Electron mobility in silicon under high uniaxial strain

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In the pursuit of enhancing the performance of semiconductor devices, the manipulation of material properties through strain engineering has emerged as a promising avenue [1]. In this work, the enhancement of the electron mobility in silicon has been experimentally investigated for uniaxial strain up to 1% applied along the [100] crystal direction.

A four-point bending setup is used to apply strain levels ranging from 0 to 1%, by steps of 0.02%, on an n-type silicon strain gauge supplied by *Kyowa* bonded on polycarbonate substrate (see inset Fig. 2a). A metallic strain gauge from *Micro-Measurements* is put next to the semiconductor one to measure the strain applied by the bending equipment. The device resistance has been obtained from current-voltage measurements using an *Agilent 4145* semiconductor analyzer in a voltage range from -0.5 V to 0.5 V with 20mV steps. To complement the experimental measurements, first-principles calculations have been conducted to determine the splitting of the conduction bands and the changes in the effective masses of the electron valleys induced by the strain. The theoretical calculations are based on density-functional theory (DFT) to obtain the band energies and effective masses, as implemented in ABINIT [2] with the generalized-gradient approximation (GGA) from Perdew-Burke-Ernzerhof (PBE) [3]. The uniaxial stress applied along the [100] crystal direction lifts the degeneracies of the six electrons valleys. The energy of the two Δ_2-valleys oriented along the strain direction increases, while the energy of the four others, called Δ_4-valleys, transverse to the applied stress, decreases with the strain as shown in Fig. 1a. On the other hand, the longitudinal effective mass increases (resp. decreases) for the Δ_2-valleys (resp. Δ_4-valleys) while the transverse one decreases (resp. increases) as shown in Fig. 1b.

The experimental results shown in Fig. 2a have been obtained from 2mm-long silicon beams with a cross-section of 250 µm by 20 µm, oriented transversely and longitudinally to the strain direction. The devices are n-doped and their doping level is about 10^{17} cm^{-3}. The mobility variations extracted from the raw measurements are shown in Fig. 2b and compared to the analytical model developed by Dhar *et al.* [4] and used by Ungersboeck *et al.* [5]. This work extends the original model by considering the variations of the effective masses, in addition to the valley splitting. The updated model enhances agreement with experimental data obtained from silicon beams and is then used to determine the undoped behavior. This is especially noticeable in the transverse contribution, where the reduction in mobility is offset by an increase in the transverse effective mass of the electron valleys. A significant improvement in the longitudinal component is observed at high strain, which was underestimated in the previous study.

To the best of our knowledge, this is the first time that the electron mobility variations at high strain have been observed experimentally in silicon for uniaxial stress applied along the [100] direction. The measurements have also validated the theoretical analysis, which extends beyond the existing model based solely on the splitting of valley energies due to strain.

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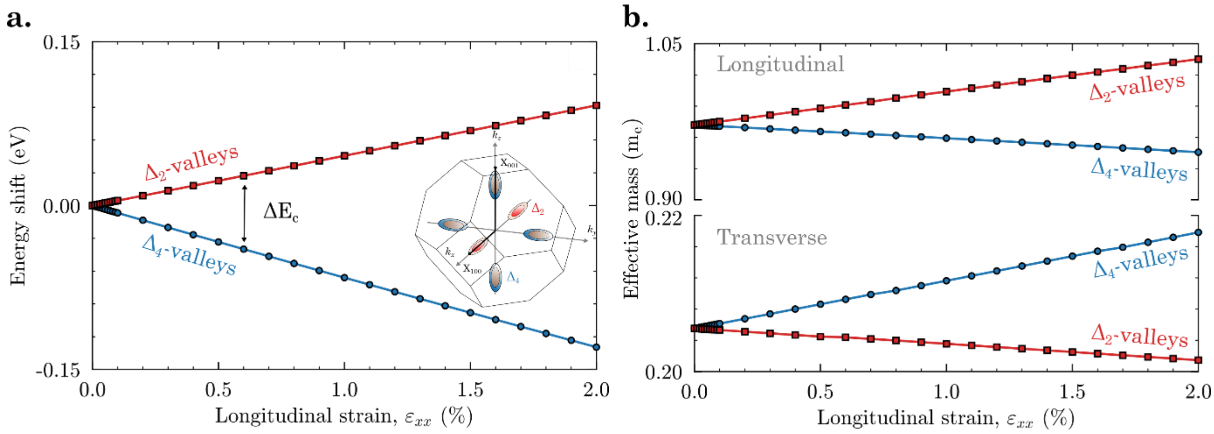

Fig. 1. (a) The energy shift of the minima of the electron valleys due to uniaxial strain along the [100] direction. The energy of the two valleys parallel to the strain (Δ_2-valleys in red squares) increases with the strain, while the one of the four valleys perpendicular to it decreases (Δ_4-valleys in blue dots). The inset shows the reciprocal space with the equipotential surface of the six electron valleys. (b) The effective masses for the Δ_2-valleys (red squares) and the Δ_4-valleys (blue dots) are given in terms of the free electron mass me. Both longitudinal (top) and transverse (bottom) masses are included.

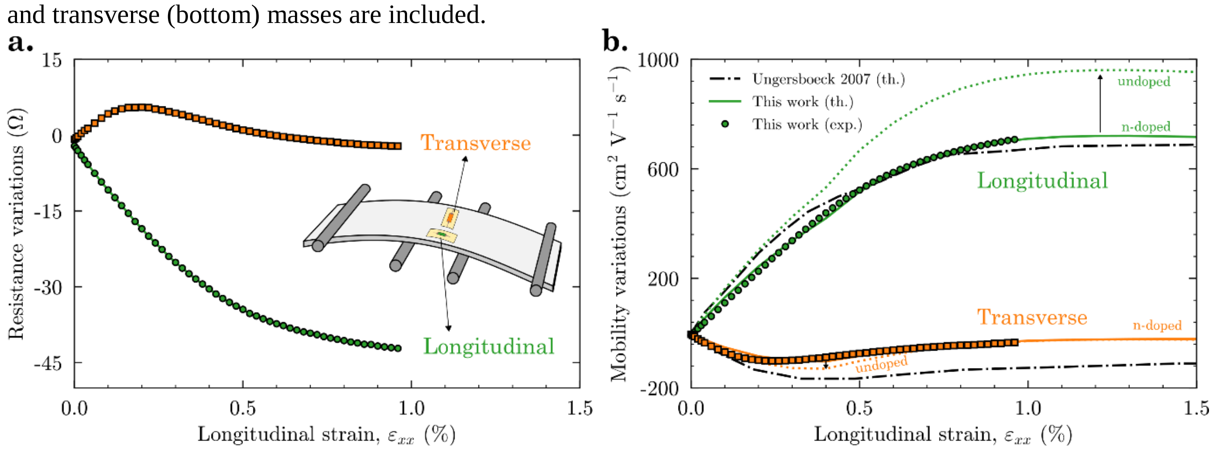

Fig. 2. (a) The resistance variations of the n-doped silicon beam were measured in both parallel (green dots) and perpendicular (orange squares) orientations to the strain direction. The picture depicts the four-point bending scheme used to strain the devices. Mobility variations were computed from the resistance measurements for the longitudinal (green dots) and transverse (orange squares) components. The figure displays the analytical model from Ungersboeck et al. [5] for undoped silicon as a dash-dotted line. The continuous and dotted lines represent the extended model for doped and undoped silicon, respectively, taking into account the effective mass variations.

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