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Multiscale Modeling of Strained Silicon

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Summary

As transistor dimensions reach 45 nm or even lower, strain engineering of silicon is becoming increasingly more important in the fabrication of high performance devices. Strained silicon has significantly improved carrier mobility and reduced power consumption enabling much higher switching speeds. Strained silicon is usually made by depositing silicon on Si1-xGex that expands the silicon lattice and hence increases the carrier mobility. Strained silicon can also have impurities such as germanium, carbon, and other point defects. A problem in the design of strained silicon is that it has not yet been possible to measure all components of strain in the finished device. It is therefore necessary to have reliable theoretical methods for modeling the strain caused by the substrate as well as the impurities in the lattice. It is also necessary to know the precise location of atoms in strained silicon in order to calculate the electron wave functions. Hence a reliable model for strained silicon containing impurities must give the local atomistic distortion in the lattice near the impurity as well as strains in the entire solid. The model must account for the local discrete lattice effects and include the contribution of surfaces and interfaces in the solid. It is thus a multiscale problem.

We shall describe a multiscale Green's function that seamlessly links the length scales from atomistic to macro. The discrete lattice contributions near a defect can be represented in terms of the Kanzaki force that is a characteristic of the host lattice as well as the defect. This force can be calculated and stored for subsequent calculations on the same system. Another useful parameter is the dipole tensor that is defined in terms of the Kanzaki force and, in principle, can be measured. We will present numerical results on the lattice distortion, 3D strain distribution, Kanzaki forces, and the dipole tensor for Ge and C impurities, and other point defects in strained silicon.

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