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Electronic band structure modulated by local surface strain in the (111) facet of the ⟨112⟩ silicon nanowires

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ABSTRACT

Based on the models built with our "cyclic replacement" method we introduced local strain into the (111) facet of the Si ⟨112⟩ nanowires. With ab initio approach, it is found that the electronic band structures of the nanowires are modulated efficiently by the surface strains: the indirect band gap declines by strong surface compression, while it always decreases and impressively changes to a direct band gap with surface tension. Moreover, the local deformations result in spatial separation of the valence band minimum to the compressed surface and the conduction band minimum to the tensed surface.

Strain has been proved to be a useful method for property modulation of various materials, which is an effective and economic way to modify the electron mobility, [1–3] band gap width, etc. [1,4–7]. For example, strain is widely used to improve the performance of the silicon materials [8,9]. Strain effect is more significant in nanostructures because subtle structure changes can lead to large modifications in properties due to the size effect. Over the past few years, strain has been extensively studied for property modulation of the nanomaterials [10]. The strain effects are often studied theoretically by changing the lattice constant for homogeneous axial strain within the one-dimensional materials or uniform biaxial strain within the two-dimensional materials [11–14]. These studies increase the understandings about the strain effects, while most strains within materials are local and constrained near the surfaces which decay fast to the bulk due to the lattice resistance stress. The surface strain is common near hetero-interfaces. For example, within silicon/germanium interfaces [8,9] compressive strain and tensile strain can be found within Ge and Si near the interface, respectively, due to their 4% lattice constant difference. Till now very few studies have been performed to explore the local deformed structures near surfaces, [15] due to experimental challenge to decompose the surface strain effect, and theoretical difficulty to construct models for the local deformations.

In this paper, we present a novel approach to study the surface strain effects by introducing local deformations within (111) facet of Si ⟨112⟩ nanowires with the "cyclic replacement" method. [16] The Si ⟨112⟩ nanowires (NWs) are chosen in our simulations because the local surface strain within their (111) facet decays fast from surface to bulk with the single bonds linking the layer-like structure along [111] direction (see Fig. 1a). Subsequently small models can be used to save calculation cost. The progress to introduce surface strain by "cyclic replacement" [16] is demonstrated in Fig. 1. The basic idea of this method is firstly introducing some surface defects (e.g. Al) to the target surface; after relaxation the surface is deformed due the defects; and afterwards the defect atoms are replaced with the original atoms (Si and H) and the (110) facet is fixed for the second relaxation. The optimized model with the deformed surface is then used to simulate the surface strain near interfaces. We define the surface strain with $\alpha = \frac{(A_0' - A_0)}{A_0} \times 100\%'$, where A_0 is width of the surface in ⟨112⟩ direction without strain, as denoted in Fig. 1a, and A_0' is the updated width of the deformed facet. Positive and negative α implies tensile and compressive surface strains, respectively. The surface strains can be controlled by amount of the defects atoms used in the "cyclic replacement" method.

Our first-principles calculations are performed with the VASP package [17–19] which is based on density functional theory (DFT) [20] using projector augmented wave potentials [21] and a plane-wave basis set. The total energy is calculated with the GGA [22,23] using the PBE functional. [23] The cutoff energy is set to 400 eV and $1 \times 1 \times 8$ Monkhorst–Pack [24] k-point mesh is used. Si nanowires with different diameters are employed in our simulations, of total 96 ($Si_{64}H_{32}$), 140 ($Si_{100}H_{40}$), and 236($Si_{182}H_{54}$) atoms. Cross-sectional aspect ratios (A_0/B_0) of the (111) to the (110) facet

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(see Fig. 1) without strain of these NWs are 1.32(96), 1.30(140) and 1.18(236) respectively [25]. The NWs are modeled in a supercell with periodic boundary conditions, with lattice parameter of 6.77 Å (vs. experimental 6.65 Å) [26,27]. The vacuum thickness between a nanowire and its images is 10 Å. All models, including those with various surface strains are relaxed until force is less than 0.02 eV/Å. In our simulations, we barely find isolated defect states within the band gap even with 9% compression in the NWs, implying that the surface strains less than 9% in the (111) facet of the Si ⟨112⟩ nanowires are always elastic deformations. Because 5% tensile or compressive local surface strain only results in less than 0.03 Å axial lattice constant change, changes of the lattice constant along the ⟨112⟩ growth direction due to the deformed surfaces are omitted in our simulations. This is explained by the strong elastic resistance of the bulk to the local surface deformation. In the following, results of surface strains less than 9% are collected and discussed.

