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Ab initio calculation of the deformation potential and photoelastic coefficients of silicon with a non-uniform finite-difference solver based on the local density approximation

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ABSTRACT

The band diagram, deformation potential and photoelastic tensor of silicon are calculated self-consistently under uniaxial and shear strain by solving for the electronic wavefunctions with a finite-difference method. Many-body effects are accounted for by the local density approximation. In order to accommodate the large number of grid points required due to the diverging electrostatic potential near the atomic nuclei in an all-electron calculation, a non-uniform meshing is adopted. Internal displacements are taken into account by adding an additional coordinate transform to the method of Bir and Pikus. Good consistency of the calculated deformation potential and photoelastic coefficients is obtained with prior experimental and theoretical results, validating the numerical methods. Furthermore, it is shown that a slight correction of the multiplicative coefficient of the $X\alpha$ approximation for conduction bands results in good agreement with experiment for both the direct and indirect bandgaps.

1. Introduction

Recent developments in electronics and optoelectronics have led to a rekindled interest in the modeling of strained semiconductors. The best known device application is the improvement of carrier mobility in strained silicon that has allowed further scaling of Moore's law [1]. Strained semiconductors are also of great interest to photonics and optoelectronics: For example, applying strain to quantum wells is a well known technique to improve the performance of semiconductor lasers [2]. More recently, strained group IV semiconductors have gained in importance for the CMOS compatible fabrication of photonic circuits (Silicon Photonics [3]). Inhomogeneously strained silicon has been shown to have a finite second order optical nonlinearity enabling photonic devices such as silicon based Pockels modulators and two photon converters [4,5]. Highly n-doped germanium has been shown to support optical gain [6]. Further narrowing of the direct bandgap via tensile strain could further improve the material's gain and enable more efficient group IV light sources [7,8]. The SiGeSn material system allows the realization of highly strained germanium and GeSn quantum wells [9] and might pave the way towards practical devices.

We solve the Kohn–Sham equation [10] for strained cubic semiconductors with a finite-difference (FD) real-space all-electron approach and apply it to the case of strained silicon. In order to assess the method's suitability to the determination of the optical properties of strained semiconductors, we carefully benchmark it by calculating the deformation potential and the photoelastic coefficients of silicon under uniaxial and shear strain.

All-electron modeling can lead to more accurate results in problems that involve a high level of interaction between valence and lower orbital electrons [11,12], certain classes of problems that require treatment of lower orbitals [13,14], or the determination of absolute energies [15] and absolute deformation potentials [16] referenced against energy levels of lower orbitals. Our interest is to apply all-electron treatment to the modeling of novel effects such as the Pockels effect in inhomogeneously strained silicon for which pseudopotentials have not yet been carefully benchmarked. However, treatment of the diverging electrostatic potential around the nucleus and rapid oscillations of the wavefunctions in its vicinity result in a multi-scale numerical problem [17] that needs to be addressed, e.g., with hierarchical finite elements bases [18,19] or real-space methods with grid refinements around the nucleus [20–24]. Real-space finite-difference methods have the general advantage of resulting in sparse matrices with a small number of off-diagonal

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terms, which can be efficiently diagonalized with parallel computing algorithms.

A number of methods have been demonstrated to adapt FD algorithms to handle the diverging potential of the nucleus. In [20,21], a rectangular cartesian grid was successively refined in concentric regions around the nucleus. In [20], orphan nodes were handled by generalizing the finite-difference expression of the Laplacian. In [21] the multi-grid problem was solved based on a V-cycle. In [22,23], a regular grid was used after applying a curvilinear spatial transformation, effectively increasing the number of grid points around the nucleus in the original coordinate system. In [24], the wavefunction was solved on a coarse rectangular grid and subsequently interpolated on a fine grid around the nuclei prior to calculating overlap integrals with pseudopotentials. Finally, in [25] the wavefunctions were solved for on a coarse grid excluding the space regions within a muffin-tin radius in the immediate vicinity of the nuclei. These excluded regions were handled by applying a boundary condition to the grid points closest to the nuclei forcing the wavefunctions on the boundary to be a superposition of atomic-like solutions. Here, we apply successive cartesian grid refinements to concentric regions centered on the nuclei, similarly to [20,21], and extend the methodology to calculate the band diagram and dielectric constant of strained semiconductors. The nested grid refinements used here allow more straight forward control over the extent and range of the grid refinements relative to methods based on curvilinear transformations [17,23], but require special handling of the derivative operators at the subgrid boundaries [20]. Here, we express the numerical problem as a sparse matrix diagonalization that can be straightforwardly handled with the Lanczos algorithm implemented in standard numerical packages.

The deformation of the crystal lattice is handled by a curvilinear coordinate transform that maps the strained onto the unstrained lattice. This allows, e.g., for the computation of the effect of internal strain with finite differences without numerical artifacts resulting from displacements of the nuclei relative to the grid points and generally for a smooth treatment of the effect of strain. The coordinate system is deformed in order for individual nuclei to remain on the same grid points irrespectively of the lattice deformation. In addition to the deformation introduced by Bir and Pikus [26,27], an additional curvilinear coordinate transform is introduced in order to accommodate internal displacements inside the unit cell [28].

