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Size and randomness effects on the temperature-dependent hopping conductivity of nanocrystalline chains

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Abstract. Developing a renormalization group approach, we study the hopping conductivity of nanocrystalline chains with different site energies. Exact calculations show that many parameters including nanosizes, randomness of grain distributions, lattice distortions, site energies, transition rates, Fermi energy, and temperature influence the conductivity. Some new singular features, for example the frequency shift, the amplitude fluctuations, and the interchange between "peak" and "valley" behavior of the imaginary part of the conductivity can be caused by certain parameters mentioned above, while the interface distortions modulate mainly the overall amplitudes of the conductivity at the whole frequency region.

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1 Introduction

The size-dependent properties of nanocrystalline (NC) solids have attracted considerable interest due to their potential applications as well as the opening of new scientific questions [1–7]. A drastic size reduction to a few nanometers may lead to many special structures with the singular physical properties. Many experiments have been made to explore into the causes of the singular physical properties induced by structural characters of NC solids [6,7]. Some interesting results such as quantum size effects, have been determined [6]. For instance, the energy gap between conduction band and valence band of NC silicon increases as compared with that of bulk silicon [7]. With the decrease of size of nano grain, the resistance of nano structured Pd metal decreases [4]. In a real NC solid, nano-grains with various numbers of atoms are distributed by a certain rule. Such nano grains consist of crystalline sites and interface sites, which take different site parameters, for example, site-energy, site distance and transition rate. With this kind of complicated structures, it seems hard to imagine that one can easily get a clear theoretical understanding of the causalities of singular properties with so many complicated structural characters and different size regimes of nano-materials [8]. This may be the reason that few theoretical works have touched on the investigation of physical properties of NC solids, especially on the interesting conductivity [12], even though some elegant theoretical efforts have been made for calculating those kinds of complicated systems [8–11].

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For the study of conductivity of solids, one of the most effective theory is the Miller-Abrahams (M-A) hopping conductivity theory [13], which was further applied for complicated systems such as quasicrystals [12,14,15]. The extended M-A equation on one-dimensional (1D) ac conductivity is derived as [14,15]

$$\mathrm{i}\omega C_n(V_n - EX_n) = \frac{V_{n-1} - V_n}{Z_{n-1,n}} + \frac{V_{n+1} - V_n}{Z_{n,n+1}}, \qquad (1)$$

linking the "voltage" variable V_n on site n of 1D chains in the presence of a time-dependent external field $E\mathrm{e}^{\mathrm{i}\omega t}$, where X_n is the co-ordinate of nth site. The factors C_n and $Z_{n,n+1}$, which are related to the temperature T, are respectively given by

$$C_n = e^2 f(\varepsilon_n)[1 - f(\varepsilon_n)]/kT, \qquad (2)$$

$$1/Z_{n,n+1} = e^2 f(\varepsilon_n)[1 - f(\varepsilon_{n+1})]U_n/kT \qquad (3)$$

where ε_n is the site energy of an electron localized at the nth site, and U_n is the transition rate from the nth site to $(n+1)$th one in the absence of external field. The Fermi function $f(\varepsilon_n)$ is defined as

$$f(\varepsilon_n) = \left[1 + \exp\left(\frac{\varepsilon_n - \varepsilon_\mathrm{F}}{kT}\right)\right]^{-1} \qquad (4)$$

where ε_F is the Fermi energy. With denotation

$$I_n = \frac{V_{n+1} - V_n}{Z_{n,n+1}},\ d_n = X_{n+1} - X_n, \qquad (5)$$

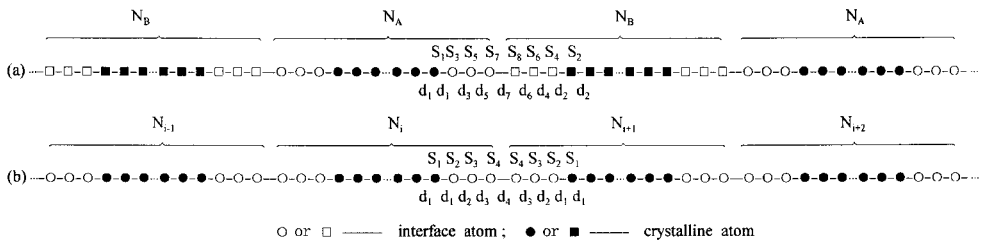

Fig. 1. Schematic representations of NC chains. (a) A periodic two type-atom chain with the primary cell of nano-grains A and B; (b) A random one type-atom chain with average atomic number $\overline{N}$.

equation (1) can be rewritten by

$$\begin{aligned} \mathrm{i}\omega C_n(V_n - EX_n) &= I_n - I_{n-1}, \\ \mathrm{i}\omega C_{n+1}(V_{n+1} - EX_{n+1}) &= I_{n+1} - I_n, \end{aligned} \tag{6}$$

corresponding to the cases of the nth site and $(n+1)$th one, respectively. The hopping conductivity is then given by

$$\sigma = \frac{1}{EL}\sum_n I_n d_n, \tag{7}$$

where L is the total length of chains studied.

