Modeling of a SiGeSn Quantum Well Laser

Supplementary Information

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Dataset 1: Tabulated material properties from 8-band $k \cdot p$ calculations

A summary of the values calculated for a central well (5th well and barrier counting from bottom), can be found in the following table. Values vary from layer to layer due to the varying strain. Energy levels correspond to values prior to applying the additional 30 meV reduction in directness described in the Modeling Results Section of the main text.

Table S1. Tabulated material properties for 5th well and barrier.

Quantity	Symbol	Value	Unit
Γ-valley energy (well)	$\boldsymbol{E_{\Gamma}}$	0.2216	eV
L-valley energy (well)	$\boldsymbol{E_{L}}$	0.3008	eV
HH-valley energy (well)	$\boldsymbol{E_{HH}}$	-0.2412	eV
LH-valley energy (well)	$\boldsymbol{E_{LH}}$	-0.2568	eV
E_{HH} − SO-valley energy (well)	Δ_{so}	0.3877	eV
Γ-valley energy (barrier)	$\boldsymbol{E_{\Gamma,b}}$	0.3160	eV
L-valley energy (barrier)	$\boldsymbol{E_{L,b}}$	0.3250	eV
HH-valley energy (barrier)	$\boldsymbol{E_{HH,b}}$	-0.2878	eV
LH-valley energy (barrier)	$\boldsymbol{E_{LH,b}}$	-0.2784	eV
$E_{\mathrm{HH,b}}$ − SO-valley energy (barrier)	$\Delta_{\mathbf{so,b}}$	0.3606	eV
1st quantized Γ-level	$\boldsymbol{E_{\Gamma 1}}$	0.2353	eV
2nd quantized Γ-level	$\boldsymbol{E_{\Gamma 2}}$	0.2764	eV
1st quantized L-level	$\boldsymbol{E_{L1}}$	0.3044	eV
2st quantized L-level	$\boldsymbol{E_{L2}}$	0.3145	eV
1st quantized HH-level	$\boldsymbol{E_{HH1}}$	-0.2437	eV
2nd quantized HH-level	$\boldsymbol{E_{HH2}}$	-0.2514	eV
3rd quantized HH-level	$\boldsymbol{E_{HH3}}$	-0.2636	eV
1st quantized LH-level	$\boldsymbol{E_{LH1}}$	-0.2652	eV
In-plane Γ-valley mass[1] (well)	$\boldsymbol{m_{\Gamma,||}}$	0.0250	m_0
z-direction Γ-valley mass[1] (well)	$\boldsymbol{m_{\Gamma,z}}$	0.0260	m_0
In-plane L-valley mass[1] (well)	$\boldsymbol{m_{L,||}}$	0.2920	m_0
z-direction L-valley mass[1] (well)	$\boldsymbol{m_{L,z}}$	0.1170	m_0

In-plane HH-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{HH},||}}$	0.0375	m_0
z-direction HH-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{HH,z}}}$	0.2184	m_0
In-plane LH-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{LH},||}}$	0.0838	m_0
z-direction LH-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{LH,z}}}$	0.0294	m_0
In-plane SO-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{SO},||}}$	0.0518	m_0
z-direction SO-valley mass[1] (well)	$\boldsymbol{m_{\mathrm{SO,z}}}$	0.0518	m_0
In-plane Γ-valley mass[1] (barrier)	$\boldsymbol{m_{\Gamma,||,\mathrm{b}}}$	0.0480	m_0
z-direction Γ-valley mass[1] (barrier)	$\boldsymbol{m_{\Gamma,\mathrm{z,b}}}$	0.0470	m_0
In-plane L-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{L},||,\mathrm{b}}}$	0.2970	m_0
z-direction L-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{L,z,b}}}$	0.1210	m_0
In-plane HH-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{HH},||,\mathrm{b}}}$	0.0382	m_0
z-direction HH-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{HH,z,b}}}$	0.2204	m_0
In-plane LH-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{LH},||,\mathrm{b}}}$	0.0851	m_0
z-direction LH-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{LH,z,b}}}$	0.0300	m_0
In-plane SO-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{SO},||,\mathrm{b}}}$	0.0527	m_0
z-direction SO-valley mass[1] (barrier)	$\boldsymbol{m_{\mathrm{SO,z,b}}}$	0.0527	m_0

[1]Effective masses are given in multiples of the free electron mass m_0.
In-plane masses are averaged over the [100] and [110] directions.

Table S2. Tabulated material properties for the $Ge_{0.9}Sn_{0.1}$ buffer layer.

