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First Principles Simulations of Nanoscale Silicon Devices With Uniaxial Strain

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Abstract—We report parameter-free first principle atomistic simulations of quantum transport in Si nanochannels under uniaxial strain. Our model is based on the density functional theory (DFT) analysis within the Keldysh nonequilibrium Green’s function (NEGF) formalism. By employing a recently proposed semi-local exchange along with the coherent potential approximation we investigate the transport properties of two-terminal Si nanodevices composed of large number of atoms and atomic dopants. Simulations of the two-terminal device based on the NEGF-DFT are compared quantitatively with the traditional continuum model to establish an important accuracy benchmark. For bulk Si crystals, we calculated the effects of uniaxial strain on band edges and effective masses. For two-terminal Si nanochannels with their channel length of ~10 nm, we study the effects of uniaxial strain on the electron transport. With 0.5% uniaxial tensile strain, the conductance along [110] direction is increased by ~8% and that along [001] is increased by ~2%, which are comparable with the other reported results. This paper qualitatively and quantitatively shows the current capability of first principle atomistic simulations of nanoscale semiconductor devices.

Index Terms—Density functional theory (DFT), first principles, nanoscale devices, nonequilibrium Green’s function (NEGF), quantum transport, uniaxial strain.

I. INTRODUCTION

As dimensional scaling of MOSFETs continues, quantum mechanical treatment of electron conduction is becoming increasingly important and necessary [1]. A large body of work has been done to simulate quantum transport phenomena in various device structures and different materials. Starting from a given device Hamiltonian, quantum transport can be analyzed by techniques such as the scattering matrix theory and Keldysh nonequilibrium Green’s function (NEGF) theory. The calculation of a device Hamiltonian is, however, a complex problem and most device simulations rely on model and/or parameterized Hamiltonians. Examples include the effective mass Hamiltonian, the k-p Hamiltonian, and the tight-binding Hamiltonian, and so on. Combined with the NEGF formalism for quantum transport, these approaches can provide important insights for our current understanding of nanoelectronic device physics [2]–[5].

To fundamentally solve emerging nanoelectronic device problems, an important next step is to carry out parameter-free self-consistent modeling of quantum transport from atomistic first principles. This is necessary not only due to the lack of reliable phenomenological Hamiltonian parameters for many emerging device materials and structures, but also due to the fact that the transport driven by an external bias is intrinsically a nonequilibrium problem while the parameterization of a model Hamiltonian is usually done at equilibrium. In the recent ITRS [6], utilization of first principle simulations to understand the new device physics of the emerging nanoelectronics have been discussed.

It is the purpose of this paper to report self-consistent atomistic first principles simulations of uniaxial strain effects in electronic structures of bulk Si and quantum transport properties of two-probe Si nanochannels. Uniaxial strain engineering has been widely applied to boost transistor performances in CMOS technology [7] and was extensively investigated from effective mass model considerations [8] to tight-binding parameterizations [9], [10]. On the other hand, first principles atomistic analysis of quantum transport in strained Si has proven to be very difficult due to several reasons. First, the self-consistent density functional theory (DFT) with the local density approximation (LDA) or the generalized gradient approximation (GGA) cannot correctly predict bandgaps and dispersions of semiconductors. While higher level theory and functionals such as GW [11] and hybrid functional [12] improve on this aspect, they require costly computation for simulating solid-state devices (which are usually comprised of large number of atoms). Second, the low doping concentration in semiconductor device channels is difficult to deal with from atomic point of view since it requires a very large number of host atoms to accommodate the few dopant atoms. Finally, the electronic structure and quantum transport properties must be accurately averaged over the multitudes of disorder configurations due to random positions of dopants. A brute force average requires prohibitively large computation for the device systems we investigate in this paper.
In this paper, we present state-of-the-art first principles simulations of quantum transport in Si nanoscale device channels. Our approach is based on carrying out DFT within the NEGF formalism. In particular, by implementing the linear muffin tin orbital (LMTO)-based NEGF-DFT [13], [14], by applying the coherent potential approximation (CPA) to deal with the configuration average [15], [16], and by adopting the modified Becke–Johnson (MBJ) semi-local exchange [17], the above mentioned technical difficulties are solved. In this paper, we first establish the quantitative accuracy of our atomistic approach by calculating the electronic potentials of Si nanochannels doped with realistic atomic impurities, and quantitatively compare them with that obtained from continuum technology computer-aided design models that are based on experimental parameters. We then report first principles self-consistent NEGF-DFT calculations of the uniaxial strain effects on both bulk Si band structures and on quantum transport properties of two-terminal Si nanochannels with up to 960 atoms in the device scattering region. Our results are qualitatively comparable with the other reported results.

