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Newsletter for semiconductor process and device engineers

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TCAD news

Latest Edition

Welcome to the IEDM 2017 edition of TCAD News. This edition has a special significance because it highlights the products from our recent acquisition of QuantumWise. For several years, we have observed a growing need among our customers for materials modeling as one of the key early research activities in new process node development. This need will only accelerate as material properties and device architectures become increasingly intertwined in their impact on device performance and reliability. In some cases, unique material attributes become the catalyst for product innovations, as we are already seeing with new memory technologies.

QuantumWise was founded in 2008, and over a time span just shy of 10 years became a leading supplier of atomic-scale materials and advanced transport modeling tools, with more than 400 commercial and academic customers worldwide. This acquisition, along with the addition of the GSS team in 2016, demonstrates our continued investment in the growing customer demand for of a Design-Technology Co-Optimization (DTCO) solution for modeling all the way from atoms to (small) circuits. We can now bridge the ab initio and TCAD worlds through the newly released product, Sentaurus Materials Workbench, enabling customers to explore, evaluate and select device, process, material and layout options in the early phases of technology research.

I hope you will enjoy reading this edition of TCAD News, dedicated entirely to the important topic of materials modeling.

With the approaching holiday season, I would also like to take this opportunity to wish you happy holidays and a prosperous New Year.

With warm regards,

Terry Ma
Vice President of Engineering, TCAD

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Materials Modeling Enables Time and Cost Savings for Advanced Process Nodes

In the 1967 film “The Graduate,” the protagonist, Ben Braddock, unsure about what career path to pursue, is given the advice “one word: Plastics.” A modern remake of the film would likely change the advice to “one word: Materials.”

Material science is indeed at the center of many product innovations across a wide range of industries and the semiconductor industry is no exception. Silicon and many of the other critical materials used in today’s semiconductor chips are among the most studied and technologically relevant materials. As semiconductor technology continues to scale, new materials need to be investigated for potential integration into new technology nodes to achieve the target performance and power. Even silicon, under mechanical stress or in spatially quantized regions, is sufficiently altered from its bulk form to warrant detailed modeling and characterization. At such scales, atomistic materials modeling becomes necessary.

With the recent acquisition of QuantumWise, a leader in atomistic materials modeling software based in Denmark, Synopsys now offers industry-proven software products to support the current and future materials modeling needs of the semiconductor industry. The Quantum ATK products are becoming integrated with Sentaurus TCAD and TCAD-to-SPICE products through the newly released Sentaurus Materials Workbench, resulting in a Materials-to-Circuits Simulation flow that enables our customers to investigate the impact of material choices at the circuit level, saving process development time and cost. This flow is one of the key components of Design-Technology Co-Optimization (DTCO).

Since this is a relatively new and rapidly growing area, we dedicate this newsletter to a description of the main physical theory underlying atomistic materials modeling and several of its key applications.

Atomistic Materials Modeling

Over the last decade, the use of software tools to model the properties of materials at the atomistic level has grown very rapidly, benefiting both from performance improvements in computer hardware and the development of more efficient models and algorithms to solve the underlying equations. In particular, Density Functional Theory (DFT) as a quantitative approach for the quantum mechanical modeling of materials at the atomistic level has now permeated many fields, of which semiconductors are a prominent example.

Since DFT is the foundational theory within QuantumATK we embark on a brief description of what DFT is before illustrating its application to several problems highly relevant to today’s and future semiconductor development.

Quantum Mechanical Modeling of Materials

The story begins in the late 1920s. As the ink began to dry on the papers [1] [2] [3] that established the foundation of quantum mechanics, the search began for applications of the new theory beyond the problems in atomic physics that motivated its initial development. Among these applications was quantum chemistry and other multi-electron problems comprising many atoms in molecular and crystalline configurations.

Soon it became apparent that while the quantum-mechanical physical laws governing such systems had just been discovered, their solution for even modestly-sized systems remained beyond the analytical techniques available then. As Paul Dirac famously put it in his seminal 1929 paper [1] entitled Quantum Mechanics of Many-Electron Systems,

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of those laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation." [1]

Perhaps as a testament to Dirac's notorious conciseness and brilliance, these statements remained true even after the advent of the modern computer in the 1940s.

