{21} cm^{-3}$, we have $\Delta \sim 8.6$ meV, [1] smaller than the Debye energy which we have reason to believe to be of the same of order of magnitude as in a normal crystal where we have $\hbar\omega_D \sim k_B T_D \sim 60$ meV, with $T_D \sim 700$ K. To estimate the renormalized electron phonon interaction we start with the bare coupling g_0 which we assume to be of the same of order of magnitude as in a normal metal and can be estimated from

$$g_0^2 = \frac{1}{V} \frac{4\pi e^2}{|k-k'|^2 + k_F^2} \frac{\hbar\omega_{k-k'}}{2} \tag{1}$$

For immediate simple estimation we set $(k-k') \sim k_F$, $\omega_{k-k'} \sim \omega_D$, and $V \sim a^3$ to obtain

$$g_0^2 \sim \frac{\pi e^2}{a} \frac{k_B T_D}{(k_F a)^2} \tag{2}$$

and $g_0 \sim 0.17$ eV, of the same order of magnitude as in an average normal metal. To estimate the renormalized electron phonon interaction we use perturbation theory to proceed and find

$$g \sim \frac{1}{\epsilon_2 - \epsilon_1} \int_{\epsilon_1}^{\epsilon_2} d\epsilon \frac{|g_0|^2}{\epsilon - \epsilon_0} = \frac{|g_0|^2}{\Delta} \ln(\frac{\epsilon_2 - \epsilon_0}{\epsilon_1 - \epsilon_0}) \tag{3}$$

where $\Delta = \epsilon_2 - \epsilon_1$, the bandwidth. The ratio $(g/g_0)^2 \sim (g_0/\Delta)^2(\ln\Delta)^2$ provides an estimate for the significant enhancement of the electron phonon interaction. The effect of a narrow bandwidth enhancing electron phonon interaction is well known and discussed in the literature; see, *e.g.*, [10]. To estimate the effect of the enhanced electron phonon interaction on conduction we note that by the golden rule the electron phonon scattering transition rate is proportional to the square of the coupling matrix element. With our assumed Debye temperature of 700 K, this produces an estimated enhancement for the quasi crystal's electrical resistivity by a factor of $(g_0/\Delta)^2(\ln\Delta)^2 \sim 390$, within a factor of ~ 3 from as observed, which is at around 1100. To see qualitatively why a narrow band may significantly enhance the electron phonon interaction we consider the effect of one phonon of typical energy, taken to be ~ 60 meV (with an assumed Debye temperature 700 K), to scatter one electron very far out from a band of typical bandwidth which, as noted above, is ~ 8.6 meV. Such an interaction can easily kick a carrier very far out of its initial "quasi band," and an enhanced electron phonon interaction can be expected to result from. It is also possible to consider the problem from an artificial, opposite limit, a jelly model with its "infinitely broad" band where there would be zero, no electron phonon coupling at all, consistent with our suggestion from the opposite direction. [11] It will be of interest to consider the effect of this enhanced electron phonon interaction on sample's temperature or frequency dependent transport properties, both are experimentally observable. A simple estimation could be made for the magnitudes of the temperature scale $T_0 \sim \Delta/k_B \sim 100K$ and frequency scale $f_0 \sim \Delta/h \sim 2 \times 10^{12}$ Hz, over which the conductivity may vary. It will, finally, also be of interest to consider what such an enhanced electron phonon interaction might have effect making high temperature quasi crystalline superconductors of conventional mechanism. Discussions about quasi crystalline superconductors can be found in [12, 13] and superconducting quasi crystals have also been found experimentally, [14] with Tc $\sim$ 0.12 K. Theoretical discussions about limits on superconducting temperature have mostly been based on considerations of stability, that too strong an electron phonon interaction could lead to lattice collapse (melting?). Those discussions are generally considered unconvincing in that they are mostly based on linear treatment of the problem thus may not apply in the strong interacting regime. The lack of full periodicity does not damage the parity of the system, and a direct Cooper paring scheme between k and -k states could still be worked out even though k may not be the appropriate variable to characterize the participating carriers. Because of that, it is still possible to imagine that what carry super current in a quasi crystalline superconductor are not necessarily Cooper "pairs" but certain, generalized, quasi Cooper "droplets" (?) Independent of these, we believe it is still useful to recognize that a quasi crystal's geometrical aspect has profound impact on its interaction. We note, finally, that an experimental observation of the Josephson effect between quasi crystalline superconductors could be useful in that it may help to identify and understand the nature of the superconducting carriers in quasi crystals. While there have been concerns that fluctuations in the relative phase between the two sides of the barrier separating the two participating quasi crystals may serve to average out the Josephson current, no detailed calculation of the effect has been performed to verify the magnitude of the effect. A theory of quasi crystal melting has apparently not been fully developed, and it is not known what likewise limit on electron phonon coupled quasi crystalline superconductor might be.

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