Cooperative interplay between impurities and charge density wave in the phase transition of atomic wires

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Abstract
Impurities interact with a charge density wave (CDW) and affect the phase transitions in low-dimensional systems. By using scanning tunneling microscopy, we visualize the interaction between oxygen impurities and the CDW in indium atomic wires on Si(111), a prototypical one-dimensional electronic system, and unveil the microscopic mechanism of the intriguing O-induced increase of the transition temperature ($T_c$). Driven by the fluctuating CDW, the O atoms adopt an asymmetric structure. By adjusting the asymmetry, a pair of O impurities in close distance can pin the one-dimensional CDW, which develops into the two-dimensional domains. First-principles calculations showed that the asymmetric interstitially-incorporated O defects induce shear strains, which assists the formation of hexagon structure of the CDW phase. The cooperative interplay between the O impurities and the CDW is responsible for the enhancement of the CDW condensation and the consequent increase in $T_c$.

1. Introduction

In reduced-dimensional electronic systems, electron–electron correlations and electron–phonon couplings are enhanced, often leading to novel properties such as Mott insulators [1], charge density waves (CDWs) [2], and Luttinger liquids [3]. The former two properties emerge through phase transitions when the systems are sufficiently cooled. Over the past decades, the phase transitions in the reduced dimensional systems have been the subject of fundamental research to understand the novel physics, which is richer than in the bulk [4, 5].

The CDW transition, manifested by a metal–insulator transition coupled to a symmetry-breaking structural transition, is an example which has been intensively studied in several one-dimensional (1D) [6–11] and two-dimensional (2D) systems [12, 13]. Impurities are known to affect the CDW phase transitions by providing inhomogeneous electronic and structural perturbations to the host systems. In general, the impurities can suppress the condensation of CDW with long-range order, causing a transition to occur at temperatures lower than that in a pure system [14–16]. On the other hand, mobile impurities, arranged into quasi-regularity through interactions with the CDW, have been predicted to assist the formation of the long-range CDW ordering [17]. Experimentally, hopping impurities enhancing the CDW condensation have been deduced indirectly in a 2D CDW system [18, 19].

An array of indium atom wires on Si(111), which is a prototypical 1D system, undergoes a phase transition from a metallic $4 \times 1$ phase to an insulating $8 \times 2$ (hereafter $8 \times 2$-LT) structure at about 125 K [6]. Extensive studies of this Si(111)-In surface have been performed in order to understand the origin of this reversible transition. The related fundamental questions are the origin of the broken-symmetry $8 \times 2$-LT phase and the nature of the $4 \times 1$ phase at room temperature (RT). Two different views have been proposed. One view is that the $8 \times 2$-LT phase is the CDW phase formed by a Peierls-type instability of the quasi-1D In chains with the static $4 \times 1$ structure [6, 20]. The existence of the Fermi surface nesting was given to support this view. Another view is to consider that the $8 \times 2$-LT phase is achieved by the energy-lowering lattice distortion [21]. The $4 \times 1$...
phase at RT was then explained as an incoherent dynamical fluctuation of the $8 \times 2$-LT phase \cite{22, 23}. These CDW and non-CDW views on the transition are still in controversy.

Impurities in this quasi-1D In/Si(111) system affect the phase transition \cite{24–30}, and produce intriguing phenomena such as phase separation \cite{31} and topological soliton excitations \cite{32} as well. While most impurities decreased the $T_c$ \cite{25–29}, oxygen was exceptional in that it increased the $T_c$ \cite{26}. Although several scenarios such as hole doping, correlated arrangement of impurities \cite{25}, and local strain \cite{33} were proposed to explain this extraordinary impurity-induced enhancement of the transition, the detailed microscopic mechanism remains veiled.