Motivated by the work on the spectrum calculations of NC solids [8], we present in this paper a set of renormalization group (RG) schemes to study effects of grain-distribution factors, site parameters, temperature and the Fermi energy on the hopping conductivity. The outline is as follows: A simple NC chain is illustrated in Section 2, for which a RG scheme is presented to calculate the hopping conductivity. In Section 3, the improved model structures of NC chains are considered, in which the atomic numbers $\{N_\mathrm{i}\}$ of nano-grains are distributed by certain rules. Series calculation results are discussed in Section 4. And a brief summary is given in Section 5.

2 Conductivity of periodic two-atom NC chain: Renormalization group

Let us consider a periodic NC chain [11], which consists of two kinds of nano-grains A and B with numbers of atoms N_A and N_B to be positioned alternately in a row (see Fig. 1a). The primitive cell of the periodic chain consists of A and B, *i.e.*, A+B. The site parameters $\{\varepsilon_n, U_n\}$ take one of eight sets of values $\{\varepsilon_1, U_1\}$, ..., and $\{\varepsilon_8, U_8\}$, of which $\{\varepsilon_1, U_1\}$ and $\{\varepsilon_2, U_2\}$ is for two kinds of crystal sites S_1 and S_2, while the six sets of values $\{\varepsilon_3, U_3\}$, ..., and $\{\varepsilon_8, U_8\}$ are for the interface sites S_3, ..., and S_8 (see Fig. 1a). Analogously, the parameter d_n can be divided into seven kinds of values d_1, ..., and d_7 for the same reasons. In order to simplify mathematical solution, we consider firstly that site energy is independent of site n, *i.e.*, $\varepsilon_n = \text{const}$. One can derive, from equations (6), that

$$(2 + \mathrm{i}\omega/U_n)I_n = I_{n+1} + I_{n-1} + \mathrm{i}\omega E d_n. \tag{8}$$

Supposing that

$$\begin{aligned} E_n &= 2 + \mathrm{i}\omega/U_n \\ t_{n,n+1} &= t_{n-1,n} = 1 \end{aligned} \tag{9}$$

we then have from equation (8)

$$E_n I_n = t_{n-1,n} I_{n-1} + t_{n,n+1} I_{n+1} + \mathrm{i}\omega E d_n. \tag{10}$$

Thus, the original chain is represent by a pseudo-chain with pseudo-parameters $\{E_n, t_{n,n+1}, d_n\}$. One can find that the pseudo-chain has the same NC construction rule as that in the original chain. The pseudo-parameter E_n also takes one of the eight values E_1, ..., and E_8 corresponding to the classification of U_n.

According to the fact that our NC chain is ordered, a RG approach can be applied to calculate the conductivity σ of the pseudo-chain. We can decimate the left- and right-neighbors of each of a certain kind of sites in the pseudo-chain by a RG transformation. So, the pseudo-chain with the pseudo-parameters $\{E_n, t_{n,n+1}, d_n\}$ is renormalized into a sub-chain with renormalized parameters $\{E'_n, t'_{n,n+1}, d'_n\}$. Iterating the RG transformation above, we decimate further the new left- and right-neighbors of the remained sites in the sub-chain. Then, the sub-chain is reduced to a sub-subchain. The renormalized pseudo-parameters $\{E_n^{(k)}, t_{n,n+1}^{(k)}, d_n^{(k)}\}$ after kth RG procession satisfy the following recursion relations

$$E'_{n\pm(k+1)} = E_{n\pm(k+1)} - \frac{t^2_{n\pm(k+1),n\pm k}}{E'_{n\pm k}},\ E'_{n\pm 1} = E_{n\pm 1}, \tag{11a}$$

$$d'_{n\pm(k+1)} = d_{n\pm(k+1)} + \frac{t_{n\pm(k+1),n\pm k} d_{n\pm k}}{E'_{n\pm k}},\ d'_{n\pm 1} = d_{n\pm 1} \tag{11b}$$

$$t^{(k+1)}_{n\pm 1,n} = \frac{t^{(k)}_{n\pm 1,n} t_{n\pm(k+1),n\pm k}}{E'_{n\pm k}},\ t^{(1)}_{n\pm 1,n} = t_{n\pm 1,n}, \tag{11c}$$