It was not until the formulation of new theories in the 1960s, followed by four decades of continuous scientific development and concomitant advances in computer hardware that we have now reached the point where Dirac's second statement about approximate practical methods and reasonable computational effort has been addressed. Along the way, the 1998 chemistry Nobel Prize awarded to Walter Kohn and John A. Pople dully recognized their fundamental contributions to Density Functional Theory.

Where Does the Complexity Come From?

The atoms in a solid are typically heavy enough that they can be described as classical particles; the difficulties arise from the electrons which need a quantum mechanical description. Since the nuclear masses are much greater than the electron mass, they move much slower, and it is a reasonable approximation to assume that the electrons experience the nuclei as fixed particles. This is the so-called Born-Oppenheimer approximation [2].

The electrons may then be described by a many-electron Schrödinger equation [3]

$$\left[-\sum_i \frac{\hbar^2\nabla_i^2}{2m} - \sum_{i,I}\frac{Z_I e^2}{|\boldsymbol{R}_I - \boldsymbol{r}_i|} + \sum_{i<j}\frac{e^2}{|\boldsymbol{r}_j - \boldsymbol{r}_i|}\right]\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_n) = E\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, ..., \boldsymbol{r}_n),$$

where the first term is the kinetic energy of the electrons, the second term the electro-static attraction between the electrons and nuclei and the last term is the electro-static electron-electron repulsion. Due to the electron-electron interaction the motions of all the electrons are correlated, and we need to solve a partial differential equation for all electrons simultaneously. This is an immense problem and the many-electron Schrödinger equation is only direct solvable for a few toy problems.

Density Functional Theory: It's All About the Electron Density

Today it is possible to perform quantum mechanical modeling of systems of practical interest thanks to Density Functional Theory (DFT). Central to DFT is the theorem of Hohenberg-Kohn [4] which states that the total energy of a many-electron system is a function (in mathematically strict terms a functional) of the electron density.

This theorem, which can be validated with just intuitive arguments, has profound consequences because if allows the computation of the ground state energy, E, of the system by simply evaluating a functional with the electron density, $\boldsymbol{\rho}$, as a parameter,

$$E = F[\rho].$$

Thus, instead of solving for 3xN dimensional partial differential equation where N is the number of electrons, we only need to solve for a 3 dimensional function. However, the problem is finding F, since in principle this requires solving the many-electron Schrödinger equation. The power of DFT lays in the approximate methods devised for calculating F, which allows for a good tradeoff between accuracy and computational efficiency.

Kohn-Sham Equations

Central to all the approximations in DFT are the Kohn-Sham equations formulated by Walter Kohn and Lu Jeu Sham in their seminal paper of 1965 [5]. In these equations the electrons are described as independent particles which move in an effective potential setup by the other electrons. Each electron is described by a one-electron Schrödinger equation where the first term is the kinetic

$$\left[-\frac{\hbar^2\nabla^2}{2m} + V^{\text{eff}}(\boldsymbol{r})\right]\phi_i(\boldsymbol{r}) = \epsilon\phi_i(\boldsymbol{r}),$$

energy of the electron, and the second term an effective potential arising from the interaction with the other electrons and the nuclei. Since the electrons are treated as independent particles, the electron density can be obtained by summing up the density of each electron

$$\rho(\boldsymbol{r}) = \sum_i |\phi_i(\boldsymbol{r})|^2.$$

The effective potential can be obtained from the electron density, it consists of the following terms

$$V^{\text{eff}}(\boldsymbol{r}) = -\sum_I \frac{Z_I e^2}{|\boldsymbol{R}_I - \boldsymbol{r}|} + \int \frac{e^2 \rho(\boldsymbol{r'})}{|\boldsymbol{r'} - \boldsymbol{r}|} d\boldsymbol{r'} + V^{\text{xc}}(\boldsymbol{r}).$$

The first term is the electrostatic interaction with the nuclei, the second term is the average electro-static interaction with the other electrons, the so-called Hartree potential. The last term is the "magical" exchange-correlation potential, which contains all the quantum mechanical effects not included in the other terms. In essence, the accuracy of DFT within the Kohn-Sham formulation boils down to finding a good approximation for the exchange-correlation potential.