In this work, we investigated how the O impurities interact with the Si(111)$4 \times 1$-In surface and enhance the transition into the $8 \times 2$-LT phase (i.e., the CDW phase in the CDW-transition view\cite{3}). The interaction between the O impurities and the CDW is visualized in atomic scale by using scanning tunnelling microscopy (STM) and their cooperative interplay enhancing the CDW condensation is demonstrated. Driven by the interaction with the developing CDW near the transition, the O adsorbates adopt an asymmetric structure that is confirmed by density-functional-theory (DFT) calculations. Interestingly, the asymmetry of O impurities can be adjusted in phase with the CDW, which triggers the nucleation of the 2D CDW domains, enhances the CDW condensation, and consequently increases $T_c$.

2. Experiments

The experiments were performed by using variable-temperature STM (VT-STM) in an ultra-high vacuum below $1.0 \times 10^{-10}$ Torr. The Si(111)$4 \times 1$-In surface was prepared by depositing a monolayer of In onto an $n$-type Si(111) (electrical resistivity of $5–10$ $\Omega \cdot$ cm at RT) substrate at $700–750$ K. The Si(111)$4 \times 1$-In was dosed with oxygen gas backfilling the chamber through a variable leak valve at RT. STM measurements were made at variable temperatures, which were adjusted by the amount of liquid nitrogen supplied to the cryostat and by an ohmic heater at the cold finger. The temperature change was controlled with the rate of $\sim 10$ K per hour to maintain the stability.

3. Theoretical methods

The DFT \cite{34} calculations were performed within the local density approximation (LDA) \cite{35} using the Vienna Ab-initio Simulation Package \cite{36}. The Si(111)$4 \times 1$-In was modeled by a repeated slab with a $8 \times 19$ surface supercell and a $19$ Å thick vacuum. The slab was made up of In wires, Si Seiwatz chains, three Si bilayers, and the passivating bottom H layer, and the theoretical lattice constant of $5.39$ Å was used. The ions were represented by ultrasoft pseudopotentials \cite{37}, the plane wave basis set was terminated by using a kinetic energy cut-off of $400$ eV, and the Brillouin zone (BZ) integration was done by employing a $2 \times 1$ $k$-point grid corresponding to a $4 \times 19$ $k$-point mesh in the $4 \times 1$ surface BZ. The atomic structures were optimized by requiring that the Hellmann–Feynman forces were smaller than $0.01$ eV Å$^{-1}$, while keeping the bottom Si bilayer and the H layer fixed.

4. Results and discussion

Figure 1 (a) shows an STM image of the Si(111)$4 \times 1$-In surface dosed with 1 Langmuir (L) of O$_2$ at RT. The image was taken at $140$ K, which is well above $T_c$. Several defect features, either native or extrinsic, are indicated. The vacancy-like defects ($V_1$, $V_2$) are native defects, which are typically found without oxygen adsorption. On the other hand, the other defects ($B$, $D_1$, $D_2$, $D_a$) are O-induced features. Three of them ($B$, $D_1$, $D_2$), which possess mirror symmetry with respect to the line perpendicular to the wire, were observed previously at RT \cite{38, 39}. In addition to these symmetric O features, a new dark O defect ($D_a$) was found on the cooled surface. The $D_a$ defect is clearly distinguishable by its characteristic asymmetry due to a single off-center bright protrusion on the opposite side of the depression. Note that period-doubling ($\times 2$) modulations were formed locally on both sides of all these isolated vacancies and O defects. These are the lattice distortions commonly formed around the defects, which are different from that of the CDW phase ($4 \times 2$-LT) \cite{40}. This suggests that isolated defects do not induce the condensation of CDW. As shown below, however, the asymmetric $D_a$ defects can enhance the CDW condensation if they are located close to each other.

\footnote{In this paper, we adopt the CDW view. However, an alternative description based on the non-CDW view is also possible. For example, ‘the CDW condensation’ can be replaced by ‘the formation of the $8 \times 2$-LT structure’.}
that the asymmetries of the Da defects as well as the tilt directions are determined to accommodate the formation of the 2-LT structure in the bounded sections depends on the distance between the two Da defects. With a distance of 1.5 \( a_0 \), the 2-LT structure in the bounded region, as depicted in the schematics. The Da defects appear to be unique and critical in assisting the formation of the LT-phase structure (condensation of the CDWs). The way that the Da defects mediate the CDW condensation is unveiled when a segment is bounded by a pair of Da defects on the same wire. On each wire, two Da defects can be located either on the opposite (in figures 2(b) and (c)) or the same (in figures 2(d) and (e)) subchains.