$$E_n^{(k+1)} = E_n^{(k)} - \frac{\left[t^{(k+1)}_{n-1,n}\right]^2}{E'_{n-(k+1)}} - \frac{\left[t^{(k+1)}_{n,n+1}\right]^2}{E'_{n+(k+1)}},\ E_n^{(0)} = E_n, \tag{11d}$$

$$\begin{aligned} d_n^{(k+1)} &= d_n^{(k)} + \frac{t^{(k+1)}_{n-1,n} d'_{n-(k+1)}}{E'_{n-(k+1)}} + \frac{t^{(k+1)}_{n,n+1} d'_{n+k+1}}{E'_{n+(k+1)}}, \\ d_n^{(0)} &= d_n, \end{aligned} \tag{11e}$$

After the RG transformation is iterated $K = \left[\frac{N_1+N_2}{2}\right] - 1$ times ("[]" denotes the well-known integralisation operator), the original NC chain is reduced to a simplest periodic chain with one renormalized site in a unit cell, which

has the renormalized site parameters $E_n^{(K)}$, $t_{n\pm1,n}^{(K)}$, and $d_n^{(K)}$. Thus the conductivity σ of original NC chain is given, from equation (7), by

$$\sigma = \frac{\mathrm{i}\omega}{2L} \times \left[\frac{2(d_n^{(K)})^2}{E_n^{(K)} - t_{n-1,n}^{(K)} - t_{n,n+1}^{(K)}} + \sum_{k=1}^{K} \frac{(d'_{n+k})^2}{E'_{n+k}} + \sum_{k=1}^{K} \frac{(d'_{n-k})^2}{E'_{n-k}} \right], \tag{12}$$

where L is the length of the primitive cell in original NC chain.

3 Common NC chains and the RG method

In fact, real NC solids have much more complicated structures and properties [5] than that of the simplified model given by Figure 1. Experiments have shown that the structural and physical characters of interface atoms in a nanograin are much different from those of crystalline center atoms. And nano-sized grains with different number of atoms N_i are arranged successively by a certain distribution rule. So we further deal with more common NC models with different site energy and different grain-arrangements such as quasiperiodic and random sequences in this section. The influences of some factors on the hopping conductivity of NC chains are discussed.

3.1 With site energies dependent on site position

Assuming site energies $\{\varepsilon_n\}$ to depend on the site position n, we obtain a universal equation, from equation (6),

$$\left[\frac{1}{C_n} + \frac{1}{C_{n+1}} + \frac{1-f(\varepsilon_n)}{1-f(\varepsilon_{n+1})} \frac{\mathrm{i}\omega}{C_n U_n} \right] I_n = \frac{1}{C_n} I_{n-1} + \frac{1}{C_{n+1}} I_{n+1} + \mathrm{i}\omega E d_n. \tag{13}$$

One can find that there exist many complicated variables in above equation so that it seems to become much difficult to calculate the conductivity of the NC solids with different site energy. However, with the definitions of

$$E_n = \left[\frac{1}{C_n} + \frac{1}{C_{n+1}} + \frac{1-f(\varepsilon_n)}{1-f(\varepsilon_{n+1})} \frac{\mathrm{i}\omega}{C_n U_n} \right], \quad t_{n-1,n} = \frac{1}{C_n},\ t_{n,n+1} = \frac{1}{C_{n+1}}, \tag{14}$$

which are different from equation (9), equation (13) is then rewritten as the same form as that of equation (10) except for the values of parameters $\{E_n, t_{n,n+1}, d_n\}$. And the chain with the site parameters $\{\varepsilon_n, U_n, d_n\}$ is changed into a pseudo-chain with the pseudo-site parameters $\{E_n, t_{n,n+1}, d_n\}$. However, the sites in the pseudo-chain are arranged by the same construction rule as in the original chain. Then, one can calculate the conductivity of the periodic two-atom NC chain with different site energies by the same RG procedures as in the above section.

For brevity, we assume that the original NC chain is a periodic single type-atom chain, which consists of two basic grains with different site numbers N_A and N_B. According to local environments of crystal sites and interface sites, $\{\varepsilon_n, U_n\}$ take one of four sets of values: $\{\varepsilon_1, U_1\}$ for S_1-type crystal sites, $\{\varepsilon_2, U_2\}$ for S_2-type interface sites, $\{\varepsilon_3, U_3\}$ for S_3-type interface sites, and $\{\varepsilon_4, U_4\}$ for S_4-type interface sites (see Fig. 1b). Accordingly, the parameter d_n is one of four values $\{d_1, d_2, d_3, d_4\}$ where d_1 is both the lattice spacing and the distance between the crystal site S_1 and the interface site S_2; d_2, between the interface site S_2 and S_3; d_3, between the interface site S_3 and S_4, and d_4 between interface site S_4 and the next one in the neighbor grain (see Fig. 1b). However, the periodic one type-atom NC chain can be represented by the double type-atom chain shown in Section 2, if we replace the values of site parameters in A-type grains for those in B-type grains. This indicates that similar RG procedures to that in Section 2 can be carried out to calculate the conductivity of the periodic one type-atom NC chains.

