Alloy Scattering and Field-Dependent Electron Transport in Direct-Gap $Ge_{1-x}Sn_x$ Alloys

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Incorporation of Sn in Ge to form $Ge_{1-x}Sn_x$ alloys has been theoretically predicted and experimentally confirmed to drive an indirect- to direct-gap transition. This signals significant potential for applications in optoelectronic devices suitable for monolithic integration on Si, stimulating ongoing efforts to develop direct-gap group-IV optoelectronic devices compatible with complementary metal-oxide-semiconductor (CMOS) fabrication [1]. Proposed device applications of (Si)$Ge_{1-x}Sn_x$ alloys – including mid-infrared lasers for Si photonics, 1 eV absorber layers for multi-junction solar cells, and tunneling field-effect transistors for post-CMOS electronics [3] – mandate detailed understanding of carrier transport in the alloy, particularly in the presence of an applied electric field.

The indirect- to direct-gap transition in $Ge_{1-x}Sn_x$, which occurs for Sn composition $x \approx 8\%$, reorders the Γ- and L-point valleys in the lowest energy conduction band (CB), with the former being lower in energy for $x > 8\%$. This has long been predicted to drive strong enhancement of the electron mobility μ at low field, due to the low Γ-valley effective mass [2]. However, there has to date been limited analysis of the impact of Sn incorporation on the low-field μ, and no explicit analysis of field-dependent electron transport in the alloy. The direct-gap $Ge_{1-x}Sn_x$ CB structure – characterized by a low effective mass zone-center Γ-valley minimum flanked by higher energy, high effective mass zone-edge L- and X-point satellite valleys – can also be expected to give rise to negative differential resistance (NDR) in the presence of an applied electric field. Achieving NDR – the so-called Gunn effect, which is present in several direct-gap III-V semiconductors and is exploited to provide efficient microwave power generation for sensing applications – represents potentially novel electrical functionality in a group-IV semiconductor.

We present the first explicit calculations of field-dependent electron transport in $Ge_{1-x}Sn_x$ alloys, informed by recent developments in our understanding of the details of the CB structure [4]. We firstly analyze the evolution of the low-field electron mobility with x, via direct evaluation of the Sn-induced intra- and inter-valley alloy scattering rates based on atomistic alloy supercell calculations. Our calculations demonstrate strong enhancement of the low-field μ in the direct-gap regime which, in the absence of defects, can exceed that of GaAs for Sn compositions $x > 11\%$. We then consider field-dependent transport, in which an electric field drives the electron population out of thermal equilibrium. We solve the Boltzmann transport equation in the relaxation time approximation, including inter- and intra-valley scattering of electrons by acoustic and optical phonons, and by the alloy potential. Our calculations reveal strong dependence of the electron mobility and drift velocity on the field strength F, characterized by prompt acceleration of Γ-valley electrons and rapid intervalley scattering to L valleys. We verify the presence of NDR in the direct-gap regime, but within a limited range of F vs. in III-V semiconductors, due to the absence of polar-optical phonon scattering in group-IV materials.

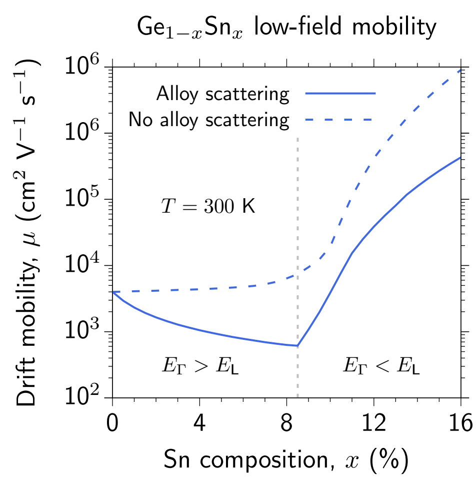

Fig. 1. Evolution of the low-field electron mobility μ with x in $Ge_{1-x}Sn_x$, calculated with (solid blue) and without (dashed blue) alloy scattering. The alloy is direct-gap for $x > 8\%$ (dotted gray), beyond which composition μ increases strongly as electrons occupy the low effective mass Γ-valley.

References

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