When two Da defects are located on different subchains, the depressions are separated by a center-to-center distance of \((2n + 1.5)a_0\) (11.5 \( a_0 \) in figure 2(b)) or \((2n + 0.5)a_0\) (10.5 \( a_0 \) in figure 2(c)) \( m \) is a positive integer, where \( a_0 \) is the Si lattice spacing defining the \( \times 1 \) periodicity, 3.84 Å. In both cases, the bounded segments exhibit a 4 \( \times \) 2-LT structure (1D CDW). Note that the tilt directions in figures 2(b) and (c) are opposite. This indicates that the asymmetries of the Da defects as well as the tilt directions are determined to accommodate the formation of the 4 \( \times \) 2-LT structure in the bounded region, as depicted in the schematics.

The situation changes when two Da defects are located on the same subchains. The formation of the 4 \( \times \) 2-LT structure in the bounded sections depends on the distance between the two Da defects. With a \((2n)a_0\) distance (12 \( a_0 \) in figure 2(d)), the bounded section exhibits a 4 \( \times \) 2-LT structure. In contrast, the 4 \( \times \) 2-LT structure is not formed in the region bounded by two Da defects with \((2n + 1)a_0\) separation (17 \( a_0 \) in figure 2(e)). Instead, the bounded segment shows a strong 4 \( \times \) 2-like modulation, which is different from the 4 \( \times \) 2-LT structure. In addition, the Da defects which are sufficiently close in the adjacent wires can also induce a patch of the 8 \( \times \) 2-LT structure (2D CDW) (see figure 2(a)).

On the other hand, pairs of the other defects (\( V_1, V_2, B, D_1, \) and \( D_2 \)) were not found to induce the 4 \( \times \) 2-LT structure in the bounded sections. Several examples of segments in 4 \( \times \) 1 wires bounded by pairs of the symmetric defects which are either native (\( V_1 \) and \( V_2 \)) or O-derived (B) are shown in figure 3. In all cases, \( \times \) 2-like modulations are formed in the bounded regions. These modulated structures are different from that of the low-temperature phase (4 \( \times \) 2-LT), but rather similar to the defect-induced \( \times \) 2 structures [40]. Therefore, it is concluded that the pairs of the symmetric defects do not induce the 4 \( \times \) 2-LT 1D CDW in the bounded sections.
One might think that the formation of the localized $4 \times 2$-LT structure may depend on the distance between the two defects regardless of their types (i.e., all the segments become $4 \times 2$-LT structures when they are bounded by pairs of defects which are close enough). However, figure 4 shows that it is not the case. The segment bounded by $D_a$ defects on the opposite subchains takes the $4 \times 2$-LT structure even at a distance as large as...
21.5 \( a_0 \) (figure 4(a)). On the other hand, the segments bounded by other defects do not form the 4 \( \times \) 2-LT structure even though the defects are located closer (see the cases in figures 4(b)–(d)). Therefore, it is concluded that this local phase transition is a genuine effect of oxygen adsorption at the Da sites, not a ubiquitous effect of all the defects.

DFT calculations were performed to confirm the existence of the asymmetric configuration of the adsorbed oxygen and to address the formation mechanism of the 4 \( \times \) 2-LT structure between the two asymmetric defects. In addition to the symmetric interstitial O structures which were reported previously [38, 39], four asymmetric and stable interstitial O structures were found. Figure 5 shows the newly-found asymmetric and stable interstitial O structures. The \( I_{11} \) and \( I_{12} \) in figures 5(a) and (b) are the reflection-counterpart of each other where the interstitial O forms three bonds with two surface In and one substrate Si ions. The incorporated O atoms in these structures are slightly displaced along the chain direction from the symmetric site, which preserves the mirror symmetry of the clean In wires. On the other hand, the neighboring In atoms are pushed, resulting in a significant deformation from the symmetric structure. The newly found \( I_{11} \)’s are higher in energy by 0.52 eV than the ground-state symmetric structure. The \( I_{61,62} \) are the analogs of \( I_{11,12} \) where the O atom lies in the opposite subchain as shown in figures 5(c) and (d).