3.2 Aperiodic NC chains

Contrary to the periodic NC systems presented above, we further consider aperiodic one type-atom NC chains.

Let us consider the quasiperiodic Fibonacci NC chain, which is constituted by two blocks of nanograins with different numbers of atoms N_A and N_B arranged by a Fibonacci quasiperiodic sequence $\{...N_\mathrm{A}N_\mathrm{B}N_\mathrm{A}N_\mathrm{A}N_\mathrm{B}N_\mathrm{A}N_\mathrm{B}N_\mathrm{A}N_\mathrm{A}N_\mathrm{B}N_\mathrm{A}N_\mathrm{A}N_\mathrm{B}...\}$. The RG transformations can be applied to the Fibonacci NC chain to calculate the conductivity. The RG method developed in Section 2 can reduce the Fibonacci NC chain into a simple Fibonacci quasiperiodic sub-chain (1 st RG step). In the kth renormalized sub-chain, pseudo-sites take renormalized parameters $\{E_n^{(k)}, t_{n,n+1}^{(k)}, d_n^{(k)}\}$ solved by repeating the relations (11). According to the local environments of pseudo-sites in the sub-chain, we can again separate them into three types α, β and γ with re-defined pseudo-site parameters $\{\varepsilon_i, d_i, t_i\}$ ($i = \alpha$, β or γ). Thus, we use the RG transformation presented in reference [15] to renormalize the Fibonacci sub-chain (2nd RG step). Iterating infinitely the 2nd RG step, the sub-chain can be reduced into a simplest periodic chain. Accordingly, pseudo-site parameters $\{\varepsilon_i^{(n)}, d_i^{(n)}, t_i^{(n)}\}$ ($i = \alpha$, β or γ) satisfy the same recursion relations as relations (11) in reference [15], where the symbol n notes the generation of iterations of the 2nd RG transformations. Thus the conductivity is given by

$$\sigma = \sigma' + \frac{\mathrm{i}\omega}{L} \left\{ \frac{N_\alpha [d_\alpha^{(\infty)}]^2}{\varepsilon_\alpha^{(\infty)} - 2t_\alpha^{(\infty)}} + \sum_{n=0}^{\infty} \frac{N_\beta^{(n)} [d_\beta^{(n)}]^2}{\varepsilon_\beta^{(n)}} \right\} \tag{15}$$

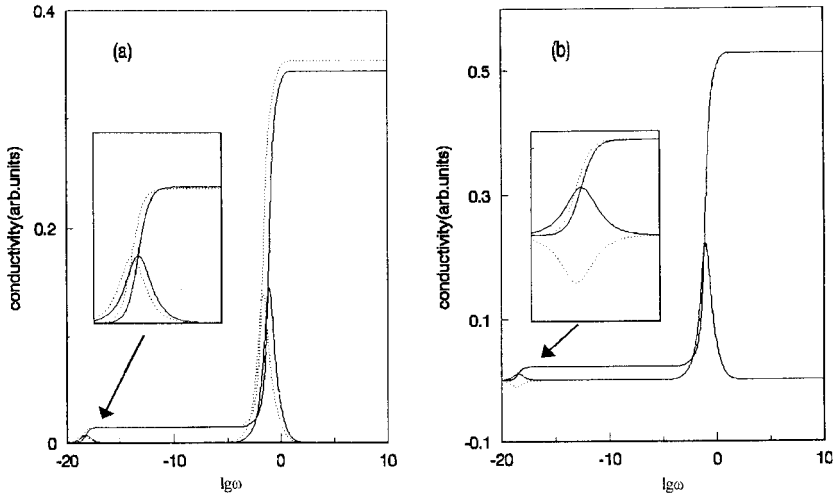

Fig. 2. The changes of the imaginary part peaked curves and the real part curves with plateaus of the conductivity of a periodic two type-atom NC chain with logarithmic frequency. The site parameters $\{U_1, U_2, ..., U_8\}$ are chosen to be {1, 0.01, 0.95, 0.0105, 0.90, 0.011, 0.85, 0.0115} (in units of U_1) and $\{d_1, d_2, ..., d_7\}$ to be {1, 0.9, 0.101, 0.89, 1.03, 0.87, 0.95} (in units of d_1). (a) The solid and dotted plots respectively correspond to the iso-energy site chains with $N_A/N_B = 10/20$ and 20/40. (b) The solid and the dotted curves respectively correspond to the case that $\{\varepsilon_A, \varepsilon_B, \varepsilon_F\}$ are {12, 11, 8} and {12, 10, 8} (arb. units) for the chain with different site energies and $N_A/N_B = 10/20$ at temperature $T = 300$ (arb. units). The frequency is in units of U_1.

