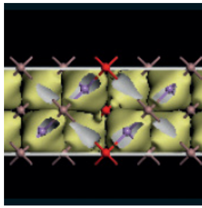

P:19 Electron and hole mobility calculation in GeSn alloys

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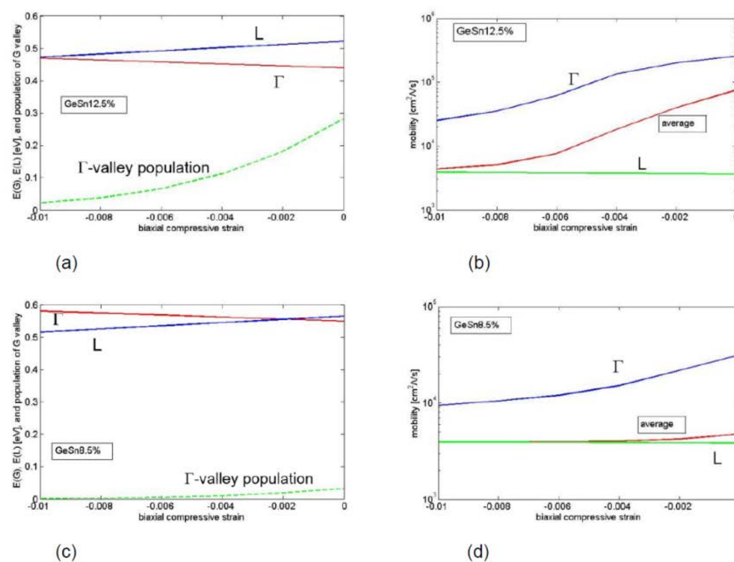
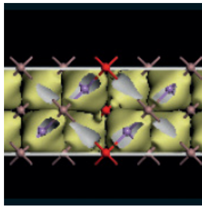
The recent advances in growth of group-IV (SiGeSn) materials are primarily directed towards their photonics applications, taking advantage of the direct band gap achievable for suitable composition and strain conditions. However, there are also good prospects of using these materials for electronic devices, where the band gap directness also offers distinct advantages (a higher electron mobility) over what is achievable in indirect gap alloys, accompanied with the benefits coming from mature and cost-effective fabrication on Si platform. Increased electron mobility is expected in direct-gap alloys because of a considerably lower Γ-electron effective mass in GeSn, compared to mass in Ge. Mobility is influenced by both the material composition and strain, and one way of using SiGeSn is as stressor material, to control the mobility in Ge, and the other would use it as active (conducting) material in CMOS type devices.

Here we present results of both electron and hole mobility calculation in GeSn bulk alloys. The band structure was calculated using effective mass with nonparabolicity for the conduction band indirect valleys, and 8-band k.p method [1], stabilised against spurious solutions, for holes and Γ-electrons, and linear deformation potentials in both cases. Mobility is then calculated in the conventional way [2,3], by finding the momentum relaxation times of carriers, due to: acoustic phonon, optical phonon (deformation potential), intervalley scattering, alloy disorder and ionised impurity scattering (however, scattering on defects / dislocations was not included because of insufficient data available, so the results may be somewhat optimistic). Examples of the dependence of mobility on alloy composition, strain, and doping density are given in Fig.1(a-f) for electrons and Fig.1(g,h) for holes. Generally, the mobility of Γ-electrons, and then also the average mobility, is indeed found to be very high provided the alloy is strongly direct, i.e. that the L valley is well above the Γ-valley, primarily because this suppresses strong intervalley Γ-L scattering. Aside from this effect, the alloy composition does not have a major influence because the alloy disorder does not give a very strong contribution to total scattering. In case of holes, the mobility primarily benefits from strain, either compressive or tensile, by removing the HH-LH scattering, while the alloy composition has a smaller influence.





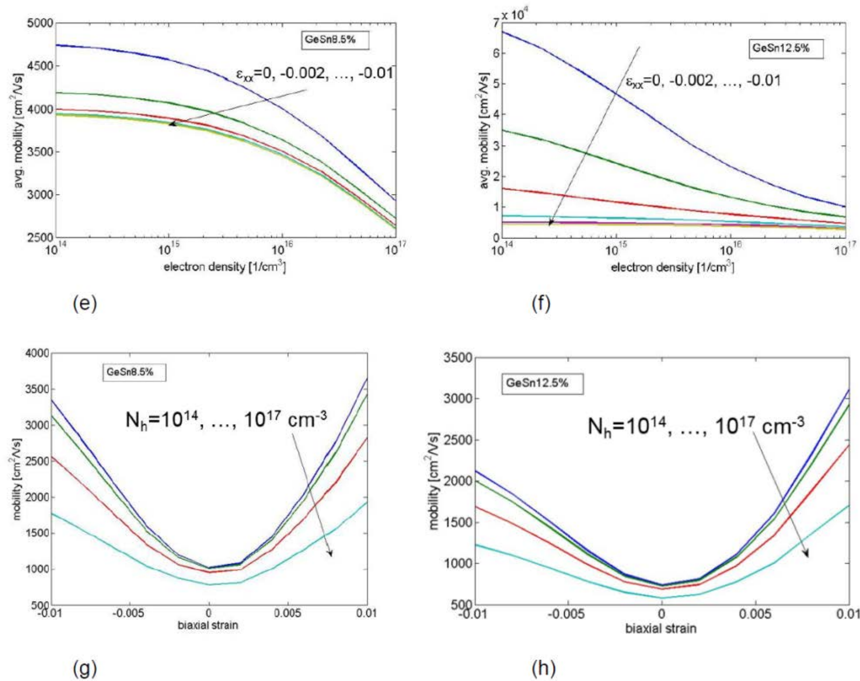


Fig.1. (a,c) GeSn c.b. valley edges (solid) and Γ-population (dashed), low-density electron mobility (b,d), its dependence on electron density (e,f), and hole mobility (g,h) in strained GeSn at T=300K.

P:20 Transport modelling and design of GaN/AlN based unipolar (opto-)electronic devices, and interface quality effects

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The AlGaN/GaN material system has been proposed as a highly promising alternative to more conventional III–V's for various optoelectronic devices, e.g. quantum cascade lasers (QCL), photodetectors and electronic devices like resonant tunnelling diodes (RTD). The high LO-phonon energy in GaN should significantly reduce the thermal degradation effects coming from phonon-assisted relaxation, which could allow lasing at higher THz frequencies, and higher operation temperature [1]. A detailed understanding of electron transport in AlGaN/GaN heterostructures is crucial for optimizing devices performance. RTDs are interesting in their own right, and also as the simplest devices in which vertical tunneling and scattering transport can be investigated, both experimentally and theoretically: the experience can then be transferred to the design of more complicated devices. We have therefore investigated electron transport in epitaxially grown nitride-based RTDs, as well as in sequential tunneling devices [2]. The density-matrix model developed for this purpose is shown to be able to reproduce the experimental I-V characteristics. Scattering-induced broadening effects (largely coming from interface roughness) are found to have a strong influence on current magnitude and peak-to-valley ratios, highlighting critical optimization parameters for III–nitride unipolar electronic and optoelectronic devices. Investigation of AlGaN QCLs, also performed by the density matrix method, shows that a realistic level of interface roughness (found from RTD modelling) would degrade the