The asymmetric deformation of In wires due to O incorporation is reflected in the STM image of \( I_{12} \) shown in figure 6(a). The simulated STM image reproduces well the characteristic features of the experimental
asymmetric D$_a$ defect (figure 1(b)); an elongated dark depression (ellipse) centered at the O site and a bright protrusion (circle) on the other subchain which is off-center with respect to the center of the dark depression. Figure 6(b) shows the configuration of two asymmetric interstitial O atoms which corresponds to the experimental D$_a$-pair in figure 2(c) at a distance of $d = 20.5 + 0.5a_0$. The bounded region, initially prepared as a $4 \times 1$ structure, adopted a $4 \times 2$-LT hexagon structure upon relaxation. The characteristics of the simulated STM image of the paired asymmetric interstitial O atoms are comparable to the experiment (figure 2(c)). Based on the good agreements between the experimental and theoretical STM features of both the single and paired asymmetric defects, the experimental D$_a$ defect can be identified as a newly-found asymmetric interstitial O structure.

The asymmetric D$_a$ defects originate from the symmetric D$_2$ defects$^4$. Figure 7(a) shows the transformation of an isolated D$_2$ defect into the D$_a$ defect on the $4 \times 1$ surface at 135 K which is above $T_c$ (top panel). A D$_2$-to-D$_a$ transformation can yield two different asymmetric defects, D$_a$L and D$_a$R, where L (left) and R (right) denote the location of the opposite-subchain bright protrusion relative to the dark depression. The D$_a$ defects can also be switched back to D$_2$. This shows that the asymmetric D$_a$ defect can alter its asymmetry (D$_a$L versus D$_a$R) even at temperatures as low as 135 K. When the temperature was cooled further to well below $T_c$, the asymmetry of the D$_a$ defect was locked in-phase with the $8 \times 2$-LT structure as shown in the STM image taken at 115 K (bottom panel of figure 7(a)).

For detailed analysis of the evolution of the O-derived defects as well as the $4 \times 1$-to-$8 \times 2$ transition, sequential STM images of the same area were obtained as the O-adsorbed surface is cooled from 160 K to 110 K. The mutual transformations between the symmetric O defects (B, D$_1$, and D$_2$), which were observed occasionally at RT$^3$, rarely occurred at LT. The O defects were distributed randomly and immobile. The fraction of the $8 \times 2$ area and the counting statistics of the O-derived defects observed in the images as a function of the temperature are presented in figure 7(b).

As the temperature decreased, the $8 \times 2$-LT area showed an abrupt increase occurring at approximately 133 K (which is higher than the $T_c = 125$ K of pristine In wire), where the condensation of 2D CDW began$^5$. The number of D$_a$ defects also increased at the expense of D$_2$ defects, whereas the total number of D$_a$ and D$_2$

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4 The atomic structure of the symmetric D$_2$ defect has not been determined by the theoretical calculations. One speculative possibility is that the D$_2$ defect is a time-averaged structure of the fluctuating D$_a$ between D$_a$L and D$_a$R (i.e., $I_1$ and $I_2$ in figure 5).

5 This temperature corresponds to the $T_c$ of the Si(111)-In surface with 1.0 L of oxygen, which is higher by about 7 K compared with the $T_c$ of the pristine surface determined in the similar procedure. This confirms the previously reported increase of the $T_c$ due to the O adsorption$^6$. 

remained almost the same. The D₂-to-D₄ transformations, however, has already started at higher temperatures and progressed considerably at 133 K. This suggests that the O-induced global CDW (4 × 1-to-8 × 2) transition is highly correlated with the local D₂-to-D₄ transformation: the 2D CDW condensation requires a considerable number of the Da defects to be formed precedingly. In contrast, the numbers of other O defects (B and D₁) show a negligible change with temperature, implying that they are not relevant to the CDW condensation.

