Thermal conductivity tensor of $In_xGa_{1-x}As/In_yAl_{1-y}As$ superlattices and application to quantum cascade lasers

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An InGaAs/InAlAs superlattice (SL) on an InP substrate is the mainstream material system for mid-IR quantum cascade lasers (QCL). The thermal conductivity tensor of SLs is critical for energy-efficient performance of QCLs; understanding the relative importance of different factors that influence heat flow in these systems is essential in device modeling and optimization [1]. It is known that thermal conduction in SLs is extremely anisotropic, with the cross-plane thermal conductivity much lower than the in-plane conductivity. Unfortunately, it is very difficult to experimentally measure the full thermal conductivity tensor, and systematic modeling of SL systems is also missing.

In this work, we calculate the full thermal conductivity tensor in the InGaAs/InAlAs SL system at a specified lattice temperature, considering full phonon dispersions, accurate phonon scattering rates, and the thermal interface resistance caused by both interface roughness and material mismatch.

We calculate the thermal conductivity tensor based on the phonon Boltzmann transport equation [2]:

$$\kappa^{\alpha\beta} = \sum_{b,\vec{q}} \tau_b(\vec{q}) C_{b,T}(\vec{q}) v_b^{\alpha}(\vec{q}) v_b^{\beta}(\vec{q}), \qquad (1)$$

where $\tau_b(\vec{q})$ is the total phonon relaxation time and $C_{b,T} = \frac{\partial\left(\frac{\hbar\omega(\vec{q})}{k_B T}\right)}{\partial T}$ is the phonon heat capacity for mode b at temperature T. Both the group velocity and the heat capacity are calculated from the full dispersion relation using the adiabatic bond charge model (Figs. 1,2).

We have previously shown [2] that we can treat the influence of surface roughness and material mismatch separately. The roughness scattering is incorporated in the scattering time $\tau_b(\vec{q})$ and the extra interface resistance caused by mismatch is added when calculating the cross-plane SL thermal conductivity. We consider a SL with $2n$ layers in a single stage, which is formed by alternating materials 1 and 2 with layer thicknesses $L_{11}, L_{12}, ..., L_{1n}; L_{21}, L_{22}, ..., L_{2n}$. The in-plane and cross-plane thermal conductivities are calculated as:

$$\kappa_{\text{in-plane}} = \frac{\sum_{i=1}^{n}(L_{1i}\kappa_1^{xx} + L_{2i}\kappa_2^{xx})}{\sum_{i=1}^{n}(L_{1i}+L_{2i})}; \qquad (2)$$

$$\kappa_{\text{cross-plane}} = \frac{\sum_{i=1}^{n}(L_{1i}+L_{2i})}{\sum_{i=1}^{n}\left(\frac{L_1 i}{\kappa_1^{yy}} + \frac{L_2 i}{\kappa_2^{yy}}\right) + n\left(\frac{1}{G_{1\to 2}} + \frac{1}{G_{2\to 1}}\right)} \qquad (3)$$

Here, $G_{1\to 2}$ and $G_{2\to 1}$ are the thermal boundary conductances from 1 to 2 and from 2 to 1, respectively. For materials 1 and 2, $\kappa_{1,2}^{xx}$ and $\kappa_{1,2}^{yy}$ are the in-plane and cross-plane thermal conductivity, respectively, and they include $\tau_b(\vec{q})$.

Thermal boundary conductance (TBC) is the dominant factor in the anisotropy of thermal conductivity in SLs. TBC has been extensively studied by molecular dynamics (MD), but very few experiments have been conducted due to difficulties in sample preparations [3]. Neither does a model exist that explains the experimental or the MD data over a wide range of temperatures and surface conditions.

There are two primary models describing phonon transmission through the interface: the acoustic mismatch model (AMM) and the diffusive mismatch model (DMM) [4]. In the AMM, an essential assumption is that phonons are governed by continuum acoustics and can therefore reflect or transmit at the boundary, following Snell's law. In the DMM,

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a phonon is destroyed on one side of the interface and a new phonon, with the same energy and a completely random momentum, is created on the other side; effectively, the DMM describes fully diffuse elastic scattering. Both experiment and MD show that real transport is somewhere between the two limits.

Here, we introduce a parameter that helps interpolate between the AMM and DMM transmission rates and get a better description of the TBC. With the SL thermal conductivity and the TBC model, we calculate the thermal conductivity tensor of InGaAs/InAlAs SLs (Figs. 2, 3). The results also includes strain effects, which are often associated with III-V superlattices and very important in QCLs. The calculated cross-plane thermal conductivity values agree very well the recent experimental results (Fig. 3) [1].

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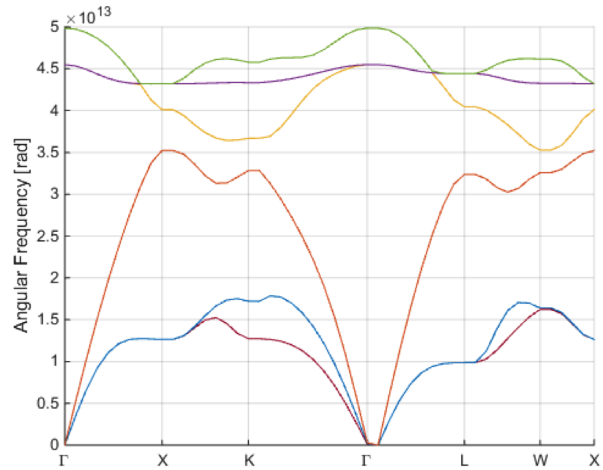

Fig. 1. Phonon dispersion of $In_{0.53}Ga_{0.47}As$ calculated from the adiabatic bond charge model.

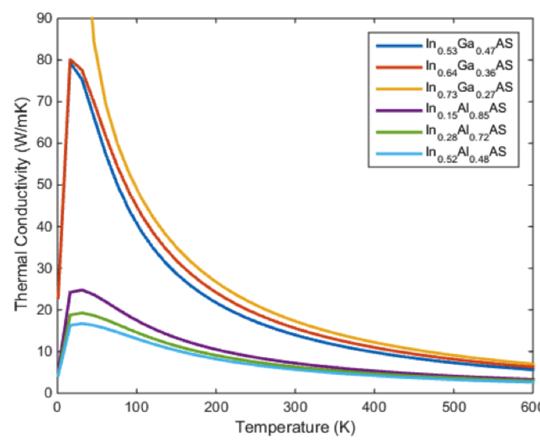

Fig. 2. Calculated bulk thermal conductivity of InGaAs and InAlAs as a function of temperature.

	$K_{in\text{-}plane}$ (W/mK)		$K_{cross\text{-}plane}$ (W/mK)			
	Exp.	Cal.	**Exp.**	**Cal.**	AMM	DMM
A2-G2	--	3.86	**1.63**	**1.27**	3.58	0.52
A2-G4	--	4.89	**1.88**	**1.75**	4.08	0.74
A4-G2	--	3.71	**1.50**	**1.61**	3.59	0.73
A2-G6	--	5.57	**2.31**	**2.17**	4.42	0.95
A6-G2	--	3.71	**1.21**	**1.88**	3.62	0.91
A4-G4	--	4.51	**1.66**	**2.00**	3.95	0.93

Fig. 3. Comparison of the calculated cross-plane thermal conductivity for different InGaAs/InAlAs SLs with experimental results from Sood *et al*. [1].