II. NEGF-DFT MODEL AND THE BENCHMARKING

The most widely used technique for atomistic first principles self-consistent simulation of quantum transport is to combine the DFT with the NEGF [13]. In NEGF-DFT, the non-equilibrium density matrix is calculated by NEGF, which is then used to construct the device Hamiltonian within a DFT-like self-consistent field theory and the process is iterated to self-consistency. Thus parameter-free device modeling is achieved. However, in order to simulate semiconductor transistor structures, all NEGF-DFT methods face some severe difficulties as mentioned above, namely: 1) transistor structures have large number of atoms leading to prohibitively large computation by typical NEGF-DFT algorithms; 2) bandgaps and dispersions cannot be accurately calculated by the widely applied exchange-correlation functional such as the LDA and GGA; and 3) it is difficult to dope small concentrations of real dopant atoms in atomistic simulation unless very large systems are calculated.

Recently, these technical difficulties of NEGF-DFT have been overcome by a new generation of the method [18] as implemented in the Nanodsim software package [19]. The technical details on the method in treating, for example, the electrodes and the flow chart of the self-consistent procedure including the solutions of Poisson equations for open systems are reported in [13] and reviewed in [14]. In particular, an LMTO-based NEGF-DFT is implemented that has an extremely sparse matrix structure to drastically reduce computation cost. To correctly predict bandgaps and band dispersions, a recently proposed MBJ semi-local exchange potential has been adopted, which is shown to provide quite accurate results for many compounds with a computational cost similar to that of LDA [17]. The usefulness of MBJ functional in producing accurate electronic structures within the LMTO description of DFT has been shown recently [20] for a wide range of III–V compound semiconductors. To deal with doping and its associated configuration average, the CPA has been applied. It is a statistical effective medium approach such that an atomic site has the x% chance to be a dopant atom and (100−x)% chance to be a host atom, the configuration average is carried out analytically hence disorder effects in bulks or interfaces can be calculated. Recently it was used to calculate the band offset of the heterointerfaces [21]. For transport properties of disordered systems, the nonequilibrium vertex correction (NVC) theory was combined with the CPA method to describe the disorder scattering [22]. Recent applications of the CPA-NVC approach include disorder scattering by the interface roughness in metal interconnect wires [23] and the impurity doping in Si nanochannels [24].

In this paper, we employ the Nanodsim software [19] to carry out the NEGF-DFT simulations of the strained Si bulk as well as the two-terminal transport nanochannels. For more technical details of the NEGF-DFT algorithm, we refer interested readers to [18] for a recent review. The atomic structures are shown in Fig. 1(a) and (b). In the LMTO-based DFT, an atomic sphere approximation (ASA) is applied where empty spheres are placed on certain sites together with the Si atoms to form a closely packed unit cell, as shown in Fig. 1(a). Atomic sphere radii are calculated by equaling the total sphere volume to the unit cell volume. In our simulations, the radii of the empty spheres and Si atomic spheres are the same. The MBJ semi-local exchange-correlation functional is used throughout the calculations, and for bulk Si with a unit cell of lattice constant $a_0 = 5.431 \text{ Å}$, our calculated bandgap $E_g$ is 1.12 eV and effective masses are: transverse mass $m_t = 0.19m_0$, longitudinal mass $m_l = 0.91m_0$, in excellent agreement to the known experimental values.
Fig. 1(b) shows the schematic of a two-terminal Si nanochannel that consists of a central scattering region sandwiched by the left and right electrodes (leads). The electrodes are degenerately doped Si (see below) crystal and extend to infinity. The scattering region consists of a channel, which is doped by boron or phosphorus atoms uniformly or locally (shown by a red stripe), it also contains part of the electrodes on either side of the channel. The transport direction along the channel is the $z$-direction, the cross-section ($x$-$y$ direction) of the two-terminal structure is assumed to be periodic and infinite. A $12 \times 12$ k-mesh is used in the self-consistent calculations and a $45 \times 45$ k-mesh is used in the transmission calculations. A logarithm mesh with a total number of 400 points is used for each atomic sphere for the real space calculations. More details about the simulations are presented below.

Without any strain, the unit cell vectors in the Si crystal coordinate system (CCS) [Fig. 1(a)] are known from textbooks. There are two Si atoms in a unit cell of the diamond structure together with two empty spheres within the ASA. Their center positions are easily derived. Before presenting results for the strained Si devices, in the rest of this section we present a quantitative comparison of NEGF-DFT model with that of a traditional simulation based on the continuum model as implemented in the Sentaurus Device simulator [25]. We use the two-probe Si nanochannel structure shown in Fig. 1(b) as an example for this benchmarking study. Here, the source and drain regions (and leads) are heavily and degenerately doped to $5 \times 10^{19}$ cm$^{-3}$ (either p- or n-type doping) using the technique of virtual crystal approximation [26]. On the other hand, the channel doping, uniform or localized, is achieved by introducing real dopant atoms of boron or phosphorus, and is handled within the CPA formalism. The length of source/drain and channel are $\sim 6.5$ and 10.9 nm, respectively, oriented to the [001] direction. The atomic structure of the central region includes 704 atoms and the entire two-terminal structure is periodically extended in the transverse $x$-$y$ directions.