after infinite RG transformation developed in reference [15], where σ', L, and N_α are the renormalized accumulation of conductivity after the first step of RG transformations, the total length of the Fibonacci chain, and the number of α-type sites in the simplest chain, respectively.

In a real random NC solid, atomic numbers of nano-grains are distributed in a certain region by a function, and arranged by random sequence. We can use Monte-Carlo methods to produce the random numbers of atoms $\{N_i\}$ of nano-grains from the normal distribution function with expectation number N_P and half-maximum width Δ_N. Then, we simulate a real random NC chain by arranging successively the nano-grains with random number $\{N_i\}$. Under certain exercisable approximations, we can also apply the RG transformations in Section 2 to decimate the original NC chain to be a random sub-chain. The renormalized pseudo-parameters of the sub-chain can be given by iterating the set of RG relation (11). Regarding the random sub-chain itself with hundreds of sites as a unit cell of a periodic sequence, one can develop further RG transformations to decimate repeatedly the left- and right-neighbors of a site in the sub-chain until it becomes a simplest one-atom periodic sequence. Then, the conductivity of the random NC chains can also be calculated exactly.

4 Calculations and discussion

We calculate conductivity of some kinds of the NC chains in order to explore the relationship of conductivity of NC systems with the quantum size effect, randomness of nano-grain arrangements, lattice distortions, distributions of numbers of atom of nano-grains, and so on, of 1D NC chains. The effect of average number of atom $\overline{N}$, site energy ε_n, site distance d_n, distribution factors N_P and Δ_N, inverse temperature $1/T$ and Fermi energy ε_f on the conductivity are also discussed.

4.1 Conductivity of periodic NC chains

To determine the basic features of the conductivity of NC solids and the influence of average numbers of atoms of nano-grains, we calculated variation of the hopping conductivity of the NC chains presented in Section 2 with frequency ω in units of U_1 as shown in Figure 2, where Figure 2a, b correspond to site-energy ε_n with the same and two different values in two kinds of grains respectively. One can find, from Figure 2a, that the shapes of the plots of conductivity σ *versus* logarithmic frequency $\log\omega$ for NC chains with iso-energy sites are similar to those of Fibonacci quasicrystal calculated by Newman *et al.* [15]. Contrary to the case in Figure 2a, however, the site-energy difference of two different grains may cause the interchange of "peak" and "valley" behavior of the imaginary part of the conductivity at low frequency $\omega = 10^{-18}U_1$ (see Fig. 2b). On the other hand, as the number of atoms of nano-grains decrease, the positions of "imaginary peaks" as well as of "real plateaus" at both high- and low-frequencies shift towards higher frequency direction, *i.e.*, blue shift. This result is equivalent to a corresponding statement for the phonon properties of NC solids [11].

Figures 3 and 4 show the influences of the inverse temperature $1/T$ and the Fermi energy ε_F on the conductivity of the periodic two type-atom NC chains with different site-energies. It can be seen that the conductivity

