Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary File: Thermal Transport in Twinning Superlattice and Mixed-Phase GaAs Nanowires

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Thermal Conductivity Versus Nanowire Length

Thermal conductivity is size-dependent in non-equilibrium molecular dynamics simulations (NEMD), increasing with the size of the unit cell. We find that this change becomes negligible near a nanowire length of 350 nm in our studies, as shown in Fig. S1 for example. The nanowire length is truncated at 350 nm to minimize the duration of NEMD simulations.

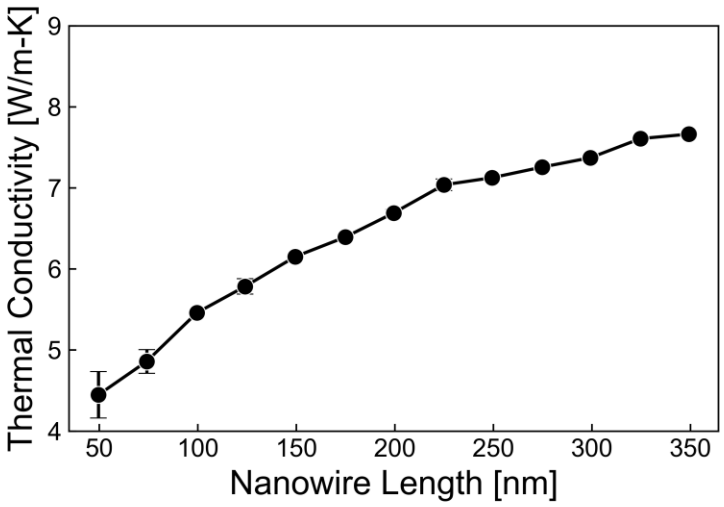

Fig. S1. Saturation of the thermal conductivity in non-equilibrium molecular dynamics simulations. Data points correspond to a pristine zincblende nanowire with constant diameter 50 Å.

Atomistic Green's Function Method

An excellent introduction to the Atomistic Green's Function (AGF) method can be found in Refs. 1 and 2. Here, we summarize the basic procedure and details relevant to our implementation.

The harmonic matrix for entire system can be partitioned into blocks:

$$\mathbf{H}_{\mathrm{tot}} = \begin{bmatrix} \mathbf{H}_1 & \boldsymbol{\tau}_1^{\dagger} & 0 \\ \boldsymbol{\tau}_1 & \mathbf{H}_d & \boldsymbol{\tau}_2 \\ 0 & \boldsymbol{\tau}_2^{\dagger} & \mathbf{H}_2 \end{bmatrix} \tag{S1}$$

where subscripts 1, d, and 2 correspond to the first contact, the device region, and the second contact, respectively. For our purposes, these labels indicate contiguous regions along an arbitrary NW structure; shown as the "device" and two "contact" regions in Fig. S2. Interactions among the N_d atoms in the device region are described by the $3N_d \times 3N_d$ submatrix $\mathbf{H}_d$ at the center of $\mathbf{H}_{\mathrm{tot}}$, which is in principle infinitely large. Similarly, the off-diagonal submatrices $\boldsymbol{\tau}_i$ contain the harmonic constants connecting atoms in the device region to either contact ($i = 1$, 2) and vice versa for $\boldsymbol{\tau}_i^{\dagger}$.

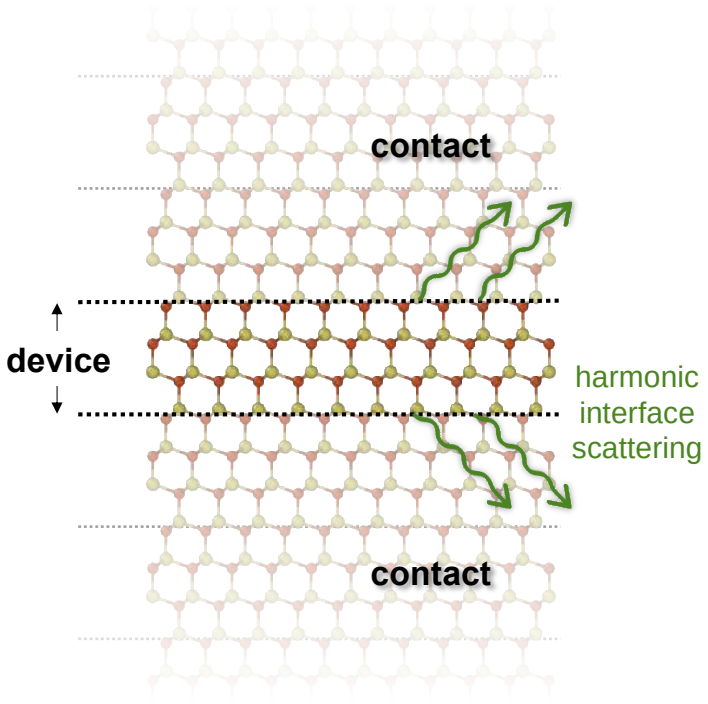

Fig. S2. An illustration of a nanowire (NW) system used for atomistic Green's function calculations. Two semi-infinite "contacts" connect to either end of the "device", here consisting of one zincblende unit cell. A NW with diameter 35 Å is shown for clarity.

To obtain the transmission function, one computes the trace of a matrix product:

$$\mathcal{T}(\omega) = \mathrm{Tr}(\mathbf{\Gamma}_1 \mathbf{G} \mathbf{\Gamma}_2 \mathbf{G}^\dagger) \tag{S2}$$

where the matrix $\mathbf{G}$ represents the Green's function for the device region:

$$\mathbf{G}(\omega^2) = [\omega^2 \mathbf{I} - \mathbf{H}_d - \mathbf{\Sigma}_1(\omega^2) - \mathbf{\Sigma}_2(\omega^2)]^{-1} \tag{S3}$$

and the matrices $\mathbf{\Gamma}_i = i[\mathbf{\Sigma}_i - \mathbf{\Sigma}_i^\dagger]$ in Eq. (S3) represent the phonon "escape rate" into either contact. Without the explicit inclusion of boundary scattering,[3] nor other disordered mechanisms, transmission is limited only by harmonic interface scattering. Hence, $\mathcal{T}(\omega)$ indicates the "connectivity" of normal modes across the device region.

Since the device region is finite, the connection matrices $\boldsymbol{\tau}_i$ are populated by finitely many non-zero elements. (This can be understood in terms of atomic interaction distances being effectively finite.) Thus, the self-energy matrices, $\boldsymbol{\Sigma}_i = \boldsymbol{\tau}_i \boldsymbol{g}_i \boldsymbol{\tau}_i^\dagger$, can be computed from finite submatrices by obtaining the surface Green's functions, $\boldsymbol{g}_i^S$, of the contacts. We employed the usual decimation technique[4,5] to approximate $\boldsymbol{g}_i^S$ by recursive renormalization, avoiding explicit inversions of a very large $\mathbf{H}_i$. Once $\boldsymbol{\Sigma}_i$ are obtained, the device Green's function is calculated by matrix inversion, as in Eq. (S3). With this, the transmission can be calculated from Eq. (S2). The process is then repeated at each frequency point, ω.

References

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