Many-body effects are accounted for by using the $X\alpha$ approximation [10,29,30] in the framework of density functional theory [31] (DFT) and of the local density approximation (LDA). While the electrostatic and LDA potentials of inner shell electrons are fully taken into account, the shape of the inner orbitals are assumed to correspond to that of isolated silicon atoms (frozen core, all-electron approximation (FCAE)). While the numerical methods described here could easily be extended to the treatment of inner shell electrons, the frozen core approximation is adequate for the numerical studies reported here and is adopted to shorten computation time. The numerical methods used here could also be applied to other semiconductors or to materials of arbitrary shape following the path shown in [21], thus providing high flexibility for the modeling of irregular shapes.

In order to validate the numerical methods, we calculate the strained band diagram, the deformation potential and the photoelastic coefficients of silicon under uniaxial and shear strain. Convergence and accuracy, as well as required computational resources are carefully benchmarked. The deformation potential is derived both directly and in the framework of perturbation theory with a linearized perturbation Hamiltonian. Numerical results for the deformation potential and the photoelastic coefficients of strained silicon are compared to the literature, with good agreement. Furthermore, in order to determine the primary factors affecting the deformation potential, the overall deformation potential is broken down in the framework of a perturbation theoretical approach into individual contributions from the LDA potential, nuclei induced dipoles, dipoles induced by valence electrons, electrostatic potential due to redistribution of the valence electron density and screening from inner shells.

2. Coordinate transformation

Given a strain ϵ_{ij}, the method of Bir and Pikus starts by introducing the transformation

$$x_i' = x_i + \sum_{j=1..3} \epsilon_{ij} x_j \tag{1}$$

where x_i' corresponds to the physical coordinates of the strained unit cell that are mapped to a new coordinate system x_i. The latter corresponds to the unstrained unit cell, in that nuclei are located at their original position. There are two atoms in the unit cell of crystalline silicon. When shear strain is applied, in addition to the overall deformation of the unit cell, the two silicon atoms undergo an internal displacement relative to one another [28,32] parameterized by a number typically denoted as ζ. When a shear strain is applied to the unit cell, the lengths of the atomic bonds between adjacent nuclei become unequal, subdividing them into two categories. This can be fully or partially compensated by the internal displacement. $\zeta = 0$ corresponds to a total absence of internal displacement, i.e., the displacement of both atoms is predicted by Eq. (1). $\zeta = 1$ corresponds to a full equalization of the bond lengths. The unit cell considered here has dimensions $[a/2, a/2, a]$, where a is the lattice constant of silicon, with atoms placed at (1a) [0, 0, 0], (1b) $[a/2, a/2, 0]$, (1c) $[0, 0, a]$, (1d) $[a/2, a/2, a]$ (each split between 8 unit cells), (1e) $[a/2, 0, a/2]$, (1f) $[0, a/2, a/2]$ (each split between 4 unit cells) and a second atom placed at (2) $[a/4, a/4, a/4]$. Atom (2) is connected with sp3 bonds to (1a), (1b), (1e) and (1f). For a shear strain ϵ_{ij}, the second atom (2) is displaced by $\delta x_k = -\zeta \epsilon_{ij} a/2$ relative to atoms of the first category (1a–1f), where $i \neq j \neq k$.

In order to accommodate the internal displacement without creating numerical artifacts in the finite-difference solver resulting from a displacement of the nuclei relative to the grid, we introduce an additional term in the coordinate transform

$$x_i' = x_i + \sum_{j=1..3} \epsilon_{ij} x_j - \sum_{i \neq j} \frac{\delta x_i}{4} \cos\left(\frac{4\pi x_j}{a}\right) \tag{2}$$

$$x_i' = x_i + \sum_{j=1..3} \epsilon_{ij} x_j + \frac{\zeta a}{8} \sum_{i \neq j \neq k} \epsilon_{jk} \cos\left(\frac{4\pi x_j}{a}\right). \tag{3}$$

This transformation maps the position of the nuclei in the unstrained unit cell to the position of the nuclei in the strained unit cell. Since the Hamiltonian will be described in the coordinate system of the unstrained lattice, x_i, rather than in the physical coordinate system of the strained lattice, x_i', this results in a description of the problem where the nuclei are always located on the same grid points, irrespectively of the strain that is applied to the lattice and irrespectively of ζ.

The Laplace operator of the physical coordinate system can be expressed in the unstrained coordinates as

$$\begin{aligned} \Delta' = \Delta &- 2 \sum_{i,j=1..3} \epsilon_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \\ &- \frac{2\pi}{a} \sum_{i \neq j} \delta x_i \sin\left(\frac{4\pi}{a} x_j\right) \frac{\partial^2}{\partial x_i \partial x_j} \\ &- \frac{4\pi^2}{a^2} \sum_{i \neq j} \delta x_i \cos\left(\frac{4\pi}{a} x_j\right) \frac{\partial}{\partial x_i} \end{aligned} \tag{4}$$

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