Note that the effective potential can be calculated from the electron density, however, the calculation of the electron density requires also knowledge of the effective potential. This chicken and the egg problem, is solved by starting with a trial electron density, and then iterating the Kohn-Sham equations until a self-consistent solution is found.

The Kohn-Sham formulation has another advantage. The independent Kohn-Sham orbitals can to some extent be treated as excitations of the system. This, gives a very simple model of a solid system, where for instance the energy dispersion of the electronic excitations, i.e. the bandstructure, is simply obtained from the eigenvalues of the Kohn-Sham one-electron Schrödinger equation.

Exchange-Correlation Functionals

As described above the essential part of DFT is to find a good approximation for the exchange-correlation functional. The first approximation that was devised is the Local Density Approximation (LDA) [6]. In LDA it is assumed that the exchange-correlation potential is a simple function of the density, i.e. the exchange-correlation potentials at a given point in space can be determined from the electron density at that point, thus, completely neglecting the effects of density variations around that point. The exchange-correlation functional can now be parameterized from full many electron calculations of the exchange-correlation functional in an uniform electron gas, which is one of the toy models where the many electron Schrödinger equation can be solved. Initially the LDA approximation was expected to be of little practical value, since in a real solid the density is far from the constant density reference. However, the LDA turned out to be so robust and accurate, that it became the preferred approximation the first 20 years of DFT. In the beginning of the 90s new robust and more accurate DFT functionals arose which also depend on the gradient of the density, so-called Generalized Gradient Approximations (GGA) [6]. This, initiated a new search of more accurate approximations, so called MetaGGA approximations [6] and Hybrid functionals [6]. These different approximations are assigned to various rungs of Jacob's ladder [6] as shown in Figure 1, according to the number and kind of added ingredients. When climbing up the ladder, the complexity increases together with accuracy with some increase in computational cost. Today there is no functional that beats them all, and the choice of which exchange-correlation functional to use depends on the type of problem and a trade-off between accuracy and computational burden.

DFT was developed to describe the ground state of a system and not constructed to describe electronic excitations like electrons in the valence band of a semiconductor, and if the LDA or GGA approximation is used to calculate the bandgap of a semiconductor, the gap usually comes out far too low. However, a number of new MetaGGA and Hybrid functionals have addressed this problem and today a number of solutions to the band gap problem exist. QuantumATK has a wide range of these band gap corrected functionals, and currently our recommended solution is the +1/2 family of corrections [7], which gives a good trade-off between accuracy and computational burden as shown in Figure 2.

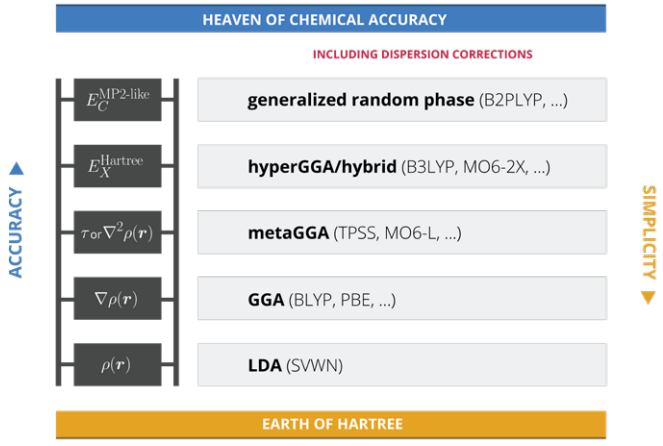


Figure 1: Jacob's Ladder of DFT functionals [6]. The earth of Hartree is no exchange-correlation correction.