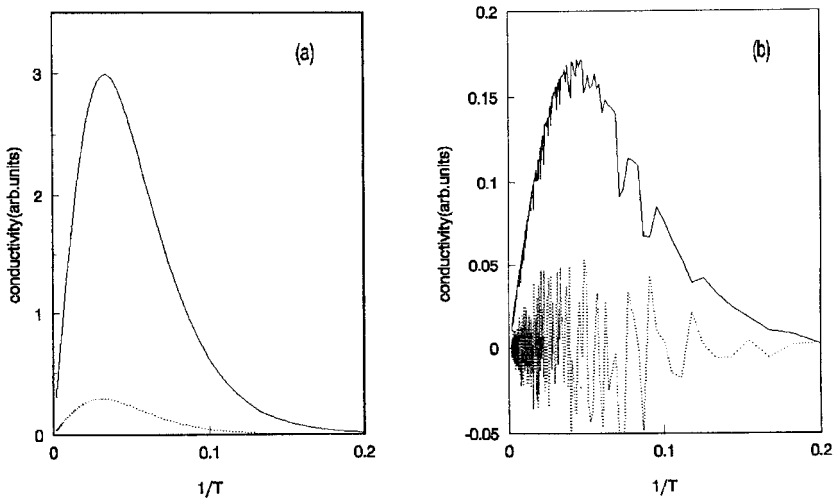

Fig. 3. The changes of conductivity of the periodic two type-atom NC chain with inverse temperature $1/T$. $\{\varepsilon_{\rm A}, \varepsilon_{\rm B}, \varepsilon_{\rm F}\}$ are chosen to be {12, 11, 8} (in arb.units) and $N_{\rm A}/N_{\rm B} = 10/20$, The site parameters $\{U_1, U_2, ..., U_8\}$ and $\{d_1, d_2, ..., d_7\}$ are the same as in the Figure 2. The solid and dotted curves represent the real and the imaginary parts of the conductivity at (a) high frequency $\omega = 1U_1$ and (b) low-frequency $\omega = 10^{18}U_1$.

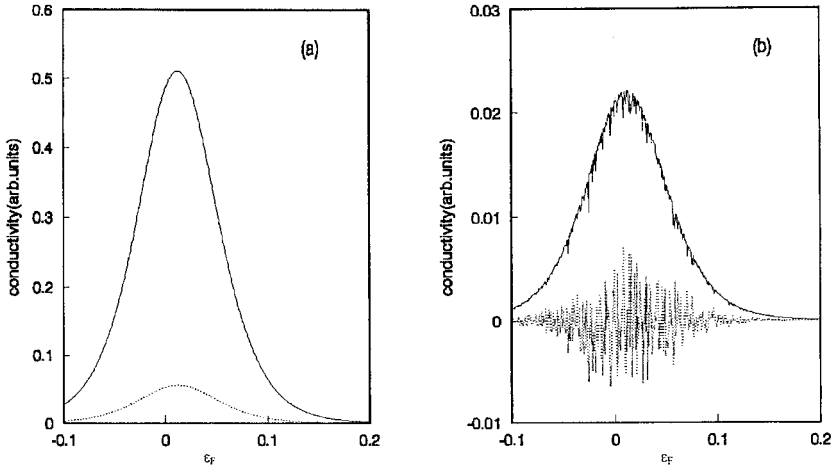

Fig. 4. The changes of conductivity of the periodic two type-atom NC chain with the Fermi energy. The solid and dotted curves represent the real and the imaginary parts of the conductivity at (a) high frequency $\omega = 1U_1$ and (b) low-frequency $\omega = 10^{18}U_1$. The parameters $\{\varepsilon_{\rm A}, \varepsilon_{\rm B}\}$ take {12, 11} and $N_{\rm A}/N_{\rm B} = 10/20$, and other site parameters are the same as in the Figure 2b.

at high-frequency $\omega = 1U_1$ assumes maximum values and is changed monotonously by $1/T$ and $\varepsilon_{\rm F}$. However, opposite to the high-frequency conductivity ($\omega = 1U_1$), the conductivity at low-frequency $\omega = 10^{18}U_1$ vibrates strongly with both $1/T$ and $\varepsilon_{\rm F}$ (see Figs. 3b and 4b).

4.2 Randomness effect on the conductivity of NC chains

In Figure 5, we show the variations of conductivity of aperiodic one type-atom NC chains with randomness of grain-distributions. For the sake of comparability, we choose that the average number of sites $\overline{N}$ in a grain equals to a common value and that site-energies are constant for all types of NC chains, while grain arrangements in NC chains get more and more random from the periodic chain to the random chain. For all types of NC chains with $\overline{N} = 30$, for example, we can take $N_{\rm A} = 31$ and $N_{\rm B} = 29$ for a periodic chain, $N_{\rm A} = 33$ and $N_{\rm B} = 25$ for a quasiperiodic Fibonacci chain, and $N_P/\Delta_N = 30/5$ and 30/10 for a random chain. The solid, dashed and dotted curves in Figure 5a correspond to the conductivity of the periodic, Fibonacci quasiperiodic and random NC chains, respectively. The amplitude of conductivity at the high frequency $\omega = 1U_1$ fluctuates with the changes of randomness, while the positions of the "imaginary peaks" as well as the "real plateaus" seems not to shift. At the low-frequency $\omega = 10^{18}U_1$, however, the positions of peaks and plateaus of the imaginary and real parts of conductivity shift to the direction of lower frequency *i.e.* red shift, with the increase of randomness of grain-arrangements in NC chains. Another interesting feature is shown in Figure 5b. It can be seen that the position of "imaginary peak"

