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Thermal Conductivity in Superlattices

半導体超格子構造における熱伝導率の解析

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Collaborators and references

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References

1. S. Tamura, Y. Tanaka, and H. J. Maris, Phys. Rev. B60, 2627 (1999)
2. B. C. Daly, H. J. Maris, K. Imamura and S. Tamura, Phys. Rev. B66, 24301 (2002)
3. K. Imamura *et al.*, J. Phys. Condensed Matter 15, 8679 (2003)
4. B. C. Daly, H. J. Maris, Y. Tanaka and S. Tamura, Phys. Rev. B67, 33308 (2002)

Outline of Talk

0. Introduction：Phonons in superlattices

1. Out-of-plane conductivity

   1- 0 Experimental results

   1- 1 Effect of Brillouin-zone folding

   1- 2 Effect of relaxation time (anharmonicity)

   1- 3 Effect of interface roughness

2. In-plane conductivity

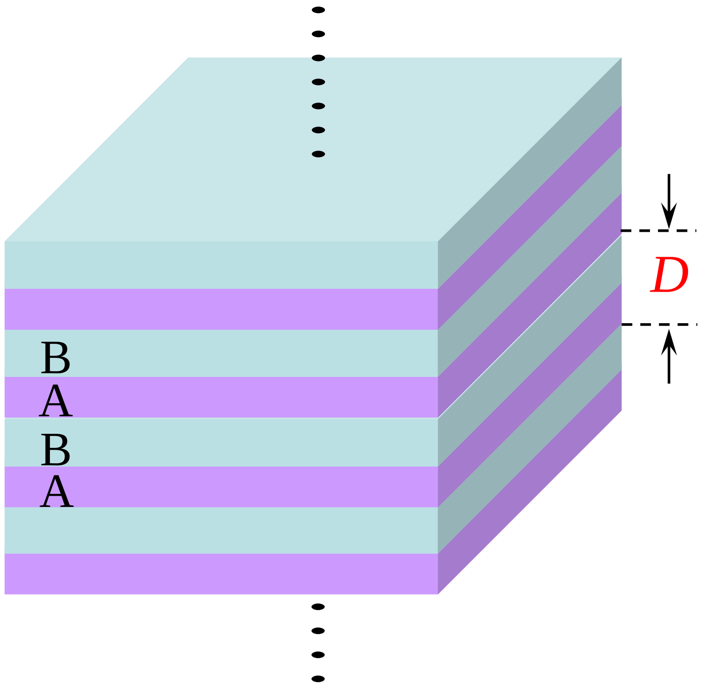
Application of superlattice structures

Operation of devices is greatly affected
by thermal conductivity κ

(1) Semiconductor laser

⇨ *large* κ is preferred

Lifetime is reduced
by the heat produced



(2) Thermoelectric devices

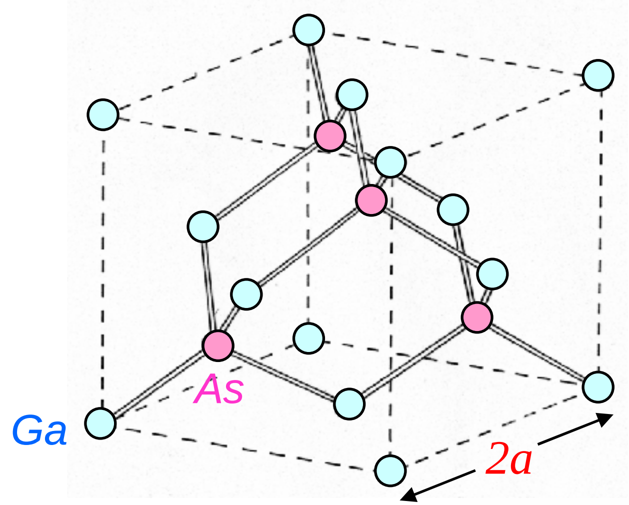
⇨ *low* κ materials are preferable

Figure of merit : $Z = \frac{S^2}{\rho \kappa}$ ($V = S\,\Delta T$, S : Seebeck coefficient)

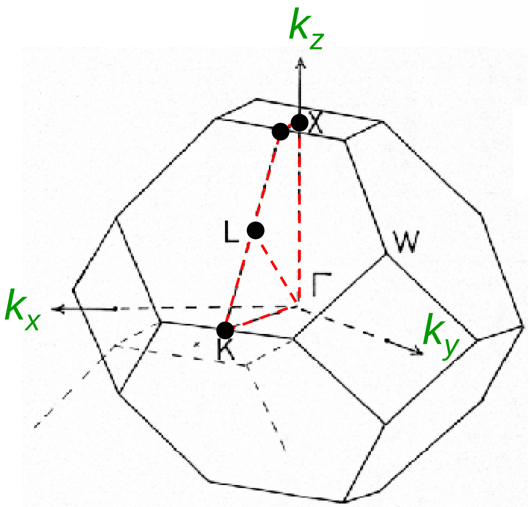
Smaller thermal conductivity produces
larger temperature difference

Phonon dispersion relations in a bulk crystal

Zincblende structure

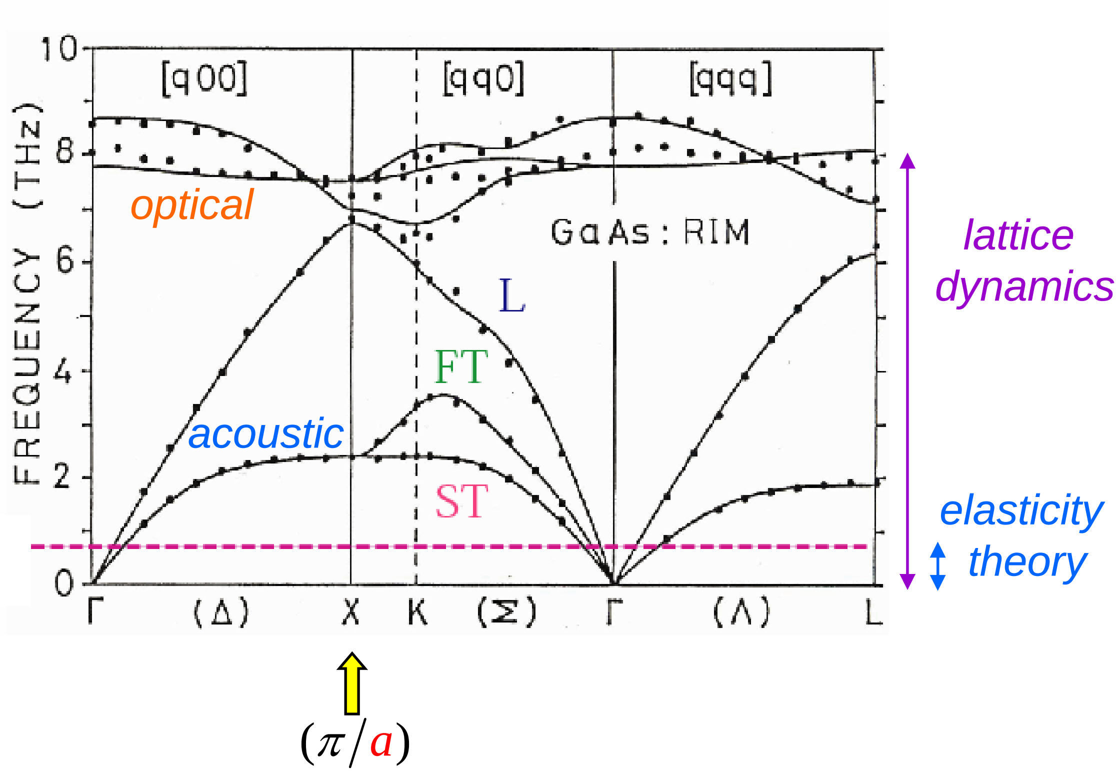


Brillouin zone



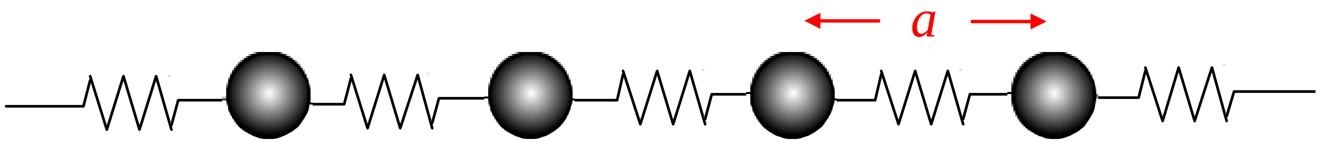
Dispersion relations $\omega = \omega(\mathbf{k}, j)$

in GaAs *(a cubic crystal)*



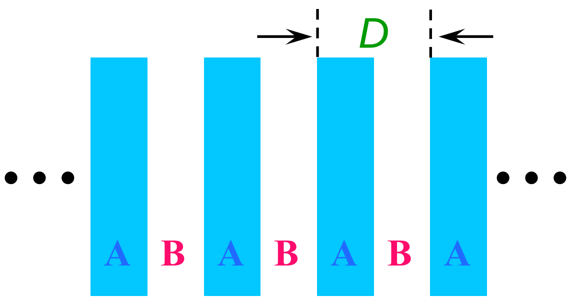
Synthetic periodicity and zone-folding

Bulk crystalline solids (1D)



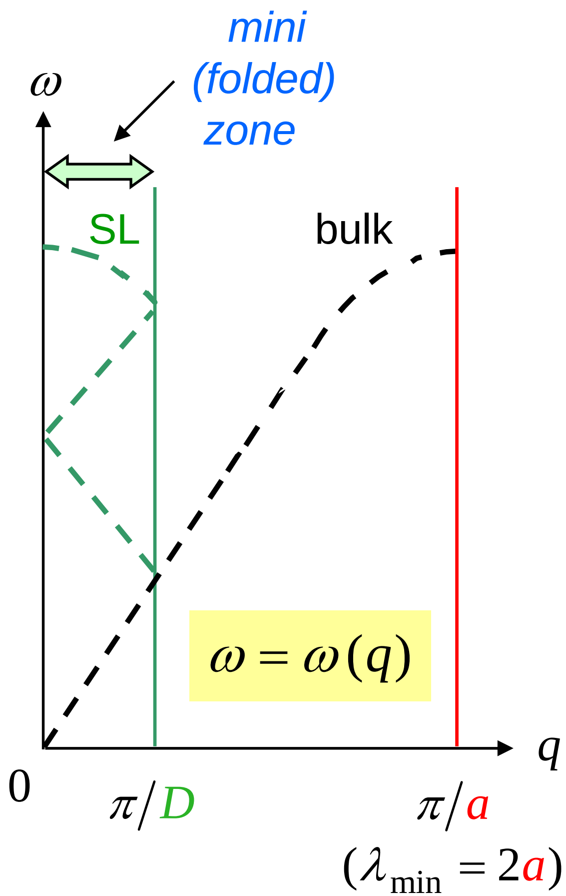
unit period a (atomic spacing)

1D Periodic superlattices (SLs)



synthetic periodicity D ($= n\, a$)

Brillouin-zone folding



$$2D = n\lambda = n\frac{2\pi}{q} \Rightarrow q = n\frac{\pi}{D}$$ (*Bragg condition*)

How to calculate the phonon dispersion relations in SLs

Elasticity theory (*valid for sub-THz phonons*)

$$\rho \frac{\partial^2 u_i(\mathbf{r},t)}{\partial t^2} = \sum_j \frac{\partial S_{ij}(\mathbf{r},t)}{\partial x_j}$$

$$S_{ij}(\mathbf{r},t) = \sum_k \sum_l c_{ijkl} \frac{\partial u_l(\mathbf{r},t)}{\partial x_k}$$

u_i : lattice displacement

S_{ij} : stress tensor

ρ : density

c_{ijkl}: elastic stiffnes tensor

$$\Rightarrow \quad \rho \frac{\partial^2 u_i(\mathbf{r},t)}{\partial t^2} = c_{ijkl} \frac{\partial^2 u_k(\mathbf{r},t)}{\partial x_j \partial x_l}, \quad (i = 1,2,3)$$: wave equations

Plane wave solution

$$\mathbf{u}(\mathbf{r},t) = a\,\mathbf{e}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

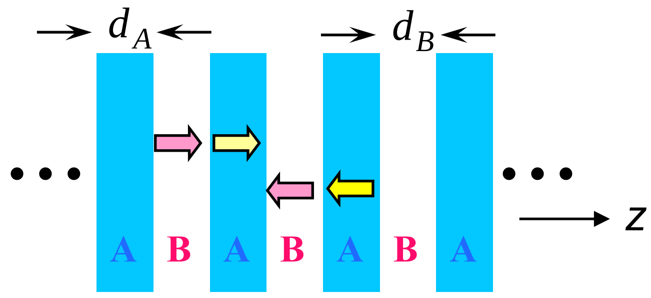
one longitudinal (L)
two transverse (T)

Christoffel equation

$$\left(\rho\,\omega^2 \delta_{im} - c_{ijmn} k_j k_n\right) e_m = 0, \quad (i = 1,2,3) \quad \Rightarrow \quad \omega = \omega(\mathbf{k}, j)$$

Wave fields and transfer matrices for superlattices

Wave fields in *A* layer



(*3 pairs of counter-propagating waves*)

$$\mathbf{W}_n^A(z) \qquad \mathbf{A}_n \qquad \Gamma_{\mathrm{A}} \qquad \Phi_A(z)$$

$$\begin{pmatrix} \mathbf{U}_n^A(\mathbf{x},t) \\ \mathbf{S}_n^A(\mathbf{x},t) \end{pmatrix} = \sum_{j=1}^{6} a_n^{(j)} \begin{pmatrix} \mathbf{e}_A^{(j)} \\ \boldsymbol{\sigma}_A^{(j)} \end{pmatrix} \exp(ik_{A,z}^{(j)}\, z) e^{i(\mathbf{k}_\parallel \cdot \mathbf{x}_\parallel - \omega t)}$$

$$= \mathbf{W}_n^A(z) e^{i(\mathbf{k}_\parallel \cdot \mathbf{x}_\parallel - \omega t)}$$