Band gaps of Si ⟨112⟩ NWs can be remarkably modified by the surface strains within the (111) facet, as shown in Fig. 2a. The band gap of a Si NW decreases with increased tensile surface strain; on the other hand, the band gap is almost maintained upon compressive surface strain less than 6% while it decreases due to intense compression. Detailed modifications of the band structure of a ⟨112⟩ Si NW by surface strains are shown in Fig. 2c. The ideal Si-140 NW without surface strain has an indirect band gap of 1.24 eV, where the valence band maximum (VBM) locates at Γ point and conduction band minimum (CBM) locates at X point. Surface compression hardly modifies the band gap, and the CBM still locates at X point (see bands marked in red and green); while the second highest band branch (marked in pink) within the valence band shifts up at Γ point. When the compression is stronger than 6%, energy of this band branch shifts up so much that it becomes the highest band below the Fermi level. As a result, large compressive strains (i.e stronger than 6% compression) result in decrease of the band gap. On the other hand, tensile surface strains also induce decrease of the band gap, and even indirect-to-direct band gap transition: the band structures near VBM change little, while the band branch marked in red shifts down in energy and to be the lowest band branch within the conduction band at Γ point when the tensile strain is larger than 4.5%. As a result, the CBM of the Si-140 NW changes from X point without surface strain to one third π/a with 4.0% tensile surface strain, and then to Γ point with 4.5% tensile surface strain. In the Si-96 NW and Si-236 NW, this indirect-to-direct band gap transition occurs with around

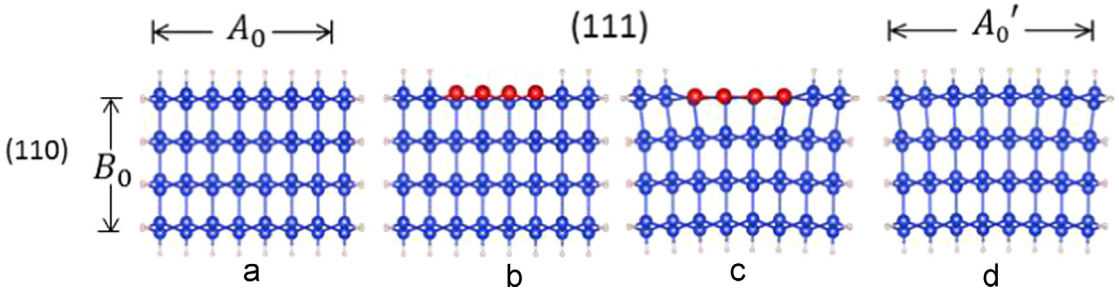

Fig. 1(Color online). (a) Cross section of an ideal ⟨112⟩ Si NW; (b) four of Si–H pairs in (111) facet are replaced by Al atoms; (c) relaxed structure of (b); (d) Al atoms are replaced back by the original Si–H and relaxed with fixed (110) facet. Blue, pink and red balls mark Si, H and Al atoms, respectively.

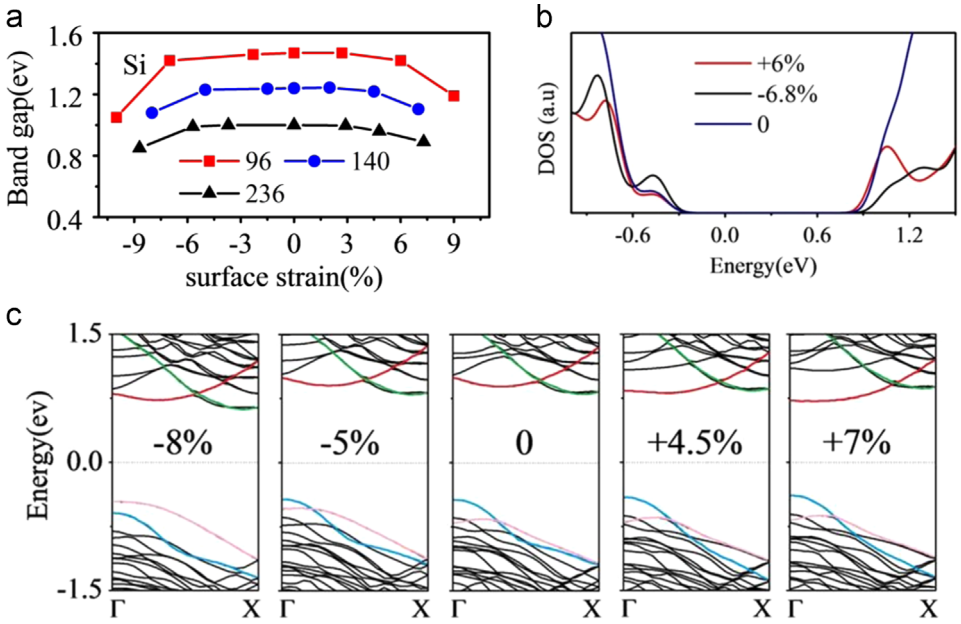

Fig. 2(Color online). (a) Band gap changes of ⟨112⟩ Si NWs in different sizes as a function of surface strain. Red, blue and black curved denote 96 ($Si_{64}H_{32}$), 140 ($Si_{100}H_{40}$), and 236 ($Si_{182}H_{54}$) nanowires; (b) total DOS for Si NWs with surface strains. (c) Near-gap bands of Si NWs with various surface strains. Four near-gap band branches are marked in different colors for clarity. 0 surface strain denotes the unstrained NWs.