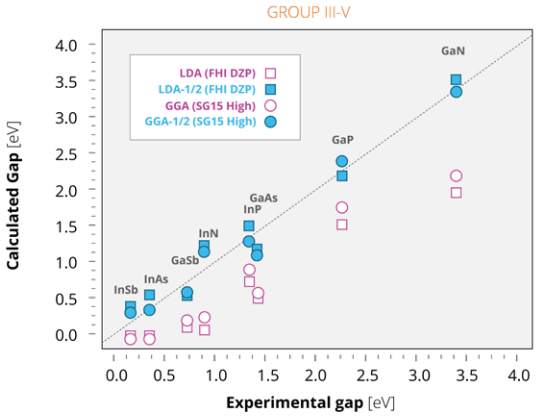


Figure 2: Theoretical bandgap of different III-V semiconductors calculated with LDA and GGA (purple points), compared with the results the +1/2 corrections are included (green points).

DFT Application: Calculation of Semiconductor Bandstructures

We now illustrate the application of DFT to the calculation of semiconductor bandstructures [8]. The goal is to extract effective masses from the bands [9] to be used in TCAD advanced transport simulators.

We consider a Si nanowire of 4.5nm diameter with the channel in the <110> direction, as shown in Figure 3. The calculation is motivated by the changes attributed to the 2D quantum-mechanical confinement of the structure which significantly alters the bandstructure relative to bulk silicon, and consequently has a primary impact on the carrier transport in the channel (refer to Figure 4).

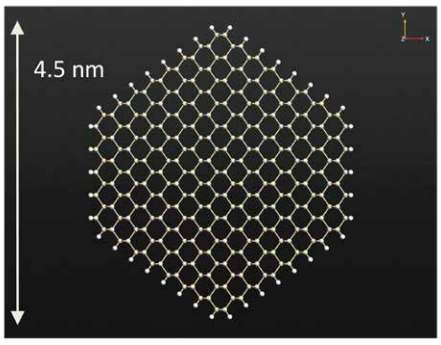


Figure 3: Si nanowire with diameter 4.5nm with <110> channel direction.

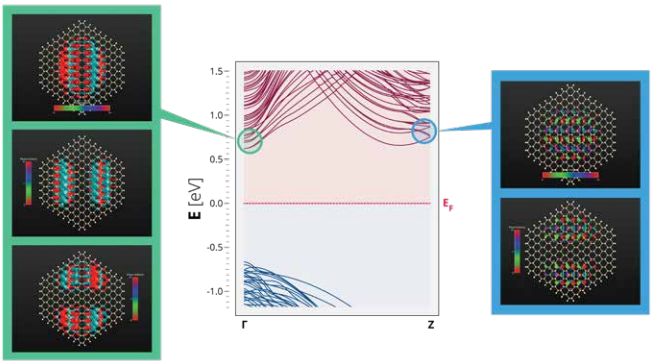


Figure 4: Band structure of the nanowire in Fig. 3 with illustration of the Bloch states at the γ and X points.

The positions of the Si nuclei are considered fixed, consistent with the immobile nuclei approximation described in the last section on the way to the derivation of the Kohn-Sham equations. The extra step that now comes into play is to take advantage of the periodicity in the crystal and to apply Bloch's theorem to the Kohn-Sham wavefunctions in a periodic potential. The resulting system is then solved for the eigen energies and periodic parts of the Kohn-Sham wavefunctions as a function of the reciprocal vector **k** and the bands.

The calculated sub-bands are then classified and the lower energy regions are used to extract the effective masses (Fig. 5). Non-parabolicity is fitted with the parameter α.

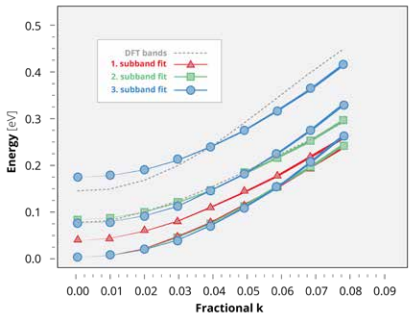


Figure 5: Each band is classified by projecting the DFT wavefunction onto an effective mass wavefunction; in this way it is ensured that the effective mass model obeys the same symmetries as the DFT model. The parameters of the effective mass models are fitted to reproduce the DFT bands.