The crucial role of Da defects in CDW condensation is exemplified in the variable-temperature STM images in figure 7, which show how the CDW condensation proceeds. The initially 4 × 1 region at 140 K with several closely-located Da defects is turned into an 8 × 2 domain at 130 K. As the temperature was lowered further to 120 K, the 2D CDW propagated over most of the area.

It was reported that defects impose strain on the wire, affecting the formation of the 4 × 2-LT structures. Similarly, the newly-found Da defect imposes strains on both subchains owing to its asymmetry and interstitially. For instance, the interstitial O in $I_{41}$ induces strain so that the In atoms move away from the O site (schematically depicted by the arrows in figure 5(a)). The magnitudes of the average In displacements are significantly different on both subchains, which induces effective shear strain in In wires. Such a shear strain is a prerequisite to form the LT-hexagon structure. In addition, a constructive superposition of the dimerizations of the outer In atoms can result in the formation of a LT-hexagon structure. This occurs when the neighboring Da defects are located in different subchains (see figure 6(b)) or are separated by even multiples of a

Because Da defects were not observed at room temperature, we can also assume that the Da defects already existing at 160 K were originated from the D₂ defects.
lattice constant \([2n a_0]\) in the same subchain. The asymmetries of the O defects are determined in a way to make the constructive superposition possible. On the other hand, the dimerization in the bounded region is not possible if the D_4 defects are separated by odd multiples of a lattice constant \([2n + 1a_0]\) in the same subchain, because of the out-of-phase superposition.

There have been two propositions for the \(T_c\)-increasing mechanism. One is the hole doping mechanism and the other is the correlated arrangement of mobile O adsorbates [25]. The hole doping scenario was not supported either by experiments [33] or by theoretical calculations [41]. Rearrangement of the impurities at temperatures near \(T_c\) [17–19] is also disproved by current observations that the O adsorbates are distributed randomly and immobile.

The observations in this work, however, provide a solid atomistic picture for the mechanism of the O-induced enhancement of the CDW \((4 \times 1\)-to-\(8 \times 2\) transition) (i.e., the increase of the \(T_c\)). The central ingredient is the transformability of a symmetric D_2 defect into an asymmetric D_a defect with the appropriate asymmetry to accommodate the developing CDW. We speculate that this D_2-to-D_a transformation is driven by the interaction with the CDW, as depicted schematically in figure 7(d). As the temperature approaches \(T_c\), from above, the fluctuating 1D CDWs likely to be formed and induce a D_2-to-D_a (and vice versa) transformation when they pass through the O defects (too fast to be imaged). The fluctuating 1D CDWs can be pinned by a pair of D_a defects which are located closely in the same chain (see figure 2): i.e. the \(4 \times 2\)-LT structure is formed locally in-between the two D_a defects.

Individual \(4 \times 2\)-LT structures existing as local, isolated, small segments have a short-range 1D ordering at best. As the surface is cooled sufficiently below \(T_c\), the long-range 2D ordering (the condensation of the 2D CDW) is triggered by both the intrawire and interwire interactions driving the D_2-to-D_a transformation further. Two conditions should be ensured when establishing the 2D-CDW condensation with a long-range order surrounding the defects: (i) along the chain, the tilt direction of the \(4 \times 2\)-LT is maintained the same on both sides of the defects, and (ii) it should alternate across the chain, forming the \(8 \times 2\)-LT phase, as shown in the bottom panel of figure 7(a). The symmetric D_2 defect, like the other O defects (B and D_1) cannot fulfill these requirements because of its mirror symmetry. On the other hand, the D_a defect can easily satisfy these requirements via its asymmetric shape and, more importantly, its flexibility to choose the asymmetry directions. By interacting with the CDWs in the neighboring chains, the D_a defect that transformed from a D_2 defect takes the suitable asymmetry \([D_{4,1}\text{ or } D_{8,8}]\) to make the tilted \(4 \times 2\)-LT segments in phase with the surroundings in both the longitudinal and transverse directions. This cooperative interplay between the O defects and the CDW leads to the enhanced condensation of the 2D CDW \((8 \times 2\)-LT phase in a large area.

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