Definitions of *transfer matrices*

$$\mathbf{W}_n^A(z) = \Gamma_{\mathrm{A}}\, \Phi_A(z)\, \mathbf{A}_n \Rightarrow T_A = \Gamma_{\mathrm{A}}\, \Phi_A(d_A)\, \Gamma_{\mathrm{A}}^{-1}$$

$$\Rightarrow \boxed{T \equiv T_B\, T_A}$$

6×6 *matrix*

Transfer matrix in *periodic* SLs

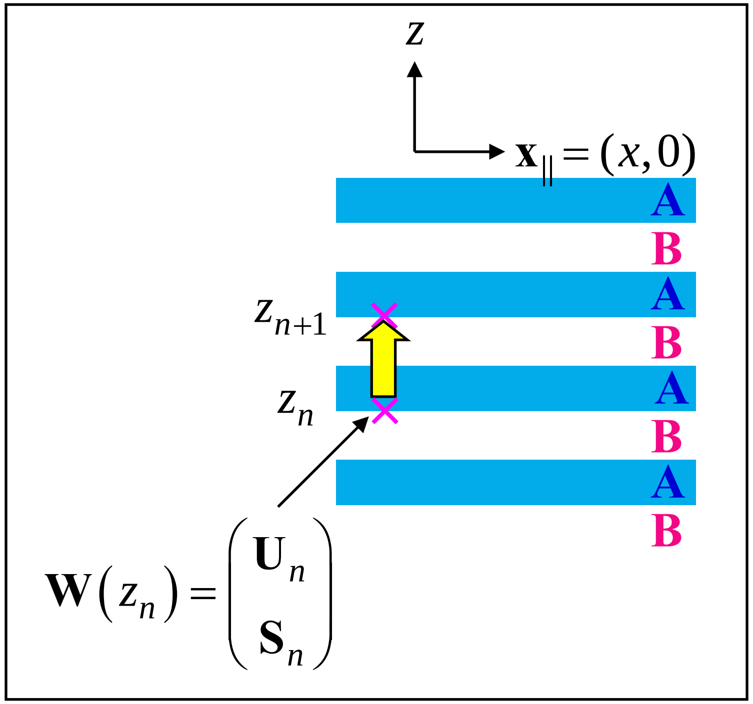
Transfer matrix T

$$\mathbf{W}(z_{n+1}) = T\,\mathbf{W}(z_n)$$

(1) Propagation normal to the layer interfaces *(z direction)* $\mathbf{k}_{\parallel} = \mathbf{0}$

(2) Single mode, *e.g.,*

$$\mathbf{u} = (0, 0, U(z,t)) \quad \textit{for L mode}$$



Matrix elements of *T*

2×2 *matrix*

$$Z = \rho \mathrm{v}$$

acoustic impedance

$$\det T = 1$$

$$T_{11} = \cos(k_A d_A)\cos(k_B d_B) - \frac{Z_A}{Z_B}\sin(k_A d_A)\sin(k_B d_B)$$

$$T_{12} = \sin(k_A d_A)\cos(k_B d_B) + \frac{Z_A}{Z_B}\cos(k_A d_A)\sin(k_B d_B)$$

$$T_{21} = -\sin(k_A d_A)\cos(k_B d_B) - \frac{Z_B}{Z_A}\cos(k_A d_A)\sin(k_B d_B)$$

$$T_{22} = T_{11}(A \leftrightarrow B)$$

$D = d_A + d_B$ *: unit period*

Perfect periodicity and phonon dispersion relation $\mathbf{k}_{\parallel} = \mathbf{0}$

Bloch theorem

$$\mathbf{W}_n = \exp(iqD)\mathbf{W}_{n-1} = T\ \mathbf{W}_{n-1}$$

q : *Bloch wave number*

Dispersion relation in periodic SLs

$$\cos(qD) = \underline{\mathrm{Tr}\,(T)/2}$$
$$= \cos\left(\frac{\omega d_A}{\mathrm{v}_A}\right)\cos\left(\frac{\omega d_B}{\mathrm{v}_B}\right) - \frac{1}{2}\left(\frac{Z_A}{Z_B}+\frac{Z_B}{Z_A}\right)\sin\left(\frac{\omega d_A}{\mathrm{v}_A}\right)\ \sin\left(\frac{\omega d_B}{\mathrm{v}_B}\right)$$

S. M. Rytov, Sov. Phys. Acoust. 2, 68 (1956)

⇨

$|\mathrm{Tr}\,(T)/2| < 1$: frequency band

$|\mathrm{Tr}\,(T)/2| > 1$: frequency gap

$-\frac{\pi}{D} < q < \frac{\pi}{D}$ *: mini-zone*

$q = 0,\ \pm\frac{\pi}{D}$ *: zone center and boundaries*

$|\mathrm{Tr}\,(T)/2| = 1 \Rightarrow \omega = \omega_m = m\pi\left(\frac{\mathrm{v}_A}{d_A}+\frac{\mathrm{v}_B}{d_B}\right)$ *: m^{-th} order Bragg freq.*

Perferct periodic SLs (normal propagation) $\mathbf{k}_{\|} = \mathbf{0}$

(001) $(GaAs)_{15}(AlAs)_{15}$ SL

$d_A = d_B =$
$2.83\ \text{A} \times 15 = 85\ \text{nm}$

Bragg reflections

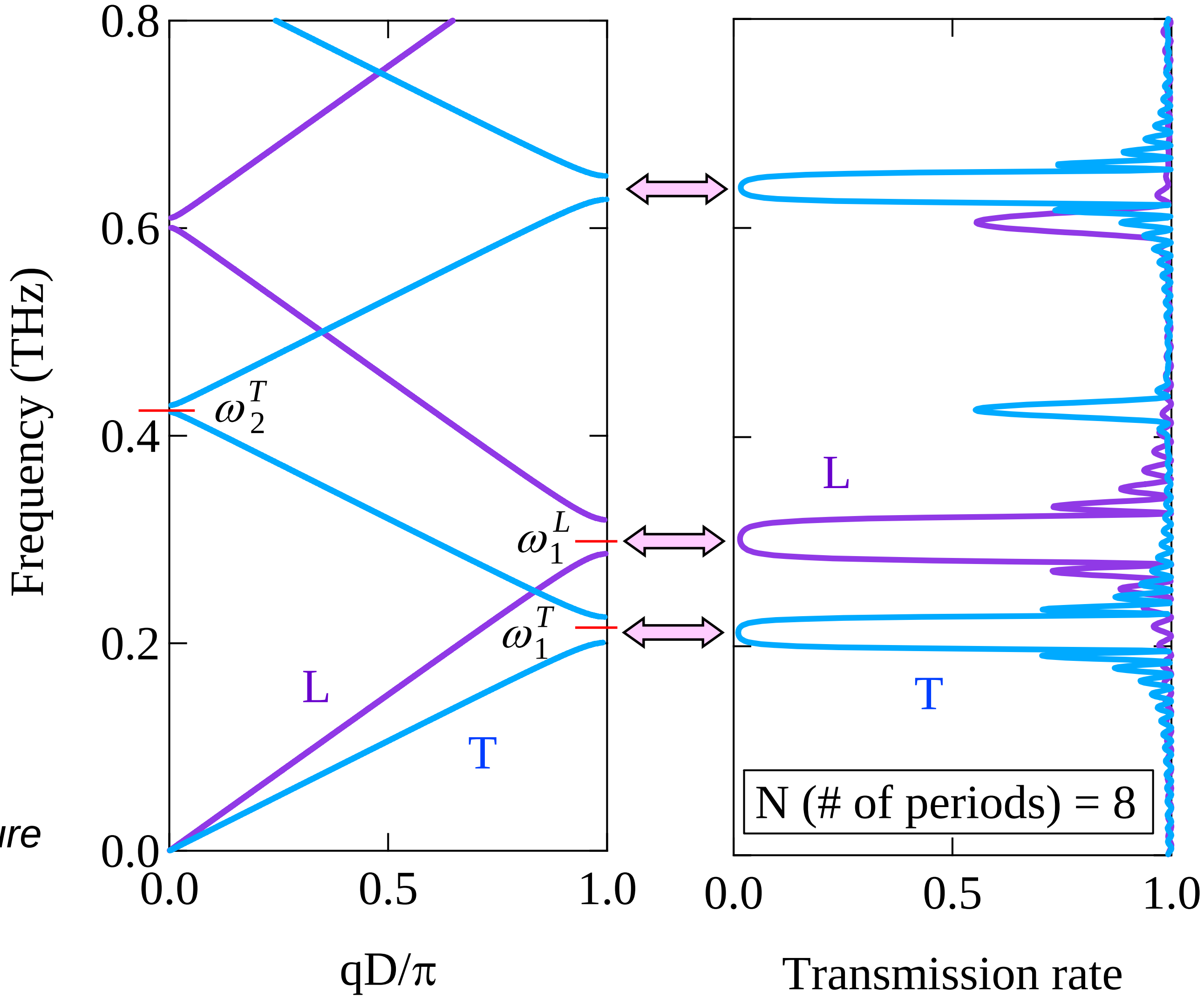
frequency gaps

transmission dips

for a finite periodic structure

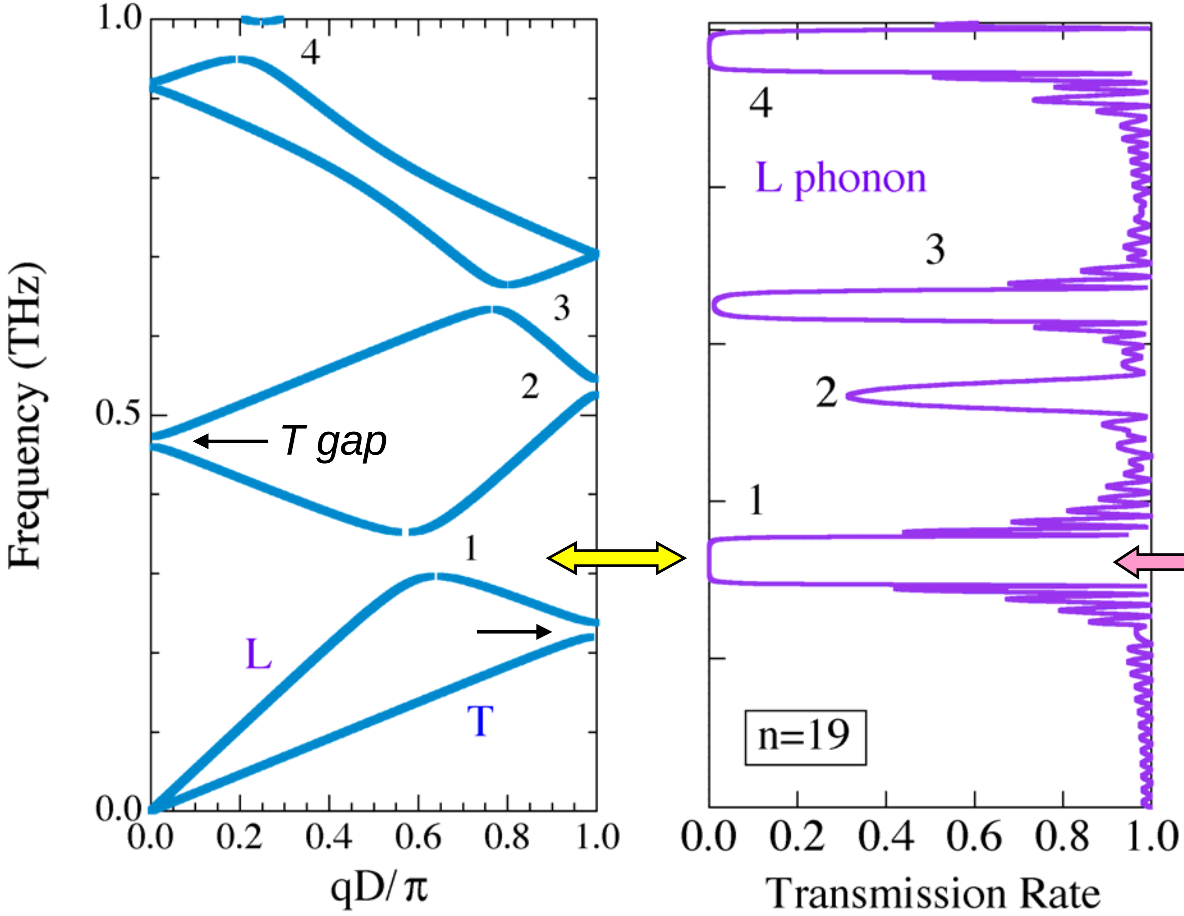
Dispersion relations

Transmission rates



Perferct periodic SLs (oblique propagation) $\mathbf{k}_{\parallel} \neq \mathbf{0}$

(001) $(GaAs)_{12}(AlAs)_{12}$ SL



L phonon incidence from a GaAs substrate

$\theta_L = 45^\circ$

$d_A = d_B = 40$ A

Intermode Bragg reflection

opening of frequency gaps

⇓

reduction of group velocity

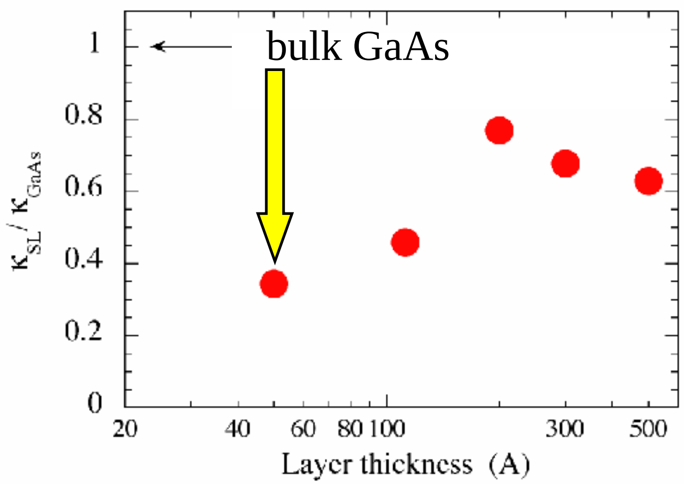
Thermal conductivity (κ) in semiconductor SLs

