भारतीय विज्ञान संस्थान
INDIAN INSTITUTE OF SCIENCE

American Physics Society
March Meeting - 2022

1945-2020
MECHANICAL ENGINEERING
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Phonon transport in ultra-high thermal conductivity materials beyond the relaxation time approximation*

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* This work is supported by the DST-SERB Core Research Grant (CRG/2020/006166) and Prime Minister Research Fellowship (192002-2069)

Thermal transport (insulator and dielectric materials)

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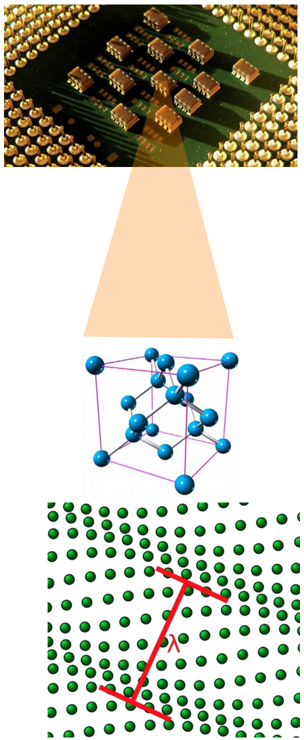

Figure: phonon propagation
https://en.wikipedia.org/wiki/Phonon#/media/File:Lattice_wave.svg

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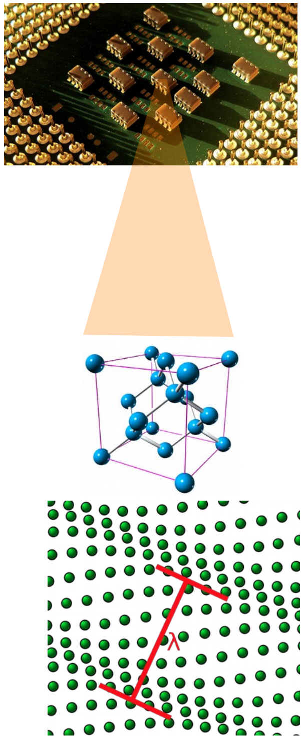

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Phonons : normal modes of lattice vibrations

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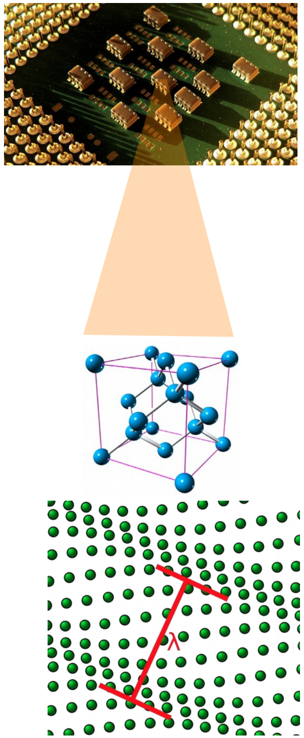

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Phonon scattering

(among themselves or boundaries, impurities and defects)

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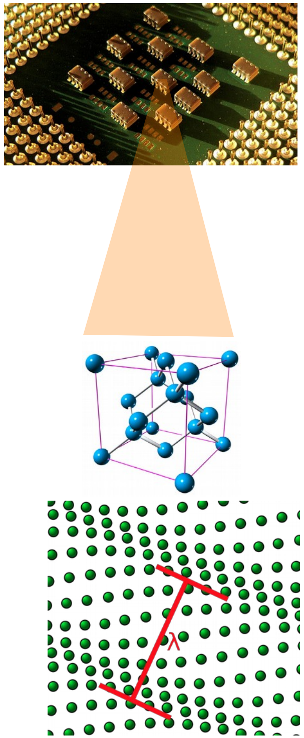

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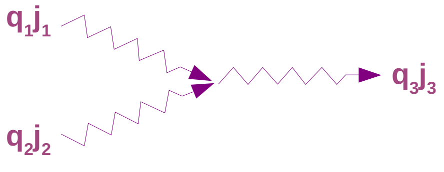
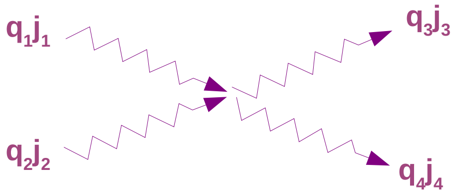
Anharmonicity in crystal



3 phonon interaction



4 phonon interaction

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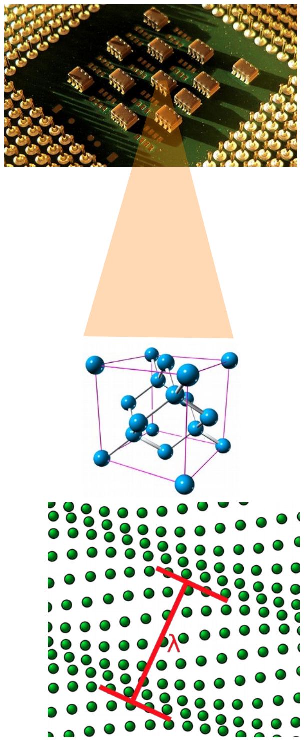

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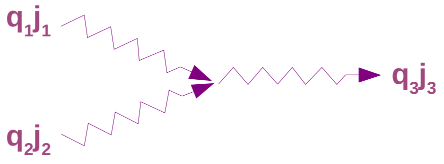

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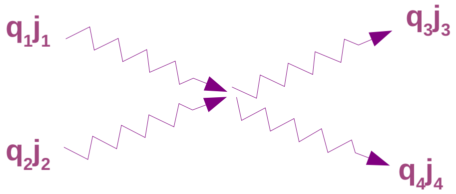

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Anharmonicity driven phonon - phonon scattering

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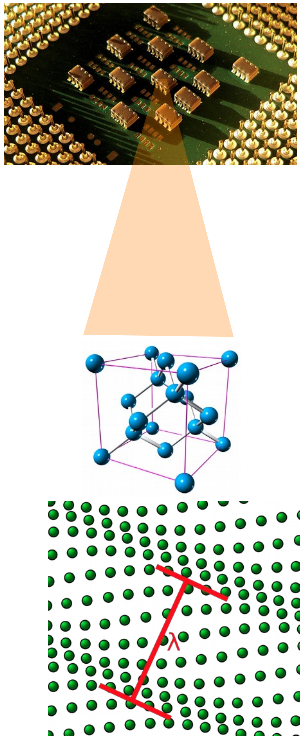

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