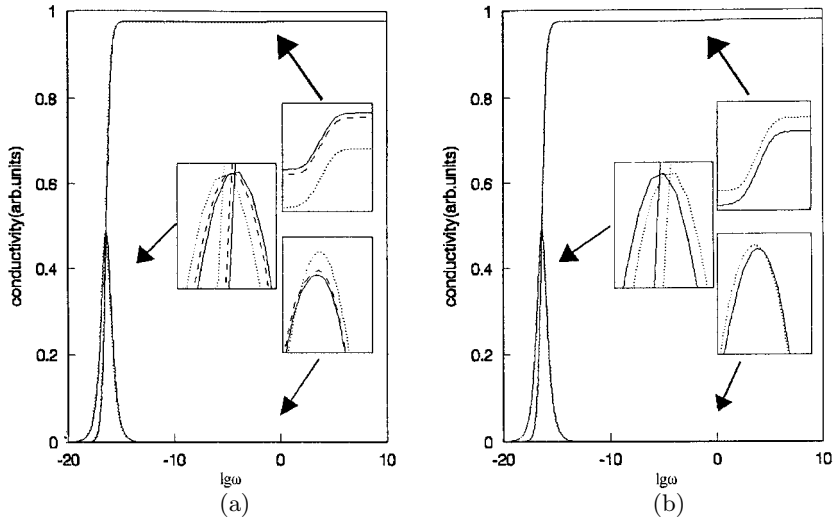

Fig. 5. The conductivity of the iso-energy one type-atom NC chains with different randomness. The average atomic number $\overline{N} = 30$, and the site parameters $\{U_1, U_2, U_3, U_4\}$ and $\{d_1, d_2, d_3, d_4\}$ are chosen to be {1, 0.95, 0.9, 0.80} and {1, 1.01, 1.02, 1.05}, respectively. (a) The solid, dashed and dotted plots correspond to a periodic chain with $N_A = 31$ and $N_B = 29$, a quasiperiodic Fibonacci chain with $N_A = 33$ and $N_B = 25$, and a random chain with normal distribution factors $N_P/\Delta_N = 30/10$, respectively. (b) The solid and dotted plots correspond to the random chain with $N_P/\Delta_N = 30/10$ and 30/5, respectively. The frequency is in units of U_1.

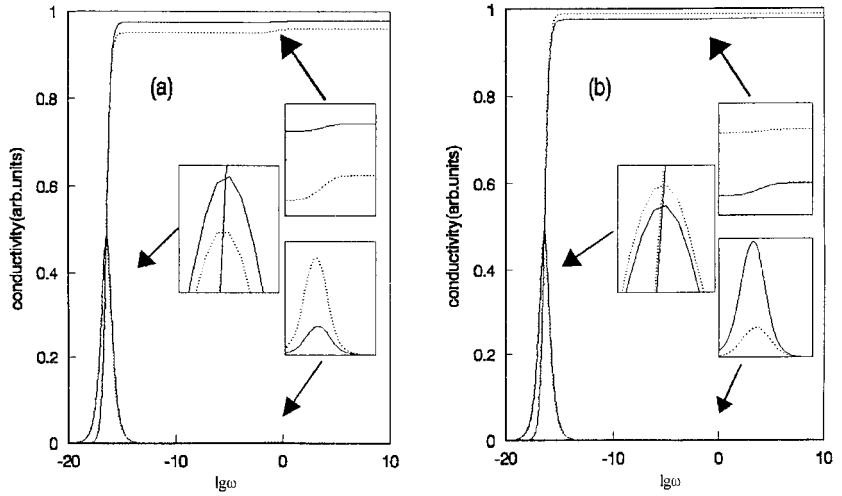

Fig. 6. The conductivity of the random iso-energy one type-atom NC chain with distribution factors $N_P/\Delta_N = 30/10$. (a) $\{d_1, d_2, d_3, d_4\}$ are chosen to be {1, 1.01, 1.02, 1.05}, and $\{U_1, U_2, U_3, U_4\}$ are chosen to be {1.0, 0.95, 0.9, 0.80} and {1, 0.9, 0.8, 0.7} corresponding to the solid and dashed plots; (b) $\{U_1, U_2, U_3, U_4\}$ take {1.0, 0.95, 0.9, 0.80}, and are chosen to be {1.0, 1.01, 1.02, 1.05} and {1.0, 1.05, 1.1, 1.2} corresponding to the solid and dotted plots. The frequency is in units of U_1.

of the random NC chain with normally distributed nano-grains shifts to low frequency direction as the distribution factor Δ_N, which corresponds to the randomness of distribution of grains, changes from 5 to 10. This may provide an indirect identification to that low-frequency conductivity treats red shift by the increase of randomness of grain arrangements.