With the atomic positions as the only input and after the self-consistency of the NEGF-DFT iterations, the potential profiles along the transport direction have been extracted and shown in Fig. 2 along with the results obtained from 1-D Sentaurus simulations [25] of devices with the same structure, dimension and doping concentration. In the Sentaurus Device simulator, continuous medium simulation is done with average charge, dielectric constant, bandgap, effective mass, and other parameters. The potentials in NEGF-DFT simulations are the Madelung potentials calculated from the charge in each atomic sphere, which are equivalent to the electrostatic potentials in the continuum model. The results, for uniformly p-type doped [Fig. 2(a)] or n-type doped [Fig. 2(b)] or localized p-type doped [Fig. 2(c)] Si nanochannels, agree very well. This quantitative comparison shows that the first principles NEGF-DFT formalism and the CPA-NVC method have quantitatively and accurately captured the microscopic physics of the Si nanochannels including the self-depletion in the junctions and the ionization of the dopant atoms at room temperature. The good agreements not only validate the NEGF-DFT formalism in general and the Nanodsim package in particular, but also bridges the first principle simulations to the traditional continuum-based methods for nanoscale devices.

### III. Effects of Uniaxial Strain on Bulk Si

With the applied strain, the unit cell vectors and atomic center positions are changed according to the elasticity theory [27] and are used as the input. The strain tensors are calculated...
Fig. 3. [001] uniaxial strain effects on (a) conduction and valence band edges and (b) effective electron masses. The band edge splitting calculated by our LMTO-DFT-MBJ method (lines) agrees well with those from the model solid theory (symbols). Conduction band effective masses from our simulations (lines) and those from VASP simulations (symbols) are quite close. Here, $X_{zz}$ and $X_{xy}$ are along and perpendicular to the strain direction.

The effects of [001] uniaxial strain on the band edges and effective electron masses of bulk Si are obtained using the Nanodsim software package, and the results are shown in Fig. 4. The band edge profiles with different strains are compared with those of the model solid theory [10], [30] in Fig. 3(a). Since the model solid theory gives a bandgap $<1.12$ eV for the relaxed Si crystal as shown in [10], a constant shift is added to the conduction band edges, which are then utilized as the benchmark. The strain-induced band splittings in different conduction band valleys agree well with the model solid theory. Fig. 3(b) plots the effect of uniaxial strain on the effective masses of the conduction band valleys. The lines and symbols are from the Nanodsim and VASP packages [31], and they agree very well. The ultrasoft pseudopotentials within a projector-augmented-wave method, together with the GGA (PBE) as the exchange-correlation functional have been used for the VASP simulations. An energy cutoff of 400 eV is used with $12 \times 12 \times 12$ k-point mesh. The results are reliable such that the electron mass values for the relaxed bulk silicon have been used as references for the tight-binding simulations of strain [10]. The [001] strain does not significantly alter the effective mass as shown before [8].

Fig. 4 shows the [110] uniaxial strain effects on band edges and effective masses in bulk Si. Fig. 4(a) shows the shifts of the conduction band and the valence band edges with different strains. Again, good agreement is observed between our LMTO-DFT-MBJ results and those obtained from model solid theory [30]. The out-of-plane conduction bands ($X_{zz}$) are brought down. Fig. 4(b) shows the electron effective masses in the split conduction bands along different directions. It indicates that the [110] strain reduces the lower $X_{zz}$ band effective mass parallel to the strain direction. Both band splitting and electron mass change contribute to an average transport mass reduction. Correct predictions of the uniaxial strain effects on bulk band structure serve as the basis for investigating strain effects on quantum transport in two-terminal devices presented in the following section.

IV. TWO-TERMINAL Si DEVICE UNDER UNIAXIAL STRAIN

Having confirmed DFT simulations of the uniaxial strain in bulk Si, in this section, we present its effect on quantum
transport in the two-terminal Si nanochannels shown in Fig. 1(b). As presented above, the cross-section of the two-terminal structure is periodic and transport is along the z-direction. The central region of Fig. 1(b) is generated by repeating a unit cell [e.g., Fig. 1(a)] along the z-direction. For example, the unit cell of a [001] orientated Si structure includes eight Si atomic spheres and eight empty spheres in the ASA and spans over four atomic layers and the distance of a lattice constant. When strained, the atomic positions in the unit cell are changed according to the strain tensor [28]. For quantum transport along [110] crystal directions, a coordinate transformation is needed. The strain tensors in [28] are derived in a CCS and a transfer matrix is needed to transform this CCS to a new coordinate system in which the transport is along its z-direction. This transfer matrix that depends on the strain is also applied to the unit cell for generating all atomic sites.