As an example the resulting anisotropic effective masses and non-parabolicity, such as listed in Table 1, can then be used by the TCAD advanced transport simulators.

	m_{zz}	m_{yy}	m_{tr}	α
1.	0.99	0.99	0.12	2.60
2.	0.46	0.45	0.11	2.10
3.	0.01	0.74	0.14	0.60

Table I: Effective masses and non-parabolicity parameter for the three lowest energy sub-bands of the 4.5nm Si nanowire example.

Simulation of Electron transport within DFT

With QuantumATK it is also possible to describe the electron transport in an electronic device using DFT. Such calculations are complicated by the applied bias which drives the electrical current from the source to the drain of the device. The bias sets up different chemical potentials in the electrodes. In order to calculate the electron density of the system, it is necessary to trace the origin of each electronic state to either the left or right electrode, and from the electronic eigen energy relative to the relevant electrode chemical potential, it is determined if the electronic state is occupied and donates an electron to the electron density. This greatly complicates the solution of the Kohn-Sham equations and in QuantumATK the solution is obtained using Non-equilibrium Greens Function (NEGF) techniques [10].

Simulation of contact resistance

A very important application of the DFT/NEGF model in QuantumATK is the calculation of metal-semiconductor contact resistances.

As the future brings continued down-scaling of modern transistor technology, the metal-semiconductor contact resistance becomes an important factor in the performance of future semiconductor devices.

It is known from experiments [11] that by increasing the doping density in the semiconductor, it is possible to reduce the contact resistance, which is crucial for sub-10 nm nodes. However, even sophisticated experimental measurements have challenges or are not able to characterize, for example, how the atomic structure of the interface impacts the metal-semiconductor resistance, what the origin of doping dependence is and what the intrinsic limits for the resistance are.

The atomic scale modeling tools in QuantumATK are designed to study metal-semiconductor interfaces and characterize the above. Importantly, QuantumATK toolbox describes the interface using the physically correct boundary conditions, and account correctly for the semiconductor band gap and doping. Examples of comparison between calculations and experimental data can be found in the studies in Figure 6, Figure 7 and Figure 8:

Study by Global Foundries and IBM Research on the TiGe/Ge Contact Resistance [12]

