Studies of the phase transition of water confined in the mesoporous adsorbent (MCM-41) using X-ray diffraction (Study of the dynamic behavior of CDW using x-ray scattering)

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In many materials with a highly anisotropic band structure, electron-phonon interactions lead to a novel type of ground state called the charge-density wave (CDW). The ground state of the coupled electron-phonon system is characterized by a gap and a collective mode formed by electron-hole pairs involving the wave vector $q = 2k_F$. The charge density associated with the collective mode is given by

$$\rho(r) = \rho_0 + \rho_1 \cos(2k_F \cdot r + \varphi)$$

where the ρ_0 is the unperturbed electron density of the metal. The phase φ of the CDW is a fundamental important term. In the previous measurement on BL12B2, using the multiple diffraction technique we investigated the interference effect between the CDWs and the host structure in a quasi-2-dimensional charge-density wave material 2H-$NbSe_2$, and observed that the related CDW phases did not change by varying the temperature. This finding suggested that the CDW phases are pinned by the imperfections of the crystal. In order to observe the dynamic phenomena due to the relative moving of CDW, CDWs must be de-pined from the imperfections. For doing so, an electric field was applied to the chain direction of a CDW material $K_{0.3}MoO_3$. Consequently, electric field exceeding the threshold value results in the nonlinear conductivity as shown in Figure 1. It is clear to see that the nonlinear behavior as the applied field exceeding the threshold, $V_C \sim 0.165$ V, namely a transition from the pinned state to the sliding state.

$K_{0.3}MoO_3$ is a linear-chain compound, and undergoes a metal-insulator transition at T=180 K due to the formation of charge-density waves (CDWs). An incommensurate CDW satellite reflection was located at (13 q –6.5), q≈0.75, at T = 70 K. Scans were performed through the longitudinal direction, which is transverse to the direction of the applied fields. Figure 2 shows the evolution of the integrated intensity of CDW satellite reflection (13 q -6.5) as a function of applied electric fields at T = 70 K.

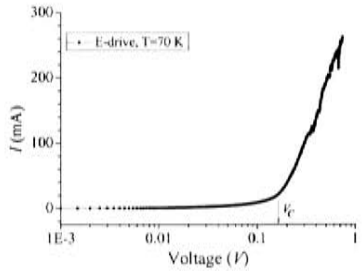

Figure 1: The non-linear conductivity as measured at 70 K on a single crystal $K_{0.3}MoO_3$. The V_C, ~0.165 V, indicates the threshold for the occurrence of sliding CDWs.

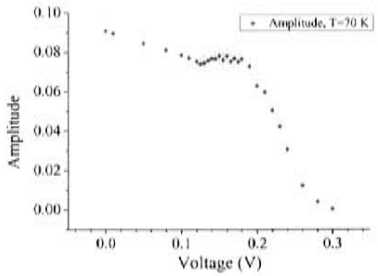

Figure 2 Evolution of the integrated intensity of CDW satellite reflection (13 q -6.5) as a function of applied electric fields at T=70 K.

X-ray scattering study on semiconductor nanostructures

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We have performed grazing incidence x-ray scattering (GIXS) and resonant x-ray scattering (RXS) on GaAs quantum wires grown on an InP(001) substrate with an InGaAs buffer layer. Figure 1 illustrates the profile of a radial scan around the InP(2 2 0) surface Bragg peak. In addition to the sharp Bragg peak, two pronounced bumps on both sides of the Bragg peak are clearly observed. These bumps are the inter-wire correlation peaks. Their positions, ~ 0.038 $Å^{-1}$ away from the InP (220) peak along the [2 2 0] direction, reveal that the wires are aligned with their axes parallel to the [2 –2 0] direction and the average inter-wire spacing is approximately 170 Å. The intensity difference between the two bumps is attributed to the lattice mismatch between the GaAs quantum wires and the underlying InP substrate. Lattice constant of bulk GaAs is ~ 3.5% smaller than that of InP. Therefore, it is expected that normal to the wire axis, the lattice is compressed on the bottom and gradually relaxes on the way to the top of the wires. As observed in the profile of the radial scan, the intensity at high q side, which is associated with the smaller lattice of the quantum wires, is higher than that of low q side, which is related to the dilated part of the substrate lattice.

It is well known that the composition of self-assembled In(Ga)As quantum dots grown on GaAs is not uniform. It is strongly speculated that the composition of these GaAs quantum wires is not uniform, either. The methods used for quantum dots compositional distribution studies depend on either the intensity ratio between the strong and weak diffractions [1] or the intensity variation of the same diffraction at different energies, i.e. the anomalous effect [2]. Nevertheless, due to the strong intensity modulation introduced by the correlation peaks, the methods mentioned above cannot be applied in this case. The resolve this problem, we employed resonant x-ray scattering, where the shape of the energy scan instead of the intensity is sensitive to the In/Ga concentration, to determine the composition of the GaAs quantum wires. Illustrated in fig. 2 are the radial (circles) and angular (squares) scans across InP (200) surface Bragg peak. ΔQ represents the deviation of the scattering vector from the (200) peak in the unit of reciprocal lattice unit (rlu). The different profiles of the two curves again manifest the anisotropy of the strain distribution in the wires. The energy spectra across the Ga k-edge collected at various radial scattering vectors, q_r, as marked by the arrows of the same color, are displayed in the inset. The systematically broadening of the dips in the spectra collected at larger q_r indicates the reduction of In concentration at regions of larger lattice mismatch with the InP substrate. Because the lattice is expected to be smaller at the top of the wires, the result implies In concentration gradually decreases from the bottom to the top of the wires. Moreover, even at the top of the wires there still exists considerable amount of In. To obtain quantitative compositional distribution, both the model simulation and numerical fitting of the experimental data is ongoing.

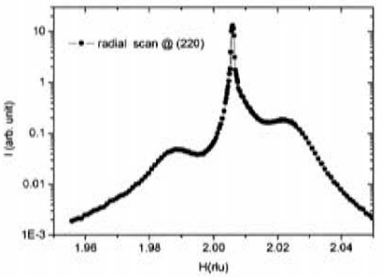

Figure 1. The intensity distribution of a radial scan along [110] direction around the InP (220) surface Bragg peak.

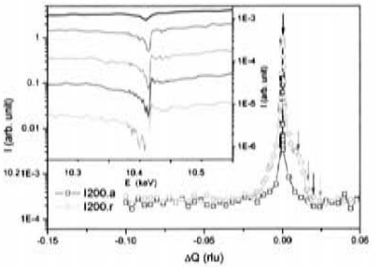

Figure 2. The open circles/squares depict the intensity distribution of a radial/angular scan along [200]/[020] direction around InP (200) surface Bragg peak. Resonant x-ray scattering scans across Ga k-edge around the InP (200) surface Bragg peak are displayed in the inset. The location of each energy scan is marked by the arrow with the corresponding color in the radial scan.

References
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