It is already known that the uniaxial tensile strain increases the ON-state driving currents of n-type MOSFETs, and in this regard the [110] strain is more effective than the [001] strain [8]. However, the experimental data of mobility enhancements are mixed effects of phonon, interface roughness, and ionized charge scatterings. To understand the uniaxial strain effect on the ultimate ballistic transport, the [001] and [110] oriented Si n-i-n devices with $5 \times 10^{20}$ cm$^{-3}$ n-type source/drain doping are simulated. The higher source/drain concentration together with the intrinsic channel doping is used to make the n-i-n device an analog to the conducting surface of ON-state MOSFETs (both with small thermionic transport barrier).

Fig. 5 shows the first principle results of the [001] oriented n-i-n device having 960 atoms in the scattering region without any strain and with a uniaxial strain. Source/drain and channel are all ~10.8-nm long. The potential profile along the transport direction is plotted in Fig. 5(a). With tensile strains the conduction band splitting (discussed in the previous section) causes a reduction of the density of state (DOS) in the source and drain. The Fermi level there is lifted up to accommodate the same charge concentration. At the same time, the self-consistent simulations reveal that the conduction band edge in the channel is also raised to keep similar amount of channel electrons. Therefore, the transmission in the device with the tensile strain is increased slightly as shown in Fig. 5(b). The tensile strain increases both the tunneling and thermionic conductance. The total conductance is calculated from the transmission coefficient [24]. Without strain, the conductance is found to be $\sim 9.7 \times 10^{-3}$ G$_0$/nm$^2$. With a 0.5% strain, it becomes $9.9 \times 10^{-3}$ G$_0$/nm$^2$, where $G_0 = 2e^2/h$ is the conductance quanta. An increase in the conductance of 2.4% is thus observed.

For the [110] oriented device, the effect of uniaxial tensile strain on the transport properties is even larger. The simulated device consists of 10 nm source/drain and channel, with a total of 624 atoms in the scattering region, and the results are shown in Fig. 6. The Fermi level in the source and drain is again lifted up due to the DOS change by tensile strain, shown in Fig. 6(a). However, the self-consistent simulations indicate that the conduction band edge does not follow the change in the Fermi level. Fig. 6(b) shows that the transmission coefficient is increased more significantly with the tensile strain compared with the [001] device. The reasons are two folds: 1) the barrier height and width for electrons at the Fermi level are reduced and 2) the electron effective mass is reduced as shown in Fig. 4(b). The barrier change contributes to the threshold voltage shift that has been observed in strained nMOSFETs [32], [33]. Both changes contribute to an increase in the conductance. The total conductance increase is $\sim 8.3\%$ with the 0.5% tensile strain, going from $1.5 \times 10^{-2}$ to $1.6 \times 10^{-2}$ G$_0$/nm$^2$. The [110] tensile strain is thus more significant for improving the conductivity of the n-i-n devices. A comparison between the transmission in the unstrained [001] and [110] devices show that the [110] oriented device has larger conductance, which agrees with the experimental observations.

Since periodical boundary conditions are applied for the cross-section of the Si nanochannels in this paper, vertical confinements in the channel, which may lead to further band splitting and contribute to the electron mobility enhancement, for example, through the surface bulging effects [34], is eliminated. It is not easy to make a fair comparison with the experimental result. Nevertheless, the percentage increases of conductance due to the uniaxial strain are comparable with those of the tight-binding simulations [10]. The effects of
finite cross-sections such as those in nanowires on the quantum transport deserve further investigations.

V. CONCLUSION

We have carried out parameter-free first principles atomistic simulations using the NEGF-DFT formalism to model the effects of uniaxial strain on quantum transport in nanoscale Si devices. The first principles approach accurately and quantitatively predicts effects of uniaxial strain on the shifts of band edges and the changes of the effective masses. Our NEGF-DFT simulations confirm that the [110] tensile strain is more effective in improving the device conductance. In addition, we provided quantitative benchmarks of the NEGF-DFT simulations comparing with the continuum model as implemented in the Sentaurus device simulators [25] using a two-probe Si nanoscale device as an example. Our results both qualitatively and quantitatively show the capability of NEGF-DFT first principles atomistic modeling for nanoscale electronic devices.

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