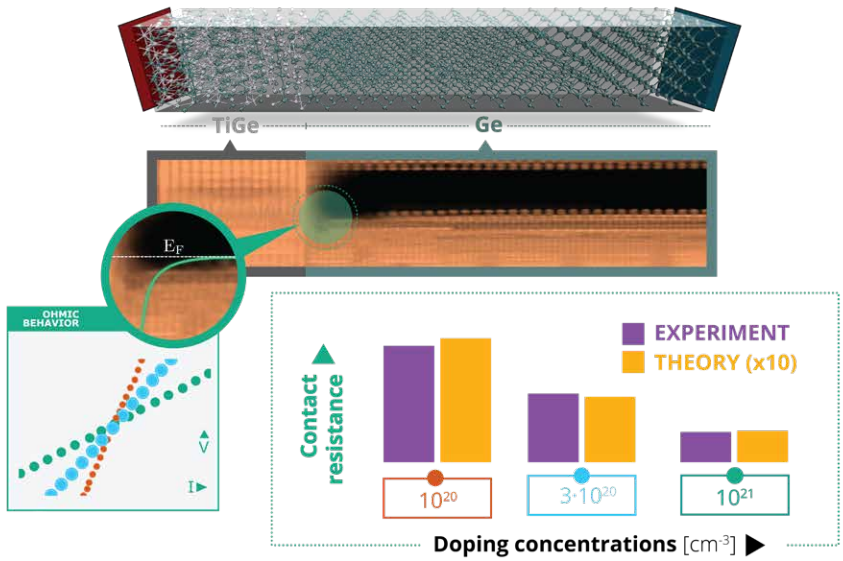


Figure 6: The structure of the TiGe/Ge interface is created with the NanoLab graphical interface [13] as shown in Panel 1. In the calculated Local Density of States (LDOS) [14] plot (Panel 2) the dark region depicts the band gap of Ge. The Schottky Barrier Heights (SBH) can be extracted from the LDOS plot as a difference between the maximum value of the macroscopic average of the Hartree potential (green line) and the chemical potential on the semiconductor side of the interface (E_F, white line). The simulations show that the SBHs of the TiGe/Ge contact depend strongly on the phase of TiGe and on the different crystallographic orientations of Ge. At the doping concentration of 10^{21} cm^{-3} the SBH for TiGe/Ge contact is very small, indicating that the contact is Ohmic, as also confirmed by the calculated linear I-V curve as shown in Panel 3. Panel 4 shows a good agreement between theory and experiment for the trend of the TiGe/Ge contact resistance extracted from the I-V curve at various doping concentrations (refer to the full publication for details).

Study by Imec, QuantumWise and Others on the TiSi/Si Contact Resistance [15]

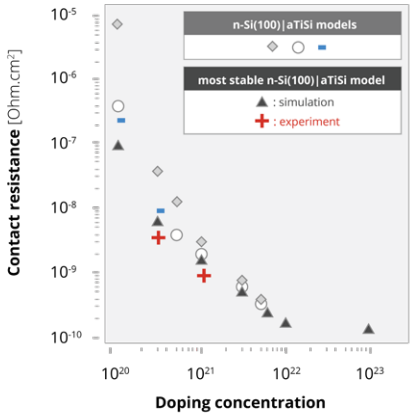


Figure 7: TiSi/Si contact resistance as a function of the doping concentration. Red crosses are experimental data points, while other symbols illustrate simulations of various interface geometries with QuantumATK [15].

The study presented in Figure 7 showed that the intrinsic contact resistivity saturates with the doping concentration. Authors suggest that as the doping concentration increases, the impact of interface composition decreases and that the intrinsic contact resistance starts being dominated by intrinsic properties of the metal and of the semiconductor, such as their effective masses and **k** vectors. Authors also suggest that metals with a high effective mass, such as, for example, Sc, could be used to maximize the transmission probability of the electron injection and thus reduce metal-semiconductor resistance.

Study by QuantumWise on the M-InGaAs (M=Ti, W, Mo) Contact Resistance [16]

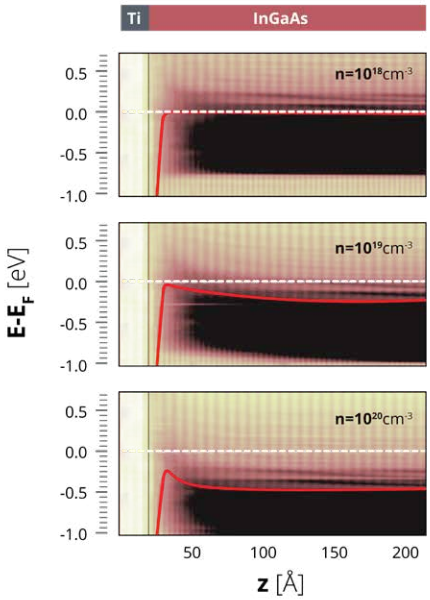


Figure 8: Band allignment at the Ti-InGaAs interface for different doping concentrations, n. Note that for all doping concentrations the SB is below the Fermi level [16]

The study highlighted in Figure 8 shed light on the origin of the contact resistance dependence on doping. The authors showed that the transport is not dominated by tunneling through a Schottky barrier (SB) as the barrier is always below the Fermi level as shown in LDOS plots. Thus, the origin of lower contact resistance as function of the doping arise from the shift of the Fermi level into energies where the transmission is high, rather than the change of SB.

In addition to showing a **good agreement with experimental results**, all three studies emphasize that the detailed understanding of the contact resistance at the atomic-scale is necessary in order to eventually optimize the devices with minimum contact resistance. Due to the limitation of space, we show only a couple of examples of how QuantumATK provides insight into how to reduce metal-semiconductor contact resistance.

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