Measurements of thermal conductivity (κ) in semiconductor SLs

1. T. Yao, Appl. Phys. Lett. 51, 1798 (1987)

In plane κ in GaAs/AlAs SLs

Reduction of 20-70 % depending on bi-layer thickness



2. S. Lee, D. Cahill, and R. Venkatasubramanian, Appl. Phys. Lett. 51,1798 (1987)

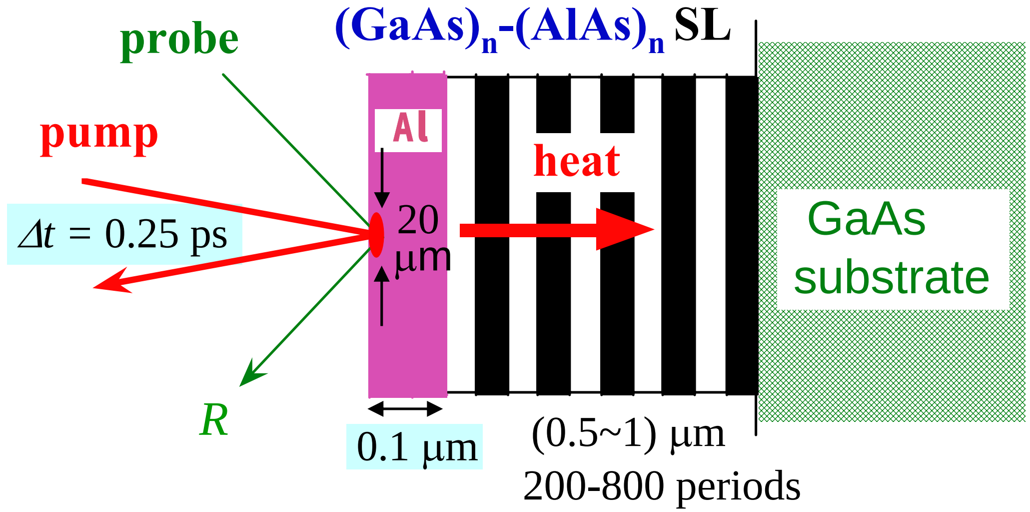
κ in Si/Ge SLs

3. W. S. Capinski, H. J. Maris *et al.*, Phys. Rev. B59, 8105 (1999)

Out of plane κ in GaAs/AlAs SLs

Out of plane thermal conductivity (κ) in semiconductor SLs

W. S. Capinski, H. J. Maris *et al.*, Phys. Rev. B59, 8105 (1999)

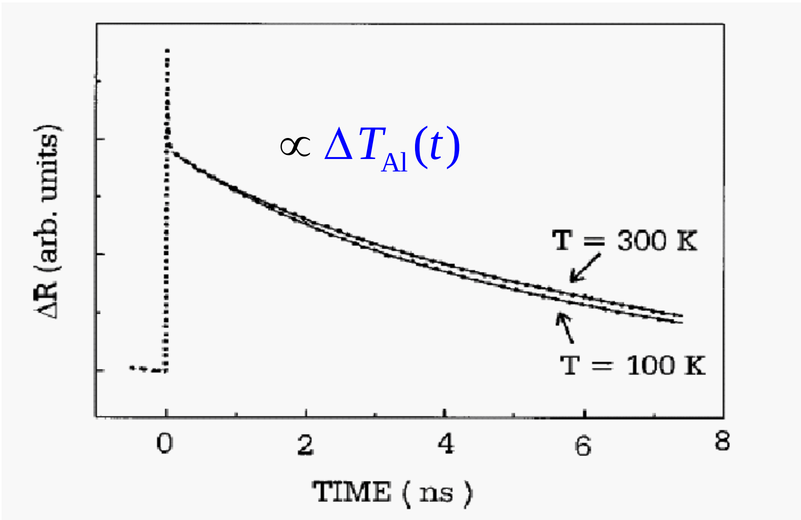


Picosecond Ultrasonics

a pump-probe optical technique

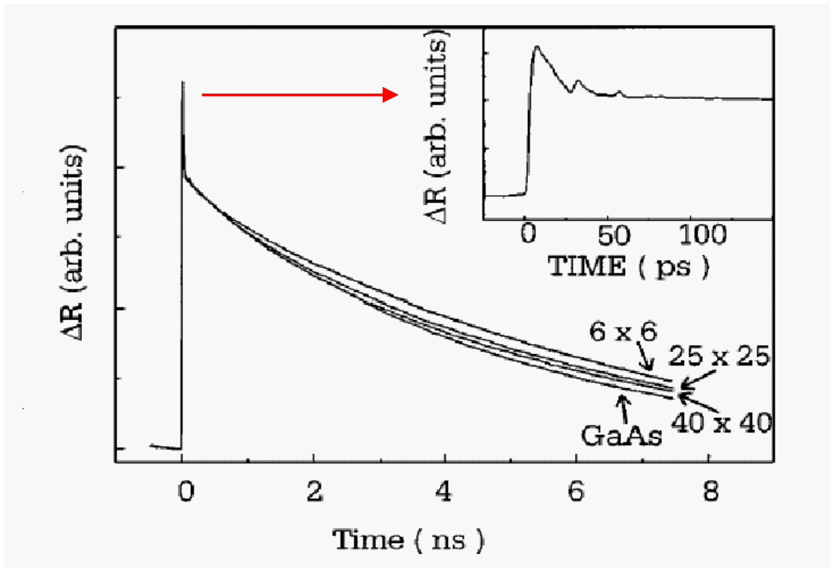
⇒ measure the change in optical reflectivity ΔR due to phonons

(A) T=100-375 K



(B) n : # of monolayers

(*repeat distance of SL*)



Thermalization time and increase in film temperature

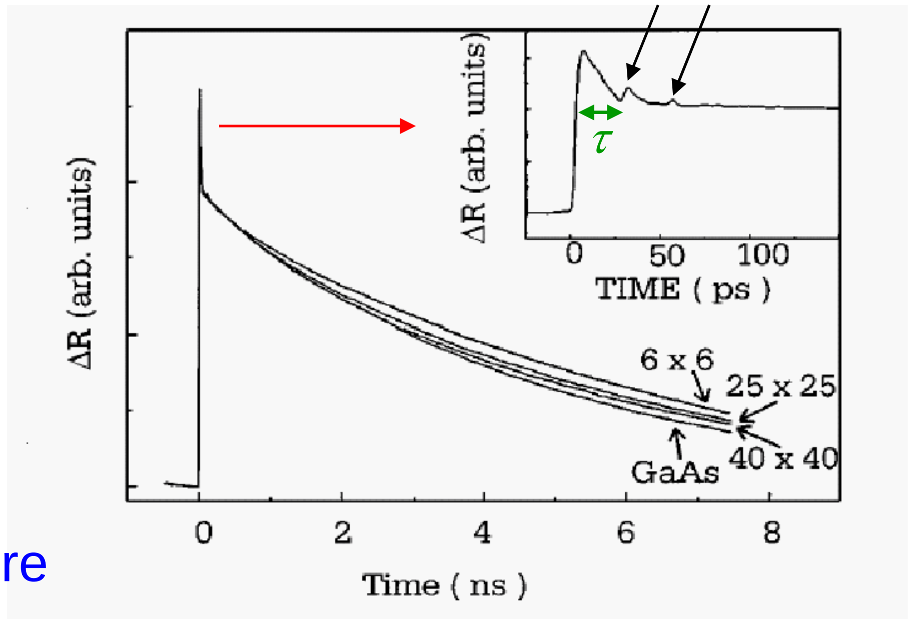
The time for *T* to become uniform inside the Al film

film thickness ~0.1 μm

$$\tau = \frac{d_{\mathrm{Al}}^{2}}{\pi^{2} D_{\mathrm{Al}}} = 23\ \mathrm{ps}$$

(300 K)

thermal diffusivity ~0.45 cm²/ s



The increase in the Al-film temperature

optical reflectivity ~0.9

energy of pump pulse 1.3 nJ

$$\Delta T_{\mathrm{Al}} = \frac{(1-R)Q}{C_{\mathrm{Al}}\, d_{\mathrm{Al}}\, A} \sim 2\ \mathrm{K} \quad \textit{at 300}\ \mathrm{K}$$

specific heat per volume

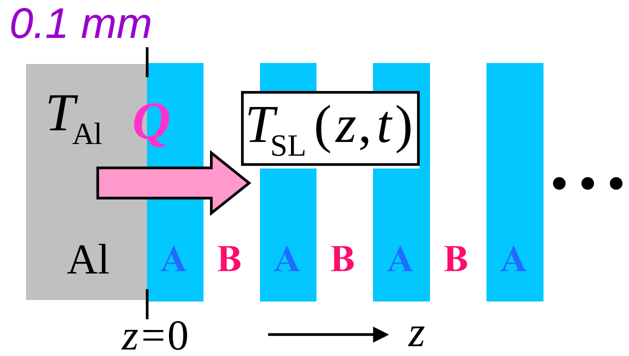
area of the spot

Determination of the thermal conductivity (κ)

The rate of heat flow across Al-SL interface

$$\dot{Q} = \sigma_K \, A\left[T_{\mathrm{Al}}(t) - T_{\mathrm{SL}}(z=0,t)\right]$$

Kapitza conductance



The rate of temperature change in the Al film

$$C_{\mathrm{Al}}\, d_{\mathrm{Al}} \frac{\partial T_{\mathrm{Al}}(t)}{\partial t} = -\sigma_K \, A\left[T_{\mathrm{Al}}(t) - T_{\mathrm{SL}}(z=0,t)\right] \quad \text{(A)}$$

Heat flow within the SL (~1D)

heat capacity in the SL
(average of GaAs and AlAs)

$$C_{\mathrm{SL}} \frac{\partial T_{\mathrm{SL}}(z,t)}{\partial t} = \kappa \frac{\partial^2 T_{\mathrm{SL}}(z,t)}{\partial z^2} \quad \text{(B)}$$

(1) *Assume* σ_K *and* κ

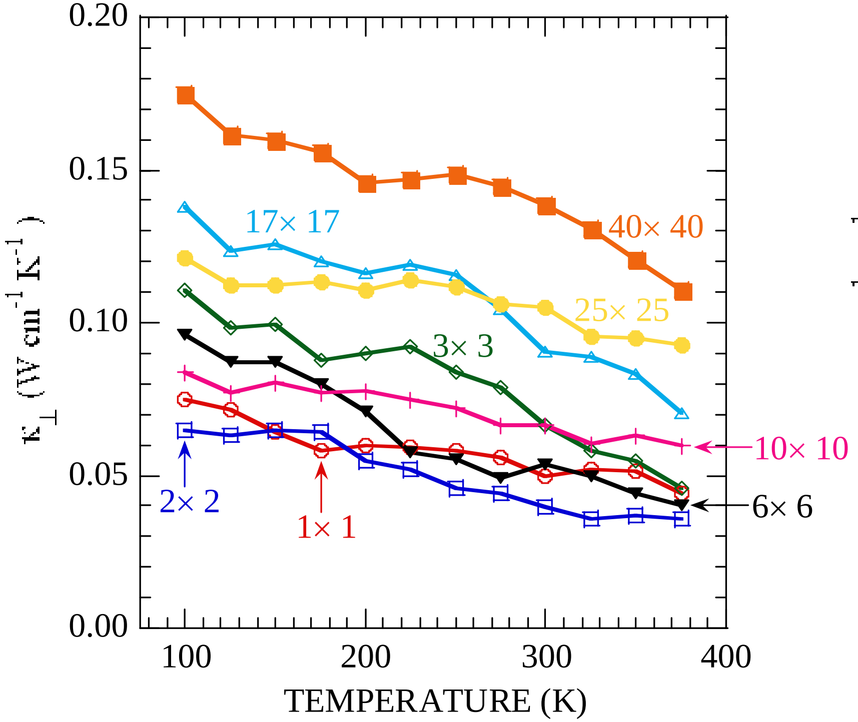
(adjustable parameters)

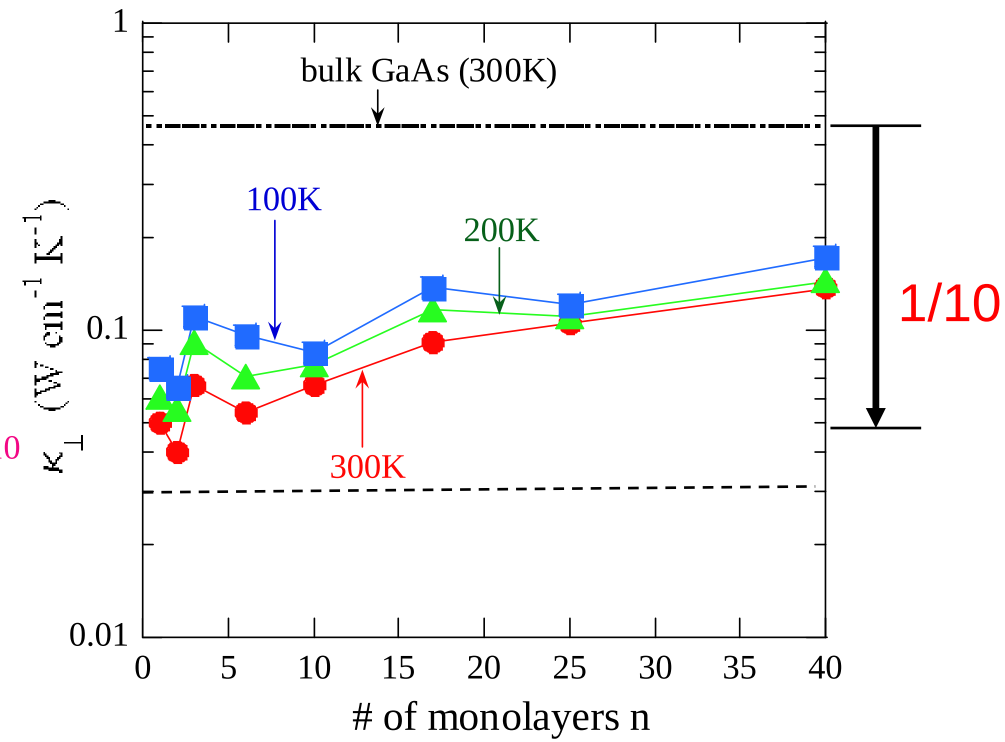
(2) *With (A) and (B), determine* $\Delta T_{\mathrm{Al}}(t)$

$$\Delta T_{\mathrm{Al}}(t) = \beta \, \Delta R(t)$$

thermoreflectance

Experimental out-of-plane thermal conductivity (κ) in SLs





(1) κ decreases as *T* increases

(2) κ decreases as the number of monolayer *n* decreases

(3) κ is much smaller than κ_{GaAs} (*~1/10 for 1x1-SL*)

How we understand these experimental results

Lattice thermal conductivity (κ)

Fourier's law

$$\mathbf{J} = -\kappa \nabla T$$

Expression for thermal conductivity

lattice specific heat

relaxation time

group velocity in the direction of ∇T

$$\kappa = \sum_{\lambda} \kappa_{\lambda} \;, \quad \kappa_{\lambda} = \underline{C_{\mathrm{ph}}(\omega_{\lambda})}\, \underline{\tau_{\lambda}}\, \underline{\mathrm{v}_{\lambda,z}^{2}}$$

$$\lambda = (\mathbf{k},\ j)$$

wave vector

phonon mode

$$C_{\mathrm{ph}}(\omega) = \frac{(\hbar\omega)^2}{kT^2} \frac{\exp(\hbar\omega / kT)}{\left[\exp(\hbar\omega / kT) - 1\right]^2}$$

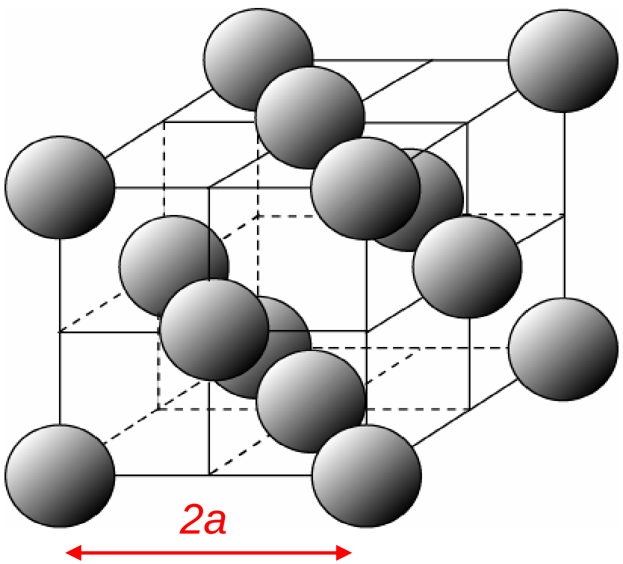
Effect of Brillouin-zone-folding in SLs

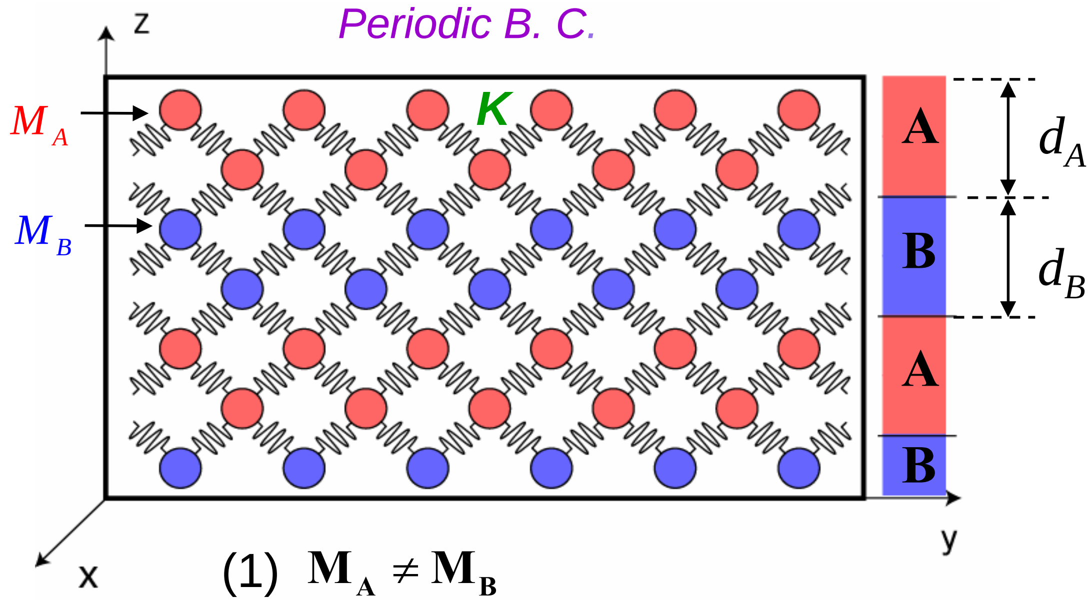
Opening of frequency gaps and the associated group-velocity reduction near the zone center and boundaries

