Electron dephasing in nanocrystalline silicon thin films

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In combination with dephasing and weak localization theories, we have presented a detailed magnetotransport investigation for the electron dephasing characteristics in hydrogenated nanocrystalline silicon thin films. It is found that the experimental magnetoconductivity can be well fitted by an integration of diffusive Fermi surface and scaling models, taking into account both the two-dimensional quasielastic small energy transfer via scattering of localized electrons on potential barriers of several different dots (Nyquist mechanism) and three-dimensional inelastic phonon scattering contribution. The dephasing time and length have also been extracted with a temperature exponent $p \approx 1.2$ for the natural semiconductor quantum dot system. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2840179]

The electron dephasing characteristics are powerful probes into transport properties and microscopic structures in metals and semiconductors. Various materials have been investigated during the last two decades,[1–5] where the magnetoconductivity is often employed to extract information on dephasing mechanisms. As is well established,[1] the electron conductance is significantly affected by scattering processes, which include elastic scatterings by potential barriers, impurities and defects, and inelastic scatterings between electrons and phonons. For elastic scatterings, the phases of the electron wave before and after a scattering event conform to a certain relationship which is called phase memory. As the temperature decreases, the lattice vibration is suppressed and the inelastic relaxation time gets longer while elastic scattering gradually dominates. When the temperature is sufficiently low, phase memory of the electron wave will cause strong quantum interference that enhances the probability with which an electron returns to its original position after a series of scattering events, giving rise to weak localization.[6] The time duration in which the electron wave remains coherent is called the dephasing time (τ_ϕ), while the dephasing length $L_\phi = \sqrt{D\tau_\phi}$, with D as the diffusion constant, is a key length scale in quantum interference phenomena. Suppose $\tau_\phi \propto T^{-p}$ at low temperatures, we have $L_\phi \propto T^{-p/2}$, where the temperature exponent p is an index on scattering mechanism, dimensionality, etc.[1]

Considerable interest has been paid recently to semiconductor nanostructures for their special properties and potential applications in optoelectronic devices, such as single photon detectors.[7] Among them, thin films containing natural Si nanodots are particularly attractive because they can be easily integrated to current silicon devices. We have demonstrated the control of electronic band structures[8] and resonant tunneling characteristics[9,10] in hydrogenated nanocrystalline Si (nc-Si:H) thin films. Nevertheless, in comparison to the extensive researches in metals and semiconductor bulk systems, the problem of dephasing has attracted much less attention in nanostructures, especially in semiconductor quantum dots. Most experimental investigations so far have focused on GaAs/AlGaAs quantum dots, where the dephasing times have been extracted from the observation of low temperature magnetoresistance.[11] A consistency has been found in these studies, where the dephasing times are best described by a temperature dependence of T^{-1} ($p=1$). The motivation of the present work is to carry out a detailed investigation combining the magnetoconductivity measurements with dephasing and localization theories for a complete understanding of the electron transport processes in the natural quantum dot system of nc-Si:H.

The studied nc-Si:H thin film sample was prepared in a radio frequency (13.56 MHz and power of 75 W) capacitive-coupled plasma enhanced chemical vapor deposition system from silane (SiH_4) and hydrogen (H_2) at a temperature of 250 °C with a chamber pressure of 1.0 Torr.[12] The percentage content of silane (SiH_4/SiH_4+H_2) was about 1.0%. The n-type nc-Si:H thin film with a thickness of ~1.0 μm was doped with phosphine (PH_3/SiH_4) of ~0.8% on a lowly doped p-type c-Si ($N_A < 10^{15}$ cm^{-3}) substrate, while the electron concentration N_D in the nc-Si:H thin film was about 5×10^{17} cm^{-3}, which was extracted from magnetic field dependent Hall effect measurements.[8,12] A long-range-ordered nc-Si:H microstructure on the c-Si substrate was revealed by high-resolution transmission electron microscopy. X-ray diffraction and Raman measurements confirmed the good quality of the nc-Si:H thin film with an average grain size of ~5 nm and a crystalline fraction of 51.7%. Indium was deposited for electrodes at four corners on the surface of the thin film. The temperature-dependent magnetoconductivity experiments were carried out to probe electron dephasing characteristics under an Oxford Instruments superconductive magnet.

Figure 1(a) shows the magnetic field B dependent magnetoconductivity of the nc-Si:H thin film at a temperature of 3.0 K. It is obvious that the magnetoconductivity under high magnetic fields (above 2.0 T) obeys the classical Boltzmann law (referred to as normal situation), where the conductivity decreases with increasing B due to the existence of magnetoresistance. However, the experimental data below 2.0 T clearly present an anomalous phenomenon of positive magnetoconductivity with increasing B. Figure 1(b) displays the detailed results under lower magnetic fields at temperatures below 17.0 K, which could be explained by the weak localization theory.[1] The magnetic field directly modifies the elec-

