Analysis of Hole Transport in Arbitrarily Strained Germanium

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Full-band Monte Carlo simulations (1) are performed to study the properties of hole transport in bulk Germanium under general strain conditions. The empirical non-local pseudopotential method (EPM) (2) is generalized to arbitrary stress/strain conditions to calculate the band structures of Ge.

The volume of the irreducible wedge, in which the band-structure is calculated, is determined by the number of symmetry elements $P(\Gamma)$ at the center of the Brillouin zone of the strained lattice via $\Omega_{\text{irred}} = \Omega_{\text{BZ}}/P(\Gamma)$. For relaxed Ge $P(\Gamma)$ is 48, for uniaxial stress along $\langle 100\rangle, \langle 111\rangle$, and $\langle 110\rangle$ $P(\Gamma)$ is 16, 12, and 8, respectively, while for stress along general directions the lattice is invariant only to inversion, thus $P(\Gamma) = 2$. For discretization of band-structure an unstructured tetrahedral mesh is used. Mesh refinement guarantees high resolution around the band minima, while a relatively low total number of mesh elements is maintained (3).

Acoustic as well as optical phonon scattering is taken into account. For impact ionization a multi-threshold formula (4) with fine tuned threshold values is used to reproduce reported velocity field characteristics (5)(6) for relaxed Ge.

Figure 1 shows the velocity field characteristics for field in [100] direction for holes in unstrained Ge and for biaxially strained Ge grown on a [001] oriented $Si_{0.3}Ge_{0.7}$ substrate. The low field hole mobility is enhanced by a factor of 2.4 to 4400 cm^2/Vs. The result for relaxed Ge is compared to values from literature and shows good agreement. Figure 2 depicts the low field in-plane mobility for holes for uniaxial compressive stress in [110] direction as a result of full-band Monte Carlo simulation. A strong anisotropy with the most pronounced mobility enhancement in stress direction can be observed. Figure 3 presents the velocity field characteristics for uniaxial compressive stress and field in [110] direction.

In conclusion, it is shown by means of full-band Monte Carlo simulations that uniaxial compressive stressed Ge in [110] direction as well as biaxially stressed Ge features high hole mobility enhancement, which makes stress engineered Ge indeed a promising material for future applications.

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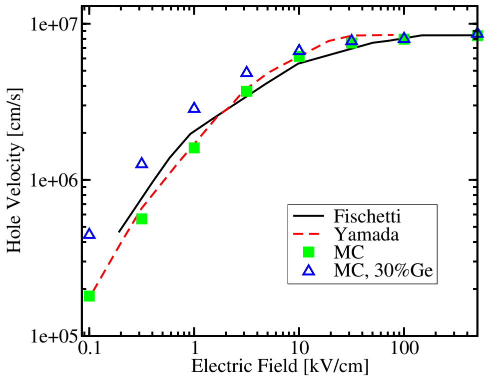

Figure 1: Hole velocity versus field in [100] direction for relaxed Ge compared to results from literature (5)(6) and for biaxial strained Ge grown on a $Si_{0.3}Ge_{0.7}$ substrate.

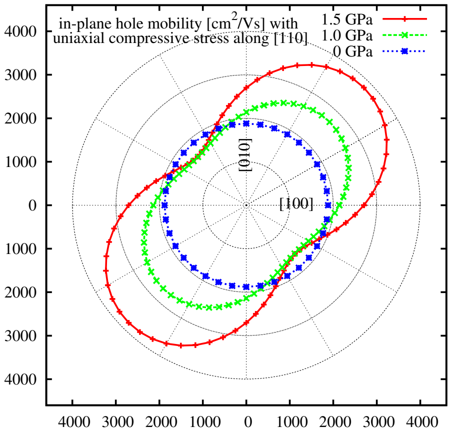

Figure 2: Low field hole mobility in bulk Ge for uniaxial [110] compressive stress computed by means of full-band Monte Carlo simulation.

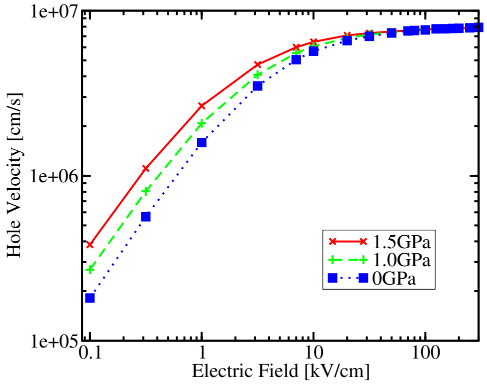

Figure 3: Hole velocity versus field for holes in compressive stressed Ge for field and stress in [110] direction.

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