(1) P. Hyldgaard and G. D. Mahan, Phys. Rev. B56, 10754 (1997) *simple cubic lattice*

(2) S. Tamura, Y. Tanaka, and H. J. Maris, Phys. Rev. B60, 2627 (1999) *FCC lattice*

3D FCC lattice model (harmonic approximation)





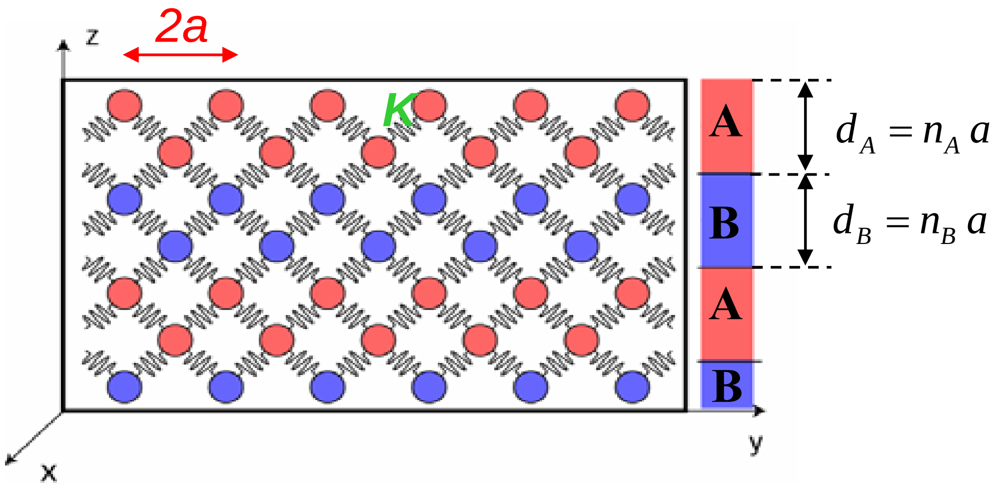
(1) $\mathbf{M_A} \neq \mathbf{M_B}$

(2) Force constant *K* is the same for the atomic pairs *A-A, A-B, B-B*

Equations of motion for the lattice displacement

A = GaAs or Si

B = AlAs or Ge



$$M_n \ddot{u}^x_{lmn} = \frac{K}{2}(u^x_{l+1,m+1,n} + u^x_{l+1,m,n+1} + u^x_{l+1,m-1,n} + u^x_{l+1,m+1,n-1}$$
$$+ u^x_{l-1,m+1,n} + u^x_{l-1,m,n+1} + u^x_{l-1,m-1,n} + u^x_{l-1,m,n-1} - 8u^x_{l,m,n}$$
$$+ u^y_{l+1,m+1,n} - u^y_{l+1,m-1,n} + u^y_{l-1,m-1,n} - u^y_{l-1,m+1,n}$$
$$+ u^z_{l+1,m,n+1} - u^z_{l+1,m,n-1} + u^z_{l-1,m,n-1} - u^z_{l-1,m,n+1})$$

$D = d_A + d_B$

$$\mathbf{r}_{lmn} = (\mathbf{x}_{lm}, z_n) = (l, m, n)a$$

⇒

$$\mathbf{u}^{(N)}_{lmn} = \underline{\mathbf{u}_n(z)} \exp[i(\mathbf{k}_\parallel \cdot \mathbf{x}_{lm} + qND - \omega t)]$$

Bloch function

$$\mathbf{u}_{n+n_A+n_B}(z) = \mathbf{u}_n(z) \quad (1 \le n \le n_A + n_B)$$

Periodic function

Determination of dispersion relations

1x1 SL $(n_A = n_B = 1)$

$$\det\begin{pmatrix} M_A\omega^2 + CC & SS & 0 & C_x(1+e^{-iqD}) & 0 & S_x(1-e^{-iqD}) \\ SS & M_A\omega^2 + CC & 0 & 0 & C_y(1+e^{-iqD}) & S_y(1-e^{-iqD}) \\ 0 & 0 & M_A\omega^2 - 4K & S_x(1-e^{-iqD}) & S_y(1-e^{-iqD}) & C_+(1+e^{-iqD}) \\ C_x(e^{iqD}+1) & 0 & S_x(e^{iqD}-1) & M_B\omega^2 + CC & SS & 0 \\ 0 & C_y(e^{iqD}+1) & S_y(e^{iqD}-1) & SS & M_B\omega^2 + CC & 0 \\ S_x(e^{iqD}-1) & S_y(e^{iqD}-1) & C_+(e^{iqD}+1) & 0 & 0 & M_B\omega^2 - 4K \end{pmatrix} = 0$$

$$\omega = \omega(\mathbf{k}_{\parallel}, q)$$

$C_x = K\cos k_x a, \; S_x = iK\sin k_x a$

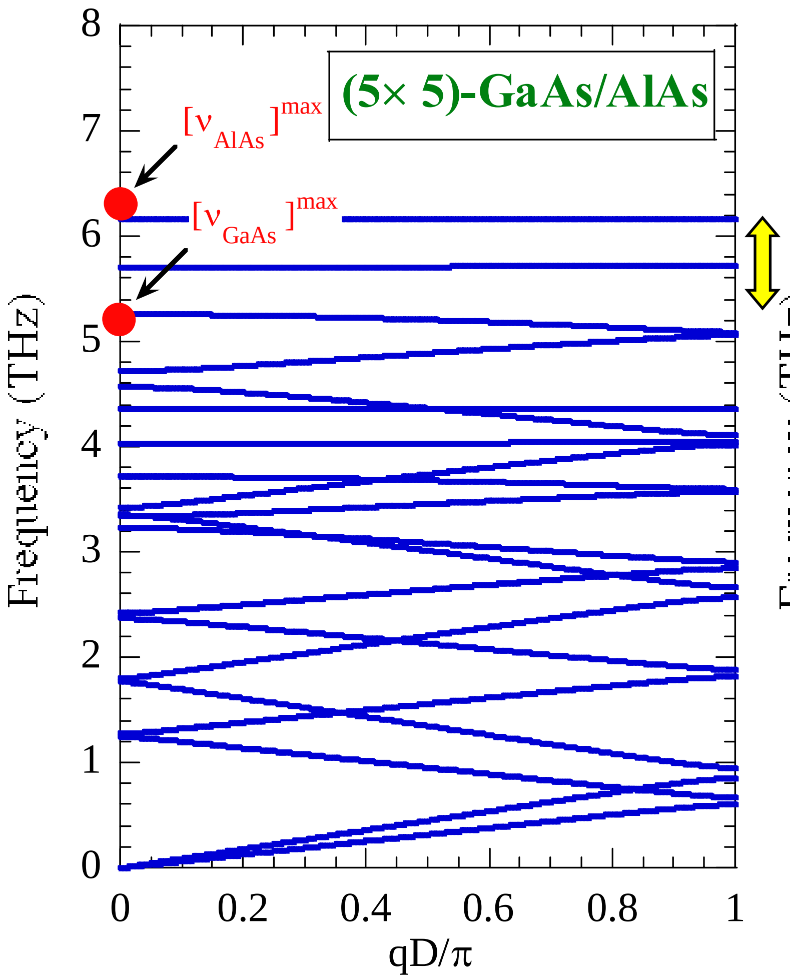
$(C_y, S_y) = (k_x \to k_y)$

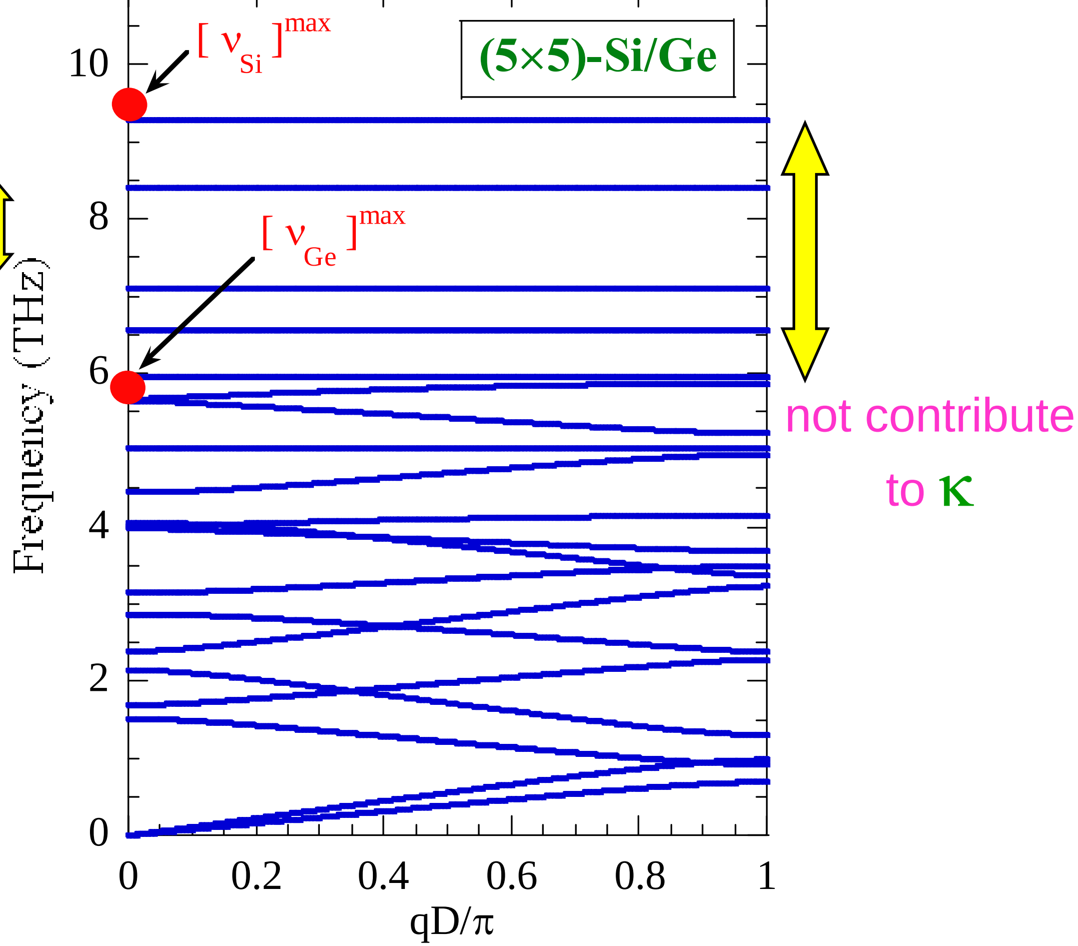
$C_+ = K(\cos k_x a + \cos k_y a)$

$CC = 2K(2 - \cos k_x a \cos k_y a)$

$SS = -2K\sin k_x a \sin k_y a$

Dispersion relations for $k_{||}=0$





Effect of group velocity and weighted density of states

To see the effect of *group velocity*, we have calculated

$$\tilde{\kappa} = \sum_{\lambda} \kappa_{\lambda} / \tau_{\lambda} \equiv \sum_{\lambda} C_{\mathrm{ph}}(\omega_{\lambda})\, \mathrm{v}_{\lambda,z}^{2}$$

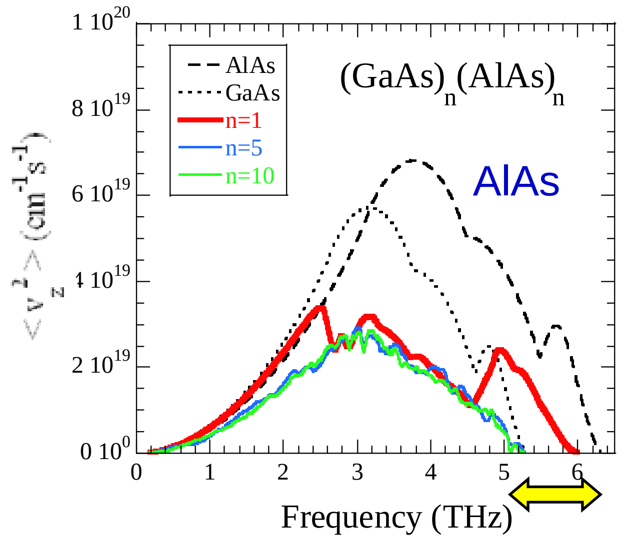
Phonon density of states weighted by $\mathrm{v}_{\lambda,z}^{2}$

$$< \mathrm{v}_z^2(\omega) > = \frac{1}{V} \sum_{\lambda} \delta(\omega - \omega_{\lambda})\, \mathrm{v}_{\lambda,z}^{2}$$

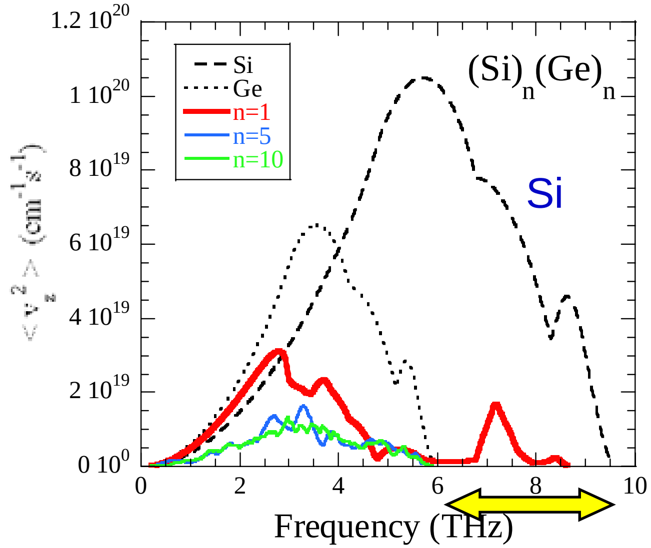
$$= \frac{1}{(2\pi)^3} \sum_{j} \int \frac{dS_{\lambda}}{\mathrm{v}_{\lambda}}\, \mathrm{v}_{\lambda,z}^{2} \Big|_{\omega_{\lambda}=\omega}$$