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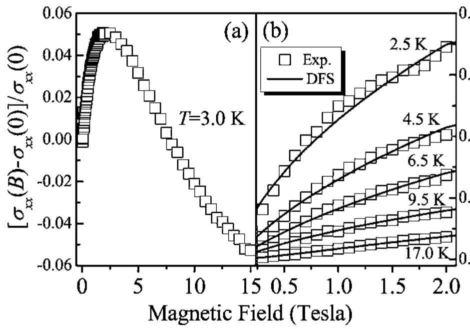

FIG. 1. (a) Magnetic field dependence of the magnetoconductivity in the nc-Si:H sample at 3.0 K. (b) Low magnetic field magnetoconductivity of the nc-Si:H sample at different temperatures. Solid curves are the DFS fittings of the experimental data (open squares).

tron wave, which gains additional phase while moving in the sample. By breaking the time-reversal symmetry, an increasing magnetic field weakens the quantum interference between two complementary electron waves traveling along a closed path in opposite directions, where the destruction of weak localization results in the increase of the conductivity. We can also observe from Fig. 1(b) that the lower the temperature is, the stronger the quantum interference becomes and, thus, the more evident this anomalous magnetoconductivity is. The solid curves are theoretical calculation results using diffusive Fermi-surface (DFS) theory[2,13,14] for the quantum interference, which are in good agreement with the experimental data in the range from $B=0.3$ to 2.0 T. The dephasing lengths for each temperature have been extracted during the fitting process, which are shown as the scatters in Fig. 2(a). The exponential fit of the experimental data represented by the solid curve gives a temperature exponent of −0.58, namely, $p \approx 1.2$, a value in agreement with other studies on quantum dots in the literature.[11,15–18]

It is clear from Fig. 2(a) that the dephasing lengths are much larger than the dot sizes (~5 nm), which implies that the electrons are not likely to be localized within one dot. To form a better comprehension of the dephasing mechanism in the nc-Si:H thin film, we first need to understand the electron transport process related to its microscopic structure, where the natural Si quantum dots are embedded in thin amorphous Si (*a*-Si) barriers.[8,12] In each dot, the electron energy is quantized due to spatial confinement, while between different dots, the centers of their discrete energy levels do not align in

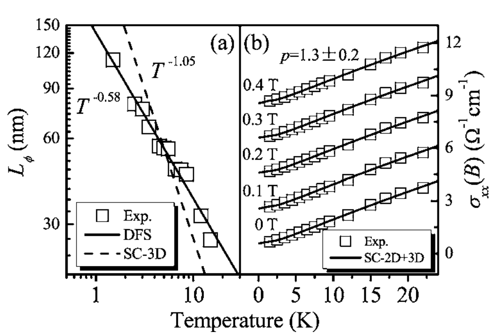

FIG. 2. (a) Temperature dependence of dephasing lengths extracted from the DFS fitting process (open squares). The solid curve represents an exponential fit which yields a temperature exponent of −0.58, differing from the result of −1.05 according to 3D scaling theory (dashed curve). (b) Temperature dependence of magnetoconductivity under low magnetic fields ($\leq$0.4 T). The experimental data (open squares) are fitted by a combined model of 2D and 3D scaling theories (solid curves), giving a temperature index $p=1.3\pm0.2$.

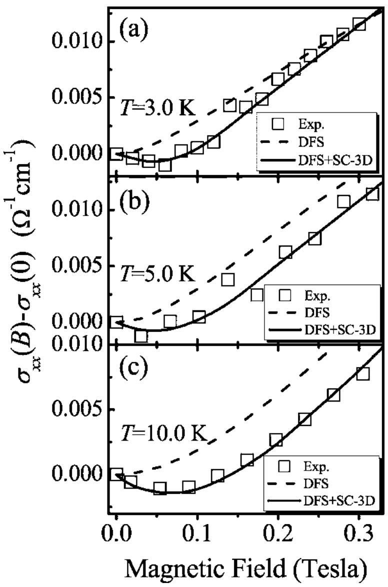

FIG. 3. Magnetoconductivity under very low magnetic fields at temperatures of (a) 3.0 K, (b) 5.0 K, and (c) 10.0 K. Dashed curves represent the DFS calculations that deviate from the experimental data (open squares), in contrast to the modified results by a combination of the DFS theory and 3D correction from the scaling theory (solid curves).

the absence of external electronic field because of the fluctuation of dot size. These energy levels will shift under bias and electrons can tunnel through the dots to form detectable resonant current when the energy levels in one dot align with another, which we have already observed.[9,10] Our observation of such long dephasing lengths suggests that the tunneling of an electron between two or more dots does not cause the electron wave to lose its phase coherence. This is possible since our nc-Si:H thin films have high mobility due to their ordered structure.[12] As often mentioned in the literature, the scattering is predominantly quasielastic in nature for low-dimensional systems at low temperatures, where phase randomization results from the cumulative effect of a number of scattering events, each involving a small energy transfer. This so-called Nyquist mechanism can be well applied to explain the electron dephasing in our sample, from which point of view we believe that in the nc-Si:H thin film, a localized electron wave travels along a closed path over several different dots, including a series of scattering events on potential barriers between the Si nanocrystals and *a*-Si surrounding.