Additionally, we will discuss the conductivity property of a random NC chains with regard to the increase of the hopping transition rates U_n and lattice distance d_n. Figure 6a shows that as the changes of transition rates Un increase, the overall amplitudes of conductivity of random NC chains decrease at the whole frequency region except that the "imaginary peak" increases at high frequency $\omega = 1U_1$. However, the influence of lattice distortions is contrary to that of changes of the transition rates U_n, which can be seen from Figure 6b. Meanwhile, an inflated example is shown in Figure 7a, for which the distance d_4 between two interface sites, belonging to two different nano-grains, gets a very large change. It is found that the peak at high frequency shifts strenuously to higher frequency direction as the change of distance d_4 increases. These features indicate that the changes of distances of interface sites modulate mainly the position of the high-frequency peak, as well as the amplitude of conductivity of NC chains at the whole frequency region. Compared to Figure 2a, Figure 7b shows the change of the conductivity with the average numbers of atoms

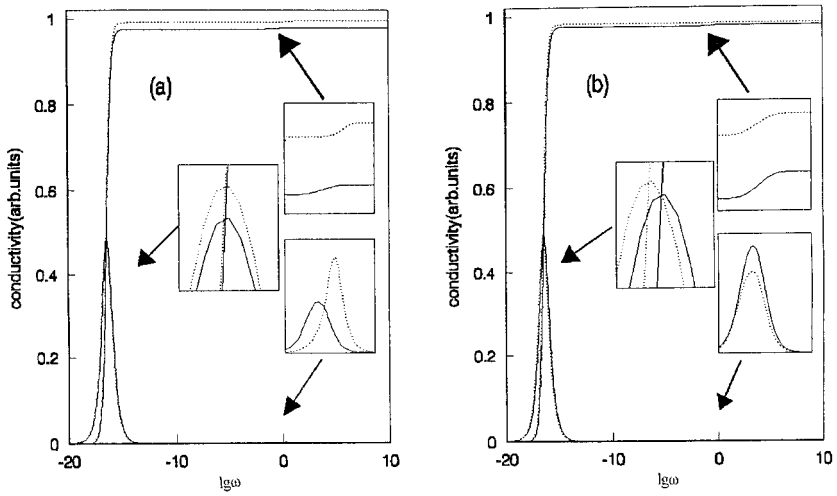

Fig. 7. The conductivity of the random one type-atom iso-energy NC chain with $\{U_1, U_2, U_3, U_4\} = \{1.0, 0.95, 0.9, 0.80\}$ and $\{d_1, d_2, d_3\} = \{1, 1.01, 1.02\}$. (a) $N_P/\Delta_N = 30/10$, and d_4 is 1.05 in the solid plot and 1.50 in the dashed plot. (b) $d_4 = 1.05$, and $N_P/\Delta_N = 30/10$ in the solid plot and $N_P/\Delta_N = 40/10$ in the dotted plot. The frequency is in units of U_1.

of the nano-grains. Similar to the case of periodic double type-atom NC chains, a blue shift of "imaginary peak" of conductivity is produced clearly at low frequency by the decrease of average atomic numbers of nano-grains for random one-atom NC chains.

5 Summary

We presented two types of NC chains: One is the two type-atom periodic chains, of which the primary cell is composed of nano-grain A and B with numbers of atoms N_A and N_B. The other is the one type-atom chain, of which nano-grains with atom-numbers $\{N_i\}$ are arranged by a rule. As for the second type, we consider three kinds of chains. One is a periodic one type-atom NC chain with two nano-grains with N_A and N_B atoms alternately arranged by a periodic sequence. Second is a quasiperiodic NC chain with two nano-grains N_A and N_B arranged in a Fibonacci sequence and third, a random NC chains with different nano-size grains $\{N_i\}$ of which atomic numbers are distributed by the normal distribution function with the distribution factors N_P/Δ_N. By developing series of RG transformations, we calculate the conductivity of NC chains in terms of above 1D NC models. For the mechanism of quantum size effects, the effects of lattice distortions and grain distributions, and several relevant physical parameters on the conductivity are discussed. It is found that the decreases of both average atomic number and randomness of nano-grain distributions lead to a blue shift of the peak of the imaginary part of the low frequency conductivity of NC chains. However, the increase of interface distances of NC chains make the high-frequency peak, not the low-frequency peak, shift to higher frequency direction. Meanwhile the amplitude of conductivity at the whole frequency region fluctuates with the changes of site distances d_n and the transition rates U_n. An additional singular feature is that the change of site energies causes the mutual interchange of "peak" and "valley" behavior of the imaginary part of the low-frequency conductivity of NC chains. Furthermore, low-frequency conductivity of NC chains vibrates strongly with the changes of inverse temperature $1/T$ and the Fermi energy ε_F.

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