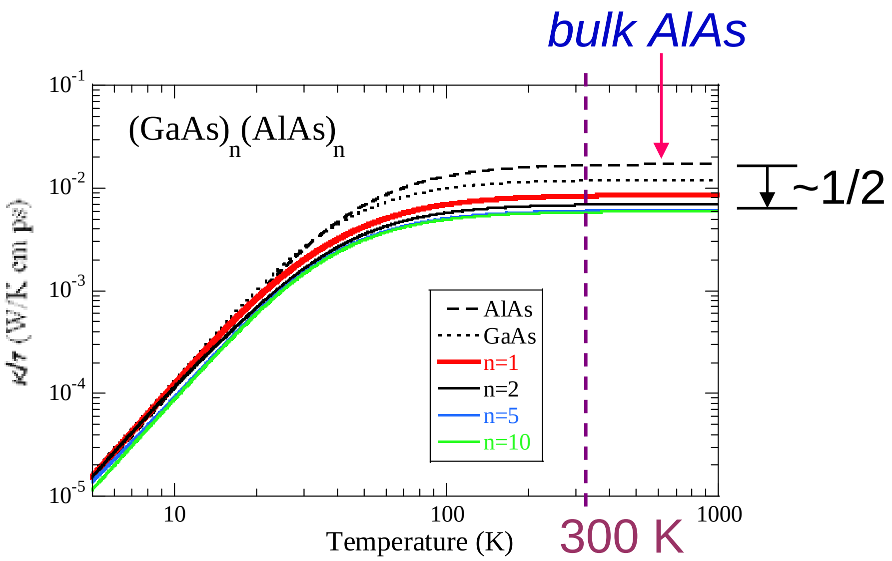
DOS weighted by $(v_z)^2$ and calculated $\tilde{\kappa} \sim \kappa / \tau$

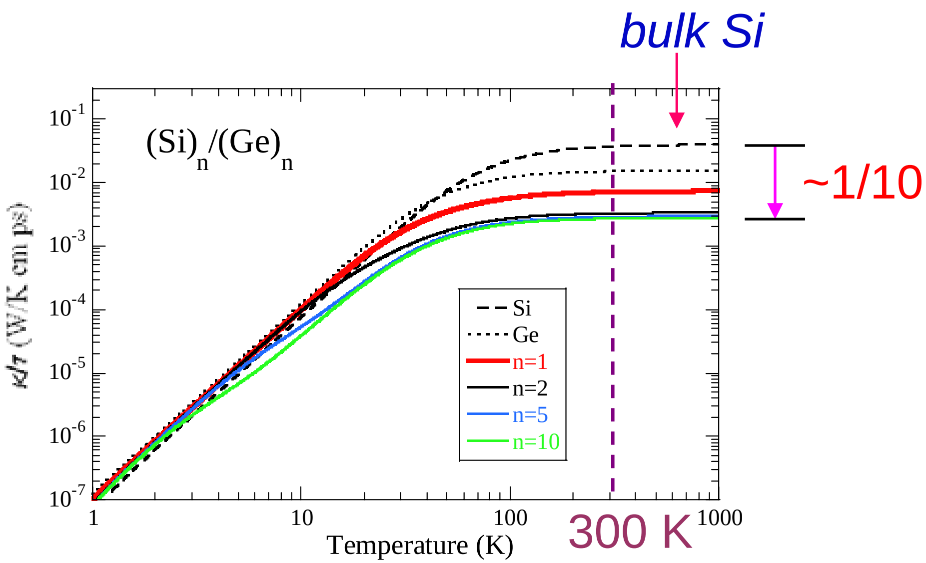
GaAs/AlAs



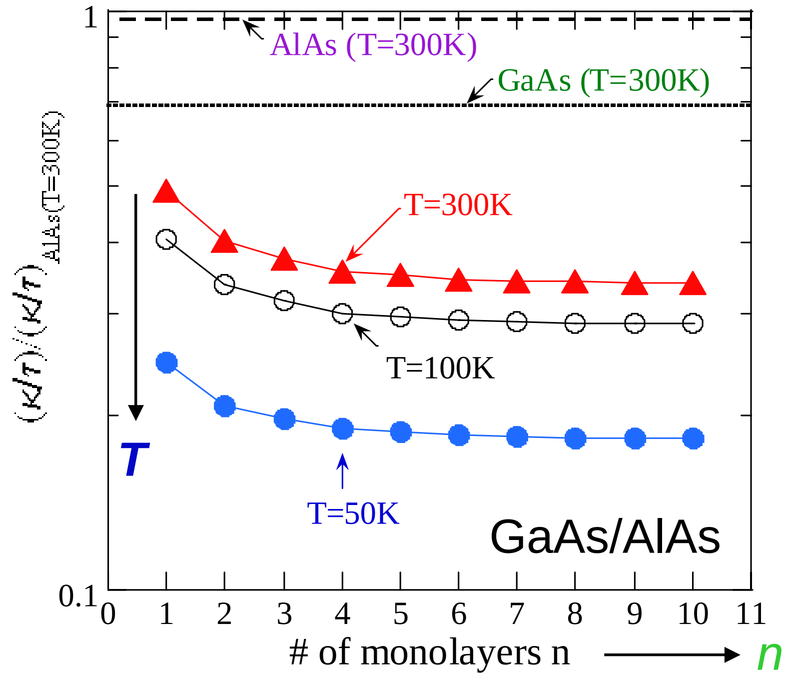
Si/Ge

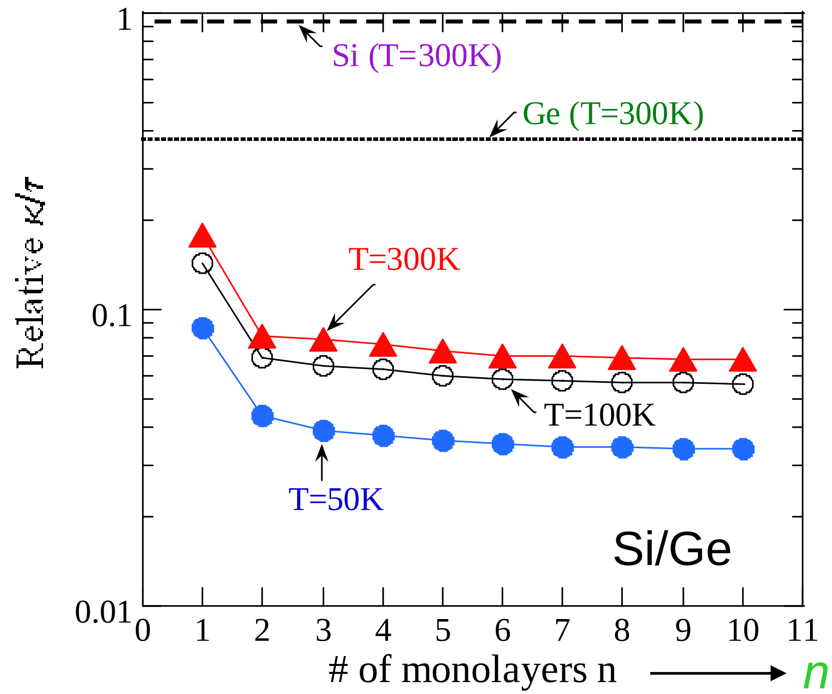


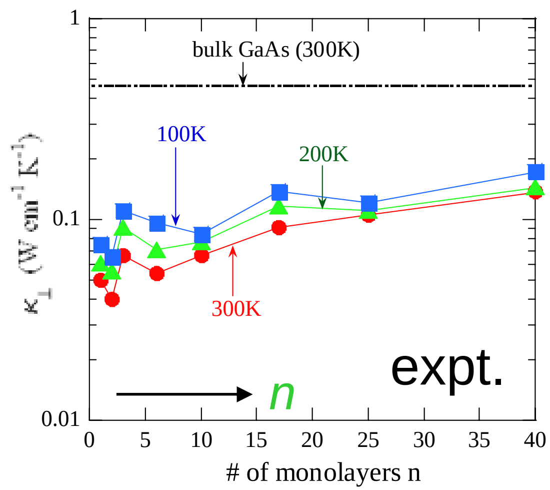




$\tilde{\kappa} \sim \kappa / \tau$ vs number of monolayers







Calculated $\tilde{\kappa} \sim \kappa / \tau$ exhibits *T* and *n* dependences *opposite to the experimental results*

Effect of τ is important !!

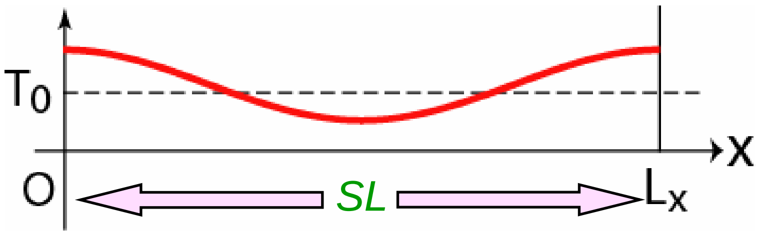
How to include the effect of relaxation time

Molecular dynamics (MD) calculations

(A) B. Daly *et al.*, Phys. Rev. B66, 24301 (2002)

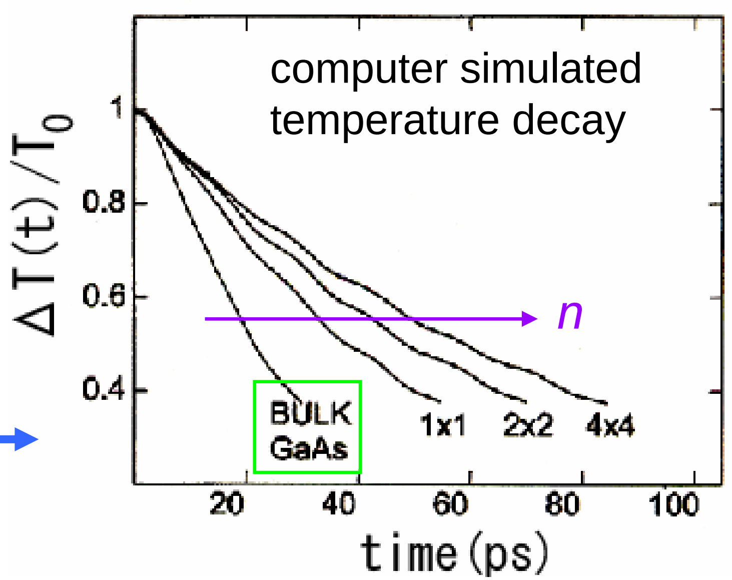
(1) Assume an initial temperature distribution of the system $T(x,t = 0)$, e. g.,

$$T(x,t=0)=T_0+\Delta T_0 \cos(2\pi x/L_x) \quad (\Delta T_0 \simeq 0.1\,T_0)$$



(2) MD is used to determine the rate at which ΔT (t) is changed by heat diffusion

$$\Delta T(t) = \frac{2}{L_x}\int_0^{L_x} T(x,t)\cos(2\pi x/L_x)\,dx$$



(3) thermal diffusion constant D is deduced from

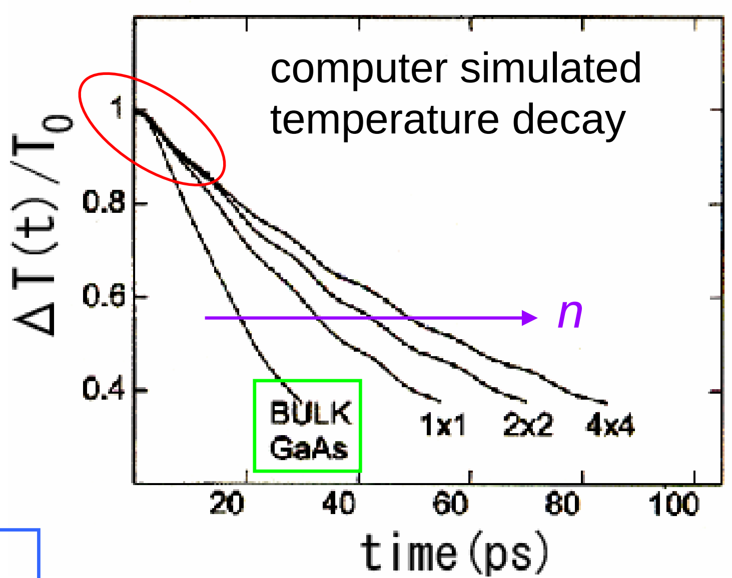
$$\Delta T(t) = \Delta T_0 \exp(-4\pi^2 D t / L_x^2)$$

(4) thermal conductivity is given by $\kappa = D\,C_{ph}$

A note on the MD calculation of Daly et al

(3) thermal diffusion constant *D* is deduced from

$$\Delta T(t) = \Delta T_0 \exp(-4\pi^2 Dt / L_x^2)$$



[*no good fit to the simulated* ΔT (t) *for a small t*]

$$v \sim (4D/t)^{1/2} \to \infty \quad (t \sim 0)$$

An *ad hoc* modification for the solution for ΔT (t)

$$x^2 \sim 4Dt \Rightarrow \frac{4Dt\, v^2 t^2}{4Dt + v^2 t^2} \Rightarrow \begin{cases} v^2 t^2 & (t \to 0) \\ 4Dt & (t \to \infty) \end{cases}$$

$$\Delta T(t) = \Delta T_0 \exp\left[-\frac{\pi^2}{L_x^2} \left(\frac{4Dt\, v^2 t^2}{4Dt + v^2 t^2} \right) \right]$$

the MD results for $\Delta T(t)/\Delta T_0$ are fit to this form using *D* and *v* as adjustable parameters

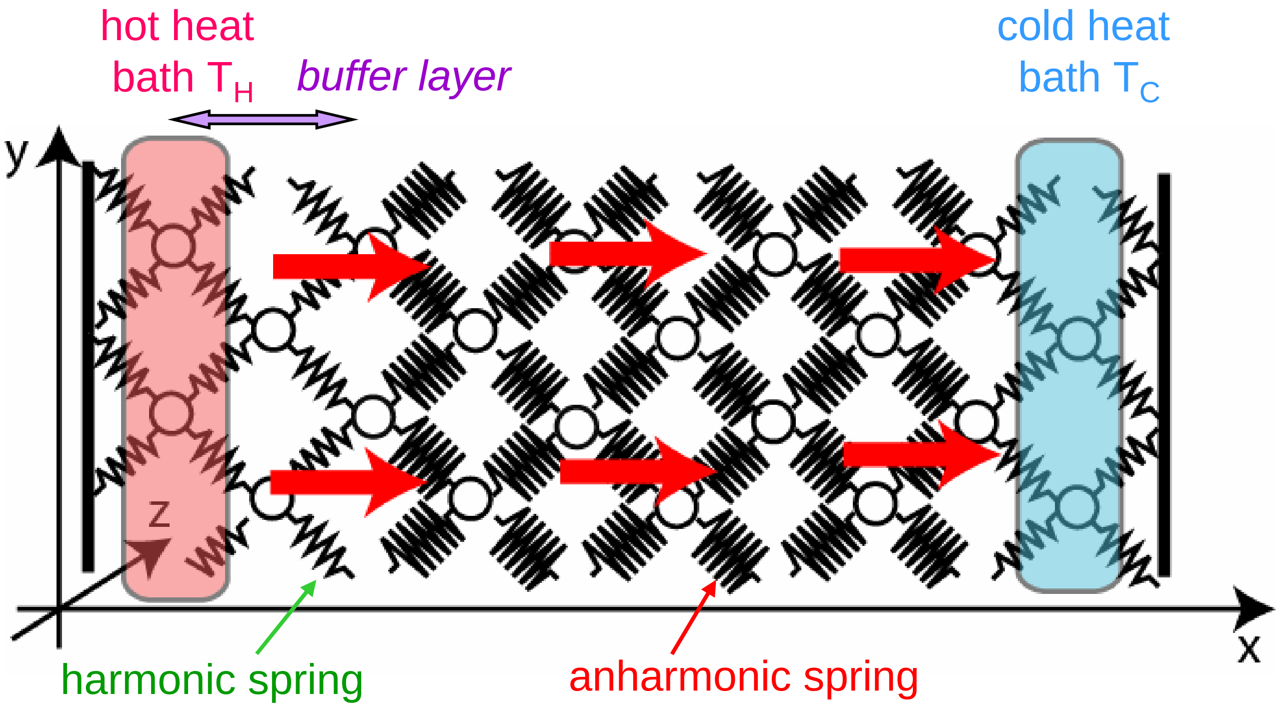
How to include the effect of relaxation time-2