In contrast to the good agreement in the magnetic field range from 0.3 to 2.0 T, the DFS theory could not fit well at low magnetic fields. The scatters in Figs. 3(a)–3(c) represent the experimental magnetoconductivity under B below 0.3 T at $T=3.0$, 5.0, and 10.0 K, respectively, where the dashed curves are the DFS fittings that obviously deviate from the experimental data. It is clear that the higher the temperature is, the larger the deviation becomes, where higher magnetic field is needed to overcome this discrepancy. The fact that DFS is not entirely applicable for low B suggests that there should be other related effects which increase with temperature but have not been included in the DFS theory. As a matter of fact, the DFS theory is deduced for quasi-two-dimensional (2D) systems,[14] implying that the deviation could arise from the mismatch between its 2D nature of the theory and the possible involvement of some three-dimensional (3D) contributions in the present nc-Si:H thin film sample. It is reasonable to assume that phonons may have played a role in the low magnetic field conductivity since the discrepancy is observed at finite temperatures and increases with the temperature.

In order to verify the validity of our assumption above, we have further performed the scaling (SC) theory of localization,[1] which has also been widely employed in the literature, to interpret our experimental data from a new aspect other than DFS. The scaling theory gives the quantum correction of the conductivity that is dependent on temperature in the forms of $T^{-p/2}$, $\ln T$, and $T^{p/2}$ for one-dimension, 2D, and 3D, respectively, offering us another method to extract the temperature exponent p. Figure 2(b) displays the temperature dependent conductivity under different low magnetic fields ($\leqslant 0.4$ T), each curve being shifted by 2.0 Ω^{-1} cm^{-1} for clarity. It is apparent that the experimental data do not conform to a $T^{-p/2}$ dependence, neither can it be well fitted by the $\ln T$ expression. Although the 3D formula of $T^{p/2}$ does provide a tolerable fit, yielding a p value of 2.1 during the process, the calculated dephasing lengths with $p=2.1$ plotted as the dashed curve in Fig. 2(a) show a remarkable discrepancy with the DFS results. To solve this inconsistency, we have proposed a combination of the SC theory with the 2D nature of DFS, taking both 2D and 3D corrections into account. The modified formula for the conductivity can be expressed as $C_1 T^{p/2} + C_2 p \ln T + C_3$, where C_1 and C_2 are the respective coefficients indicating the significance of each contribution and C_3 is the residual term. It is notable that C_1 contains a microscopic length scale according to the SC theory while C_2 should include another quantity of length, where we have employed the dephasing length and the size of the nc-Si:H sample, respectively. This model has resulted in satisfactory fittings for the experimental data under low magnetic fields, as shown by the solid curves in Fig. 2(b). The temperature exponent $p = 1.3 \pm 0.2$ extracted during the process confirms the reliability of $p \approx 1.2$ from the DFS fittings of Fig. 1(b).

Furthermore, this combined expression can also help us solve the imperfection of DFS at low magnetic fields. As the 3D correction successfully serves the SC fittings above, we utilize this term to revise the DFS values as well. The fundamental concept of this modification is that the magnetoconductivity calculated by the DFS theory at a certain temperature under a fixed B only takes 2D correction into consideration, and that we can involve the 3D contribution to realize an improvement, the quantity of which is computed using the coefficients C_1 and C_2 obtained from the fitting process in Fig. 2(b). The solid curves in Fig. 3 are the modified results integrating DFS with SC theory, which turn out much better agreements with the experimental data. As the magnetic field increases, the significance of the 3D SC correction compared to the 2D DFS contribution decreases, where its modification to the DFS values gradually becomes negligible. Therefore, the sole DFS theory can fit well when B is higher than 0.3 T, as already demonstrated in Fig. 1(b).

The above achievements of good fittings for the overall experimental magnetoconductivity illuminate that our nc-Si:H thin film possesses both the 2D and 3D characteristics. The 2D microscopic structure of the thin film sample leads to an electronic energy band diagram similar to a semiconductor superlattice, as already observed in the resonant tunneling measurements.[9,10,19] The 3D behavior indicates that the electrons are not restricted in a definite plane but are possible to move along all directions like in a bulk system, where the phonons have been attributed to make the contribution. Phonon scatterings reduce the number of electrons tunneling resonantly through quantum dots (and, hence, the conductance) due to the misalignment of the energy levels. Under very weak magnetic fields (<0.1 T), the further decrease of conductance with increasing B in Fig. 3 can be explained within the weak localization theory as the result of spin-orbit (SO) interactions.[4] The small quantum corrections of the localization effects can be positive or negative depending on the importance of the SO scatterings. In the presence of SO scatterings, the constructive interference (positive magnetoconductivity) could turn to destructive interference, where the magnetic-field-induced electron dephasing results in negative magnetoconductivity phenomenon. Both the 3D distribution of electron spatial orbits and phonon scatterings are included in the present 3D SC correction, which describes well the negative magnetoconductivity phenomenon through complementing the DFS at the lowest magnetic fields. With the further increase of the magnetic field, the destruction of localization overwhelms the phonon effect, resulting in the increase of magnetoconductivity. Moreover, the phonon contribution is expected to increase with temperature, which has been clearly shown in the temperature dependent magnetoconductivity of Fig. 3.

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