Quantity	Symbol	Value	Unit
Γ-valley energy (buffer)	$\boldsymbol{E_{\Gamma,\mathrm{c}}}$	0.2717	eV
L-valley energy (buffer)	$\boldsymbol{E_{\mathrm{L,c}}}$	0.3188	eV
HH-valley energy (buffer)	$\boldsymbol{E_{\mathrm{HH,c}}}$	-0.2845	eV
LH-valley energy (buffer)	$\boldsymbol{E_{\mathrm{LH,c}}}$	-0.2773	eV
$E_{\mathrm{HH,b}}$ − SO-valley energy (buffer)	$\boldsymbol{\Delta_{\mathrm{so,c}}}$	0.3527	eV
In-plane Γ-valley mass[1] (buffer)	$\boldsymbol{m_{\Gamma,||,\mathrm{c}}}$	0.0290	m_0
z-direction Γ-valley mass[1] (buffer)	$\boldsymbol{m_{\Gamma,\mathrm{z,c}}}$	0.0290	m_0
In-plane L-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{L},||,\mathrm{c}}}$	0.2920	m_0
z-direction L-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{L,z,c}}}$	0.1170	m_0
In-plane HH-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{HH},||,\mathrm{c}}}$	0.0454	m_0
z-direction HH-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{HH,z,c}}}$	0.2204	m_0
In-plane LH-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{LH},||,\mathrm{c}}}$	0.0964	m_0
z-direction LH-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{LH,z,c}}}$	0.0359	m_0
In-plane SO-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{SO},||,\mathrm{c}}}$	0.0617	m_0
z-direction SO-valley mass[1] (buffer)	$\boldsymbol{m_{\mathrm{SO,z,c}}}$	0.0617	m_0

[1]Effective masses are given in multiples of the free electron mass m_0.
In-plane masses are averaged over the [100] and [110] directions.

Effective masses are obtained by numerically fitting the second derivative of the density of states around the high-symmetry points corresponding to the valley centers. Sufficient strain is present in all the layers with sufficient splitting between heavy hole (HH) and light hole (LH) energy levels for these numbers to be well defined.

Dataset 2: Tabulated optical modeling results

Table S3 shows tabulated properties of the main modes discussed in the main part of the paper, TE_3, TM_3 and TM_0. It is apparent that TE_3 has near zero Γ_{TM} at well number 3, that is close to the center of the structure, due to its quasi-TE symmetry, but has finite Γ_{TM} at the other wells. Conversely, TM_3 and TM_0 have zero Γ_{TE} at well number 3, but finite Γ_{TE} for the other wells. While for TE_3 and TM_0, TE and TM confinement factors are respectively dominant, TM_3 actually has stronger TE confinement factors. Effective and group indices are referenced relative to the outer circumference of the ring, which is why higher order modes, with main lobes deeper inside the structure at lower radii, have lower effective indices (they effectively travel along a shorter circumference). Bending losses for all these modes were found to be negligible.

Table S3. Summary of the properties of optical modes.

Property	TE_3	TM_3	TM_0	Unit
Effective index	2.1925	2.2049	3.3186	
Group index	3.6684	4.0853	4.3758	
Bending losses	0.0000	0.0000	0.0000	cm^{-1}
Γ_{TE} (well 1)	0.0599	0.0200	0.0028	
Γ_{TE} (well 2)	0.0659	0.0069	0.0009	
Γ_{TE} (well 3)	0.0687	0.0006	0.0001	
Γ_{TE} (well 4)	0.0681	0.0023	0.0003	
Γ_{TE} (well 5)	0.0641	0.0122	0.0016	
Γ_{TE} (well 6)	0.0572	0.0270	0.0038	
Γ_{TE} (well 7)	0.0489	0.0405	0.0064	
Γ_{TE} (well 8)	0.0390	0.0503	0.0093	
Γ_{TE} (well 9)	0.0289	0.0519	0.0118	
Γ_{TE} (well 10)	0.0197	0.0450	0.0136	
Γ_{TM} (well 1)	0.0003	0.0208	0.0525	
Γ_{TM} (well 2)	0.0001	0.0240	0.0602	
Γ_{TM} (well 3)	0.0000	0.0254	0.0637	
Γ_{TM} (well 4)	0.0000	0.0250	0.0627	
Γ_{TM} (well 5)	0.0002	0.0227	0.0572	
Γ_{TM} (well 6)	0.0005	0.0189	0.0479	
Γ_{TM} (well 7)	0.0006	0.0146	0.0371	
Γ_{TM} (well 8)	0.0006	0.0096	0.0248	
Γ_{TM} (well 9)	0.0005	0.0052	0.0136	
Γ_{TM} (well 10)	0.0002	0.0019	0.0051	