Molecular dynamics (MD) calculations

(B) K. Imamura *et al.*, J. Phys. Condensed Matter 15, 8679 (2003)

A heat-reservoir method

(1) Heat current $\mathbf{J}$
(2) Temperature profile $T(x)$
→ *Fourier's law* $\mathbf{J} = -\kappa \nabla T$ → κ



Hamiltonian and interatomic potential

Hamiltonian

$$H = \sum_{\ell} \frac{\mathbf{p}_\ell^2}{2m_\ell} + \frac{1}{2}\sum_{\ell \neq \ell'} \Phi_{\ell\ell'} + \begin{pmatrix} \textit{interaction with} \\ \textit{heat reservoirs} \end{pmatrix}$$

$$\ell \equiv \mathbf{r}_{lmn} = (l,\ m,\ n)a$$

$$(m_\ell = m_{\mathrm{GaAs}} \quad or \quad m_{\mathrm{AlAs}})$$

Interatomic potential

3rd order anharmonicity → $\frac{\beta'}{6}u_{\ell\ell'}^{3}$

$$\Phi_{\ell\ell'} = \Phi(u_{\ell\ell'}) = \frac{\beta}{2}u_{\ell\ell'}^{2} + \frac{\beta'}{6}u_{\ell\ell'}^{3}$$

$u_{\ell\ell'} = |\mathbf{u}_\ell - \mathbf{u}_{\ell'}|$ *relative displacement*

$$\beta = \frac{3\tilde{B}a}{2}, \qquad \tilde{B} = \frac{C_{11} + 2C_{12}}{3} \quad \text{Bulk modulus}$$

$$\beta' = -\frac{9\tilde{B}\gamma}{\sqrt{2}} \quad \text{Gruneisen parameter } (\gamma = 2)$$

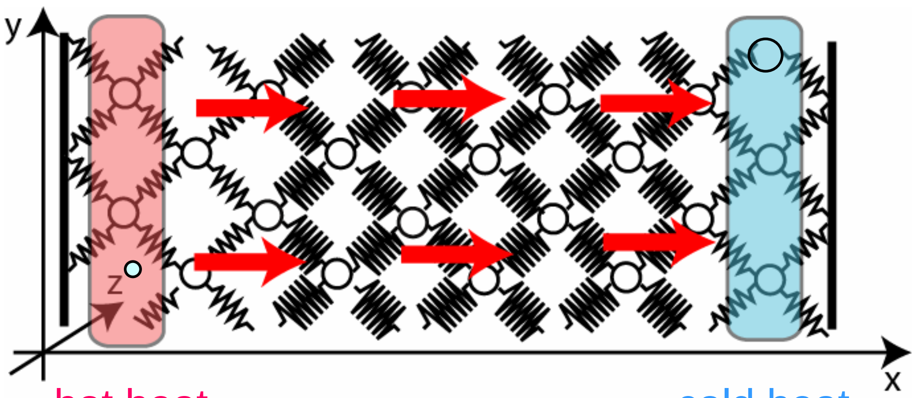
Algorithm: Symplectic Integrator (SI) method

Heat reservoirs and energy exchange with atoms

Heat reservoirs

(1) consist of particles with energy (E_H and E_L) given by Boltzmann distribution at T_H and T_L

(2) A particle collides elastically with an atom at the end of the SL with a given probability *w* (~*0.1*) at each time step



(3) Energy given to (removed from) the atom at the site $(n_x = 1, n_y, n_z)$

$[\,(n_x = N_x, n_y, n_z)\,]$

$$Q^{(s)}_{\mathbf{H},(n_y,n_z)} = E_H - \frac{\left[\mathbf{p}^{(s)}_{(\mathbf{1},n_y,n_z)}\right]^2}{2m}, \quad Q^{(s)}_{\mathbf{L},(n_y,n_z)} = \frac{\left[\mathbf{p}^{(s)}_{(\mathbf{N_x},n_y,n_z)}\right]^2}{2m} - E_L \quad \text{(with collision)}$$

$$Q^{(s)}_{\mathbf{H},(n_y,n_z)} = Q^{(s)}_{\mathbf{L},(n_y,n_z)} = 0 \quad \text{(without collision)}$$

Heat current and steady state

The *heat* flowing into (from) the SL at a time *t*

(averaging over time steps *s'* to reduce fluctuations)

$$\left\langle Q_{\mathbf{H}}(t)\right\rangle = \frac{1}{s'\Delta t}\sum_{s=1}^{s'}\sum_{n_y,n_z} Q^{(s)}_{\mathbf{H},(n_y,n_z)} \qquad \left\langle Q_{\mathbf{L}}(t)\right\rangle = \frac{1}{s'\Delta t}\sum_{s=1}^{s'}\sum_{n_y,n_z} Q^{(s)}_{\mathbf{L},(n_y,n_z)}$$

$\Delta t = 4\ ps$: an interval of time step
(from energy conservation)

Steady state for *t* > τ_0

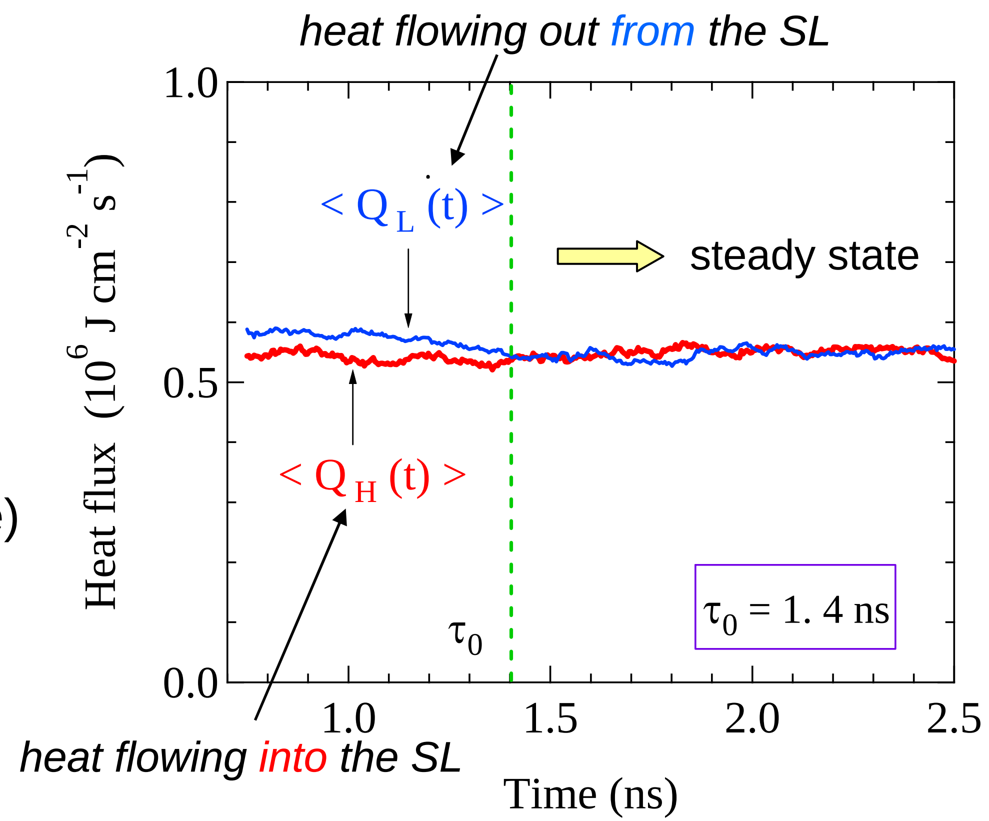
$$\left\langle Q_{\mathbf{H}}(t)\right\rangle = \left\langle Q_{\mathbf{L}}(t)\right\rangle$$

$$\left\langle Q_{\mathbf{H}}(t)\right\rangle : t-\text{indep.}$$

Heat flux (defined in the steady state)

$$J = \frac{1}{A(\tau_1-\tau_0)}\int_{\tau_0}^{\tau_1}\left\langle Q_{\mathbf{H}}(t)\right\rangle dt$$

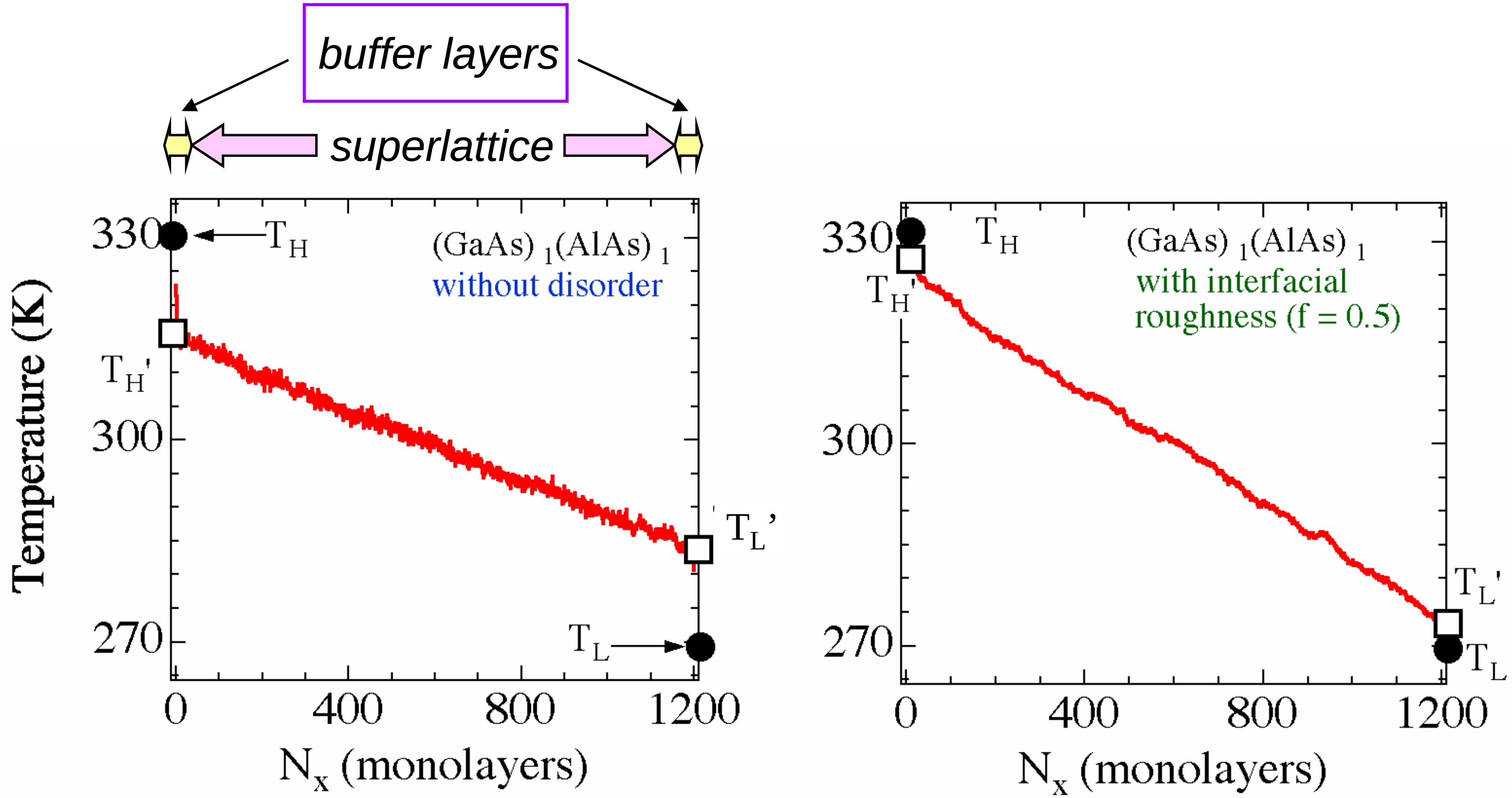
cross-sectional area of SL



Temperature profiles

$$T(x = n_x a) \equiv \frac{4}{3\,k_B\ N_y N_z} \sum_{n_y,\,n_z} \frac{\left\langle \mathbf{p}^{\,2}_{(n_x,\,n_y,\,n_z)} \right\rangle_t}{2m_{n_x}}$$

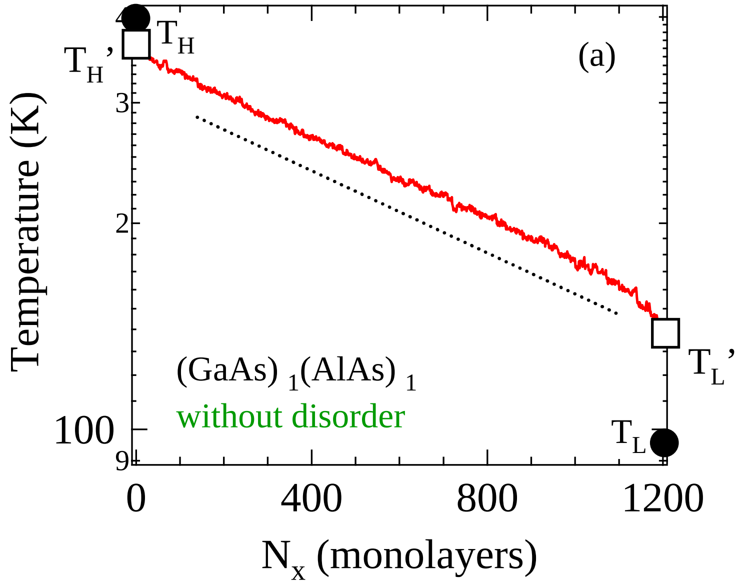
total # of lattice points in the lateral plane $=N_yN_z\,/\,2$



a good conductor

a poor conductor

A note on the temperature profiles



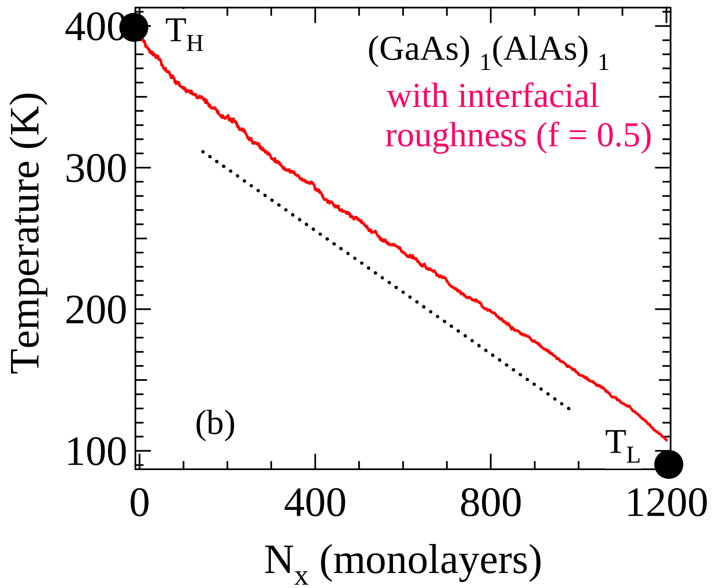
(1) No disorder is present

⇨ *T* decreases exponentially with distance

$$T(x) = T_H' \left(\frac{T_L'}{T_H'} \right)^{x/L_x} \Rightarrow \boxed{\kappa \propto \frac{1}{T}}$$

1/T-law

anharmonicity resists the heat flow



(2) Disorder is present

⇨ *T* decreases linearly with distance

$$T(x) = T_H + \frac{T_L - T_H}{L_X} x \Rightarrow \boxed{\kappa \propto T^0}$$

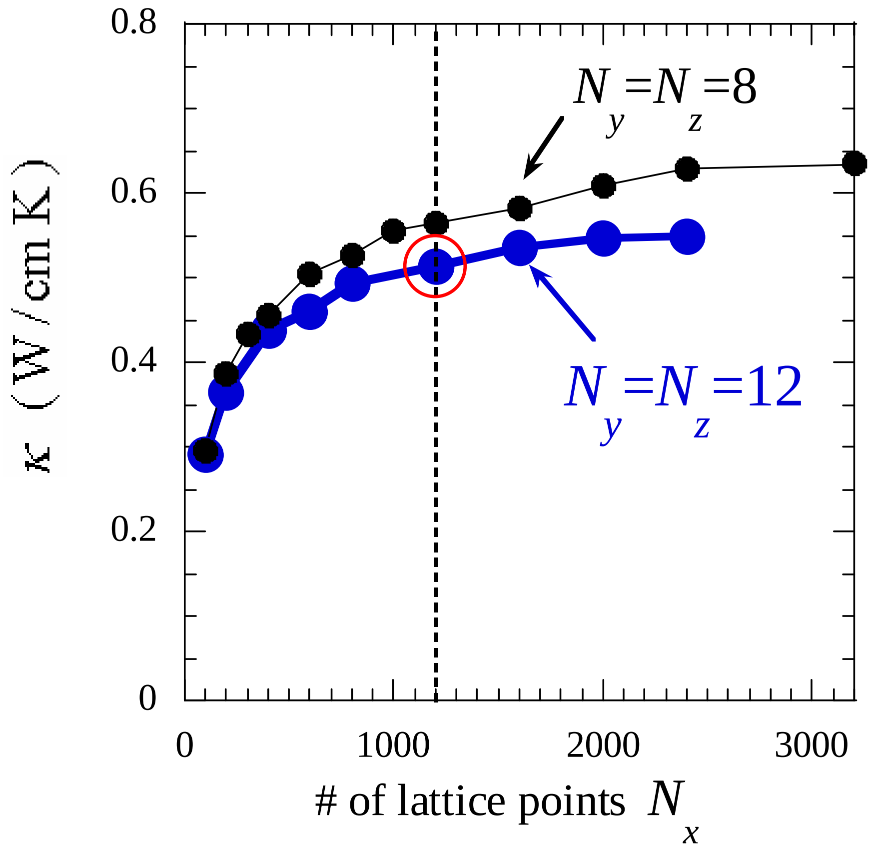
scattering from disorder is *T*-indep.

Size independence and thermal conductivity

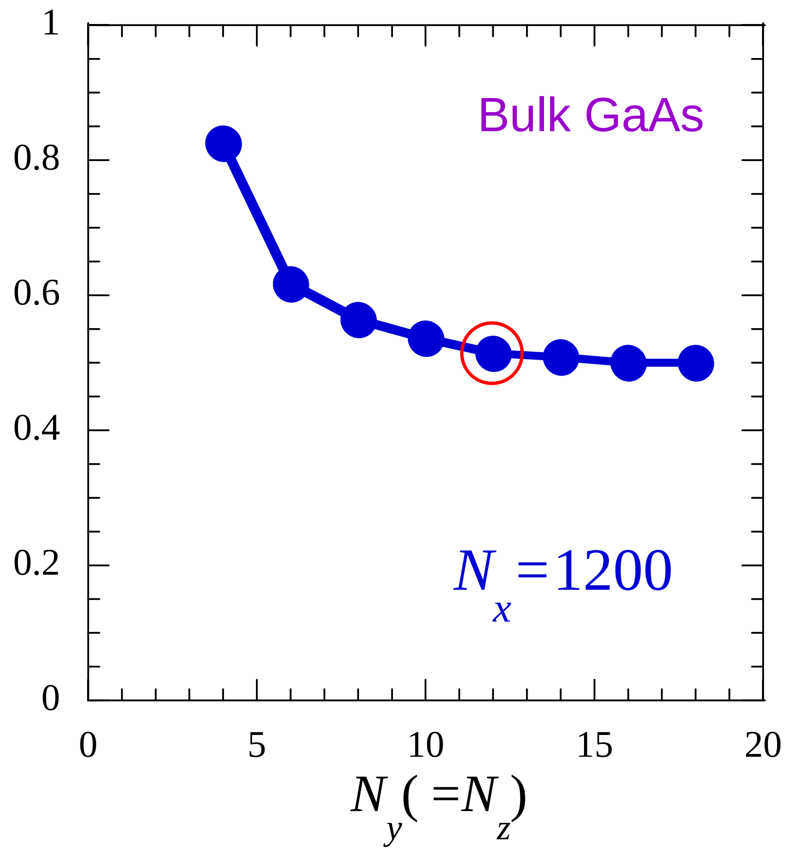
For a small system size some phonons travel ballistically between the reservoirs ⇨ Fourier's law is inapplicable

(κ depends on the system size)

Longitudinal direction

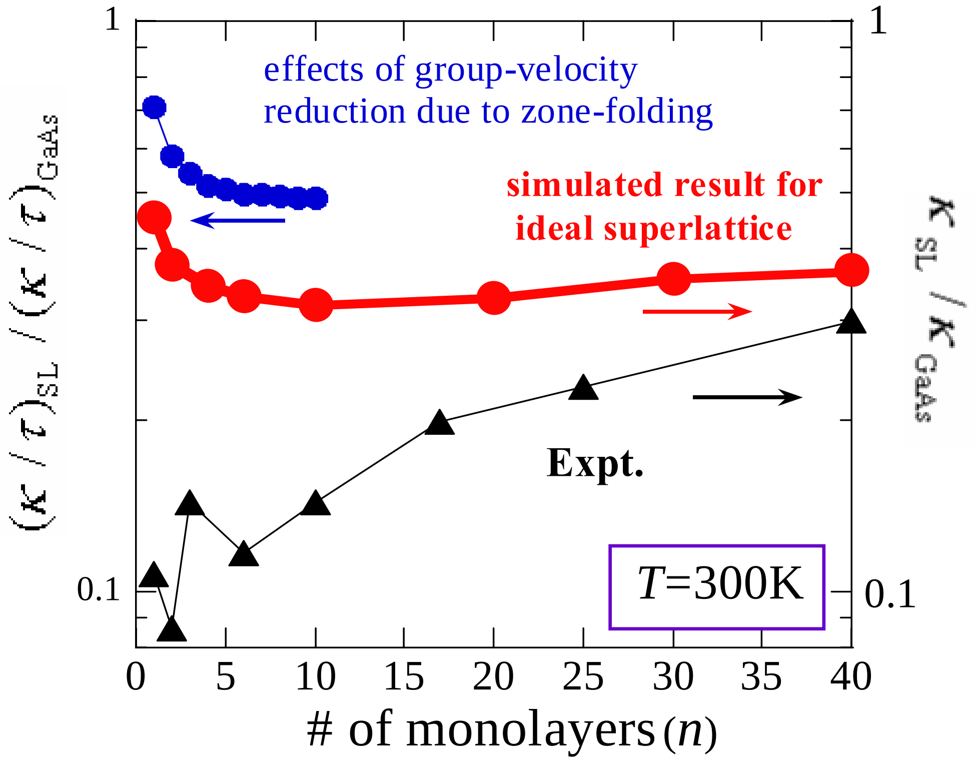


Lateral direction



Thermal conductivity in ideal SLs

The simulated κ includes the effect of *lattice anhamonicity*



(1) For *large* # of monolayers, κ approaches to the experimental values

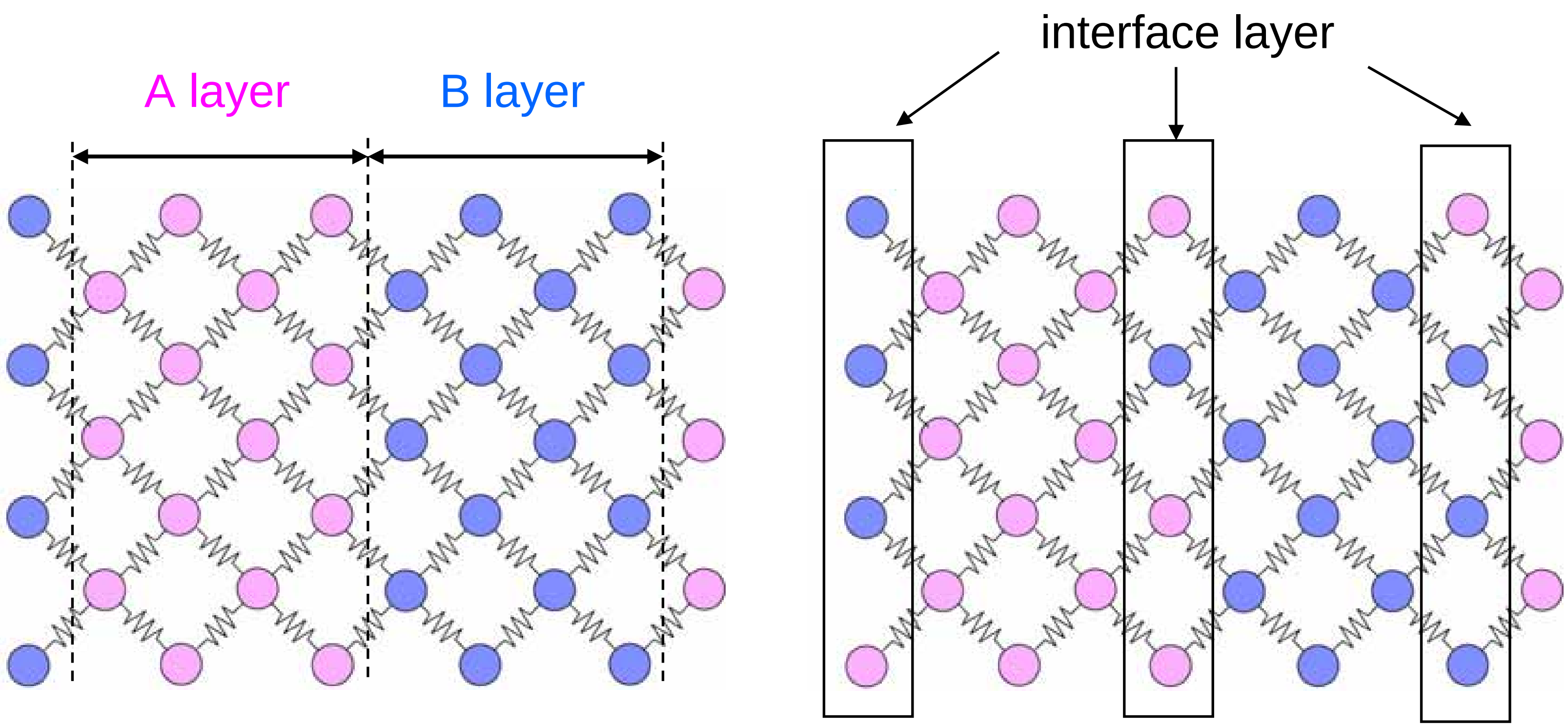
(2) For *small* # of monolayers, κ does not explain the expeimental results

⇨ ***Anharmonicity*** *is not the main origin of the reduction of κ for small n*

Thermal conductivity in SLs with interface roughness-1

How to include the interface roughness

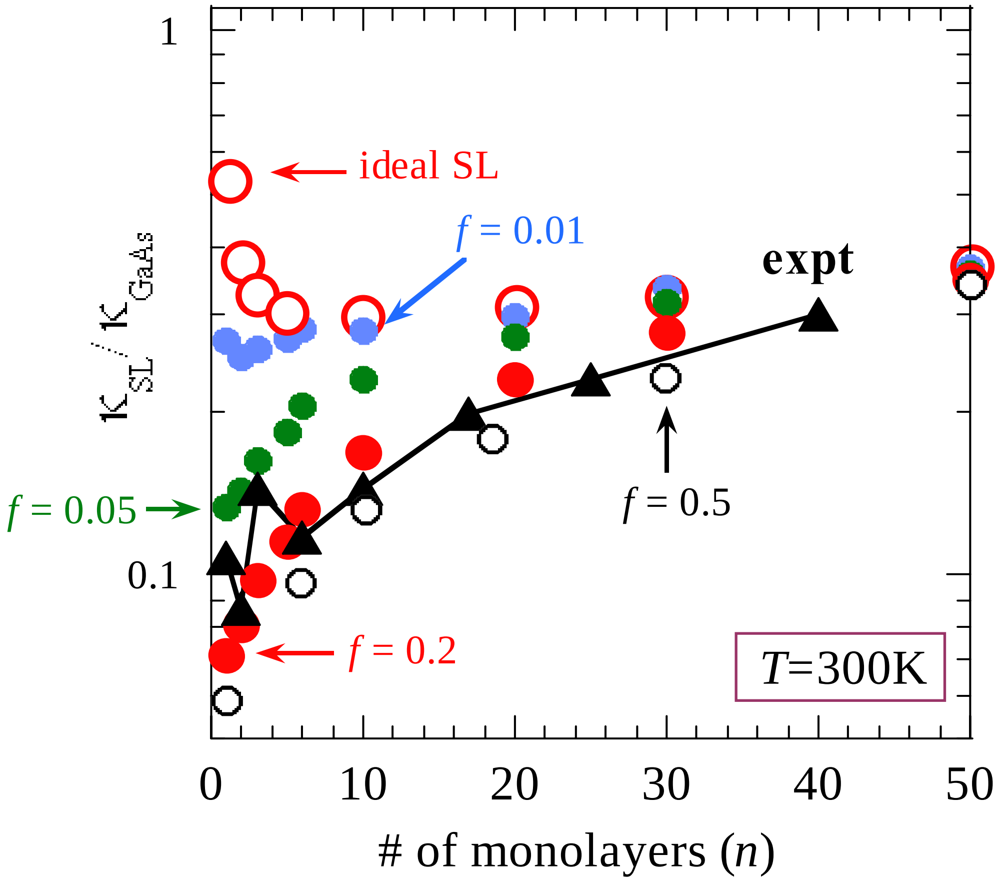
For the *last atomic monolayer* of each SL layer, we assign to each atom the mass either M_{GaAs} or M_{AlAs} randomly with a probability f



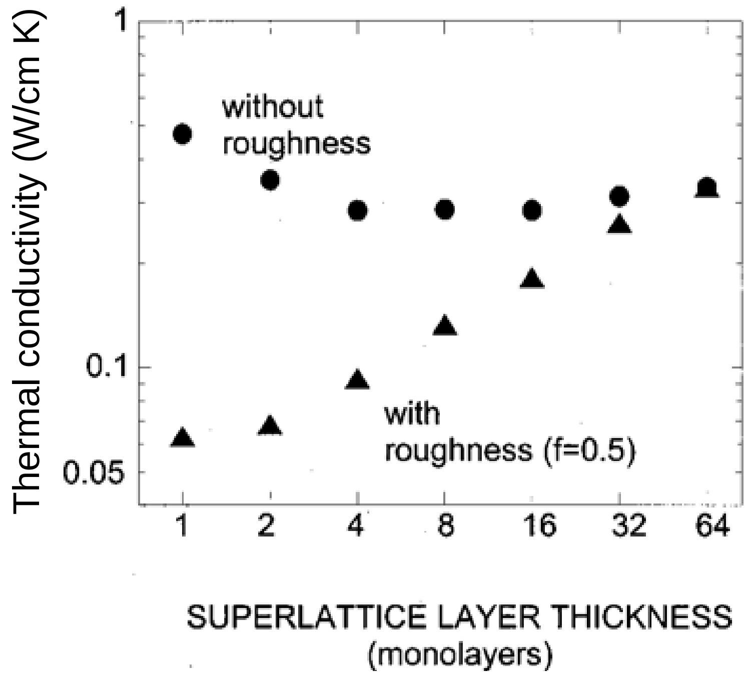
ideal SL

with roughness $f=0.25$ $(f_{max}=0.5)$

Thermal conductivity in SLs with interface roughness-2



MD results of Daly *et al.*



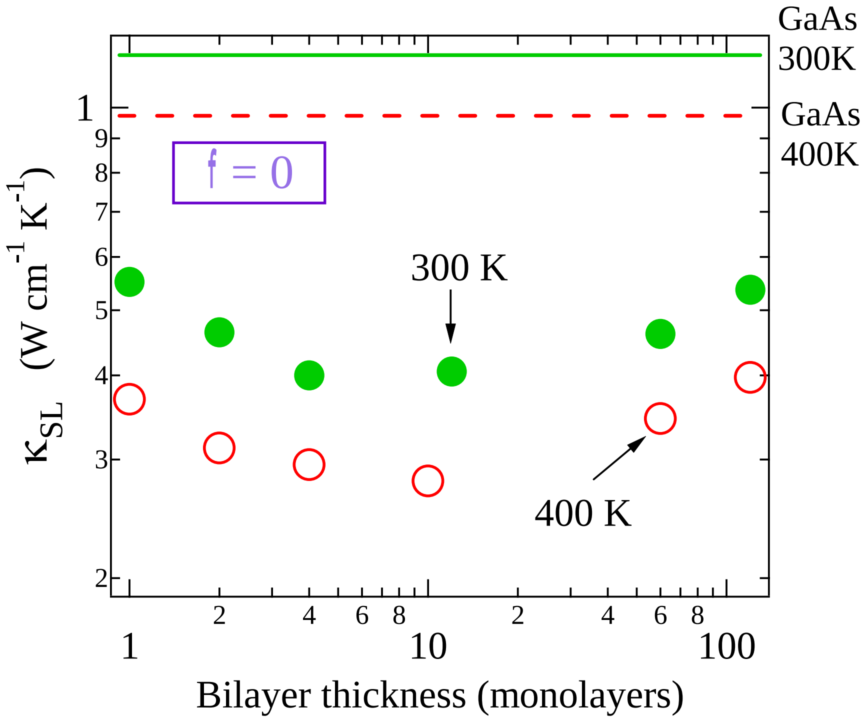
(1) κ in SLs with $n < 10$ is strongly affected by the interface roughness

(2) κ in SLs with f = *0.2- 0.5 coincides well with* κ_{exp}

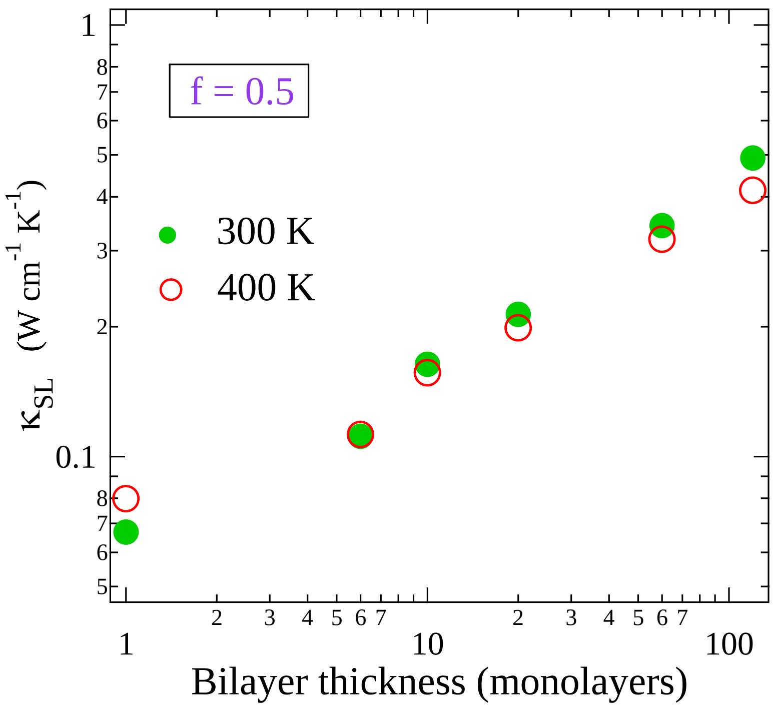
Thermal conductivity in SLs with interface roughness-2

Temperature variations

Ideal SL



Disordered SL

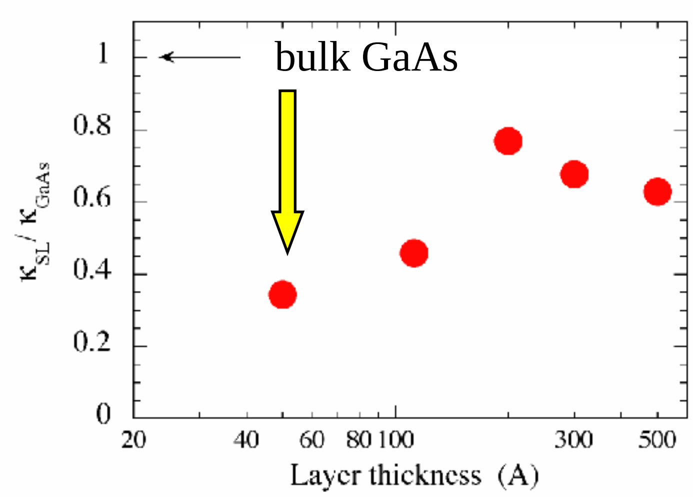


(1) κ in ideal SLs ⇒ κ_{min} with respect to *n*

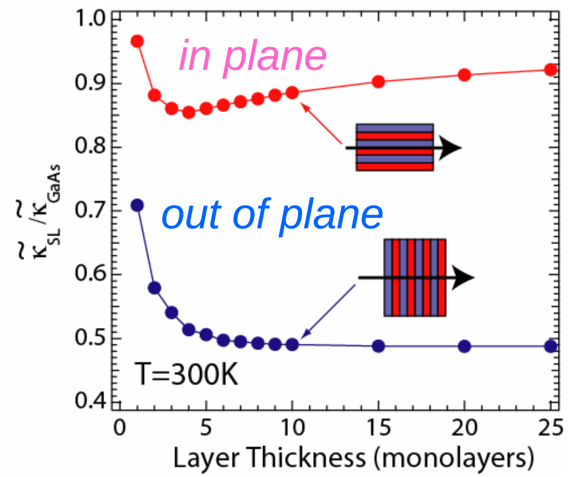
(2) κ in strongly disordered SLs ⇒ T-indep.

2. In-plane thermal conductivity

Expt. (by Yao)



Zone-folding effect for the in-plane

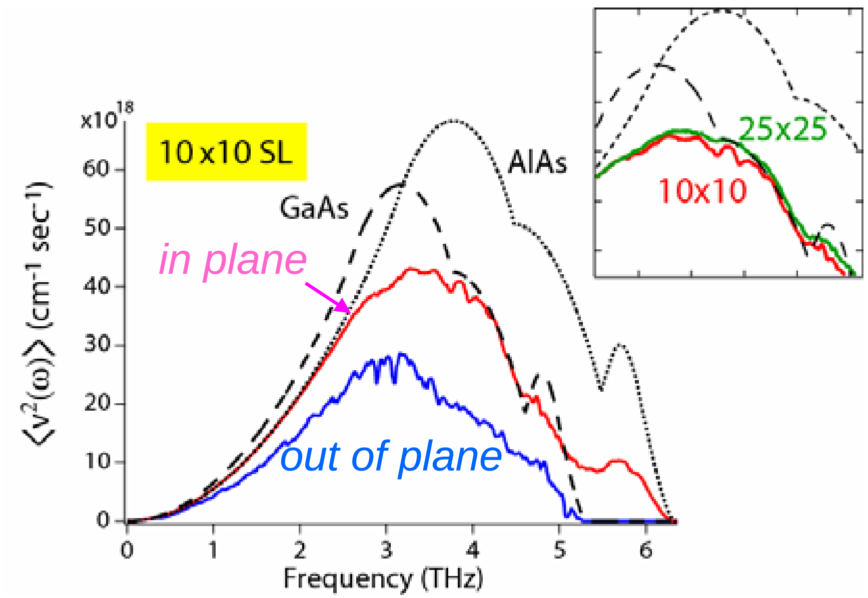


reduction ~15 %

unable to explain Yao's experiment

Weighted density of states

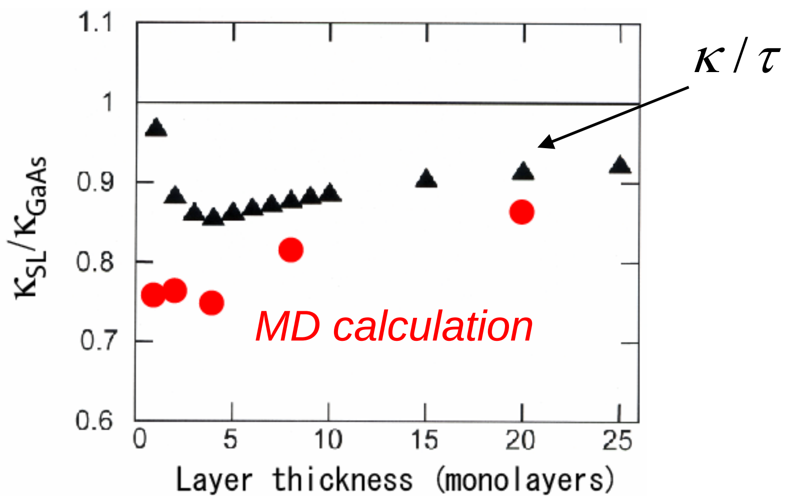
$$< v_z^2(\omega) > = \frac{1}{V} \sum_{\lambda} \delta(\omega - \omega_{\lambda}) v_{\lambda,z}^2$$



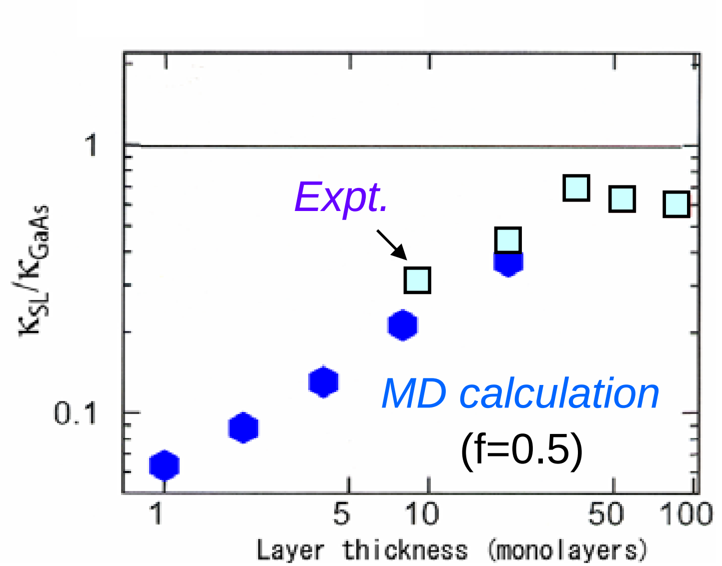
Comparison between the SLs without and with roughness

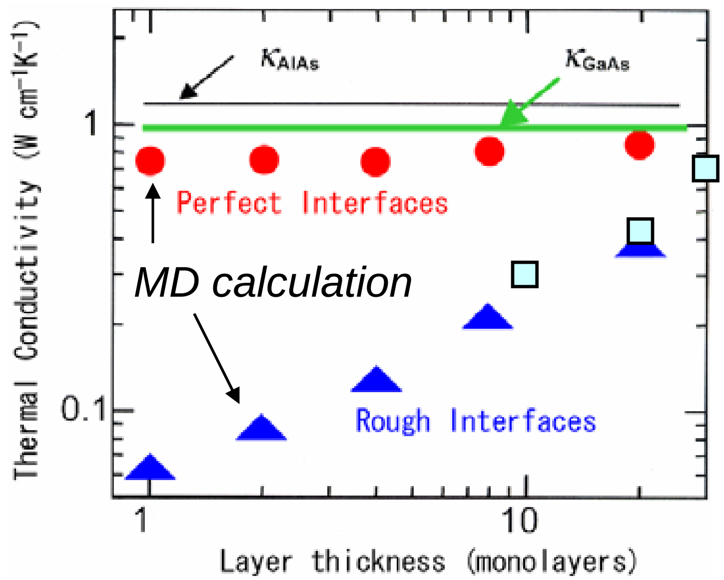
Ideal SLs

T=300 K



SLs with interface roughness





Summary

I. MD calculation with a classical fcc lattice model for the thermal conductivity (κ) of semiconductor SLs

1-1) For perfect, periodic SLs, the reduction of κ is in good agreement with the calculation based on the effect of Brillouin-zone folding

1-2) With the addition of interfacial roughness, the dependence of κ on SL period similar to that seen experimentally is obtained

II. These results are obtained with

(1) conventional MD simulations which assumes the hot and cold thermal reservoirs

(2) a MD simulation for the relaxation of an inhomogeneous temperature distribution

III. The MD calculation have proven to be a powerful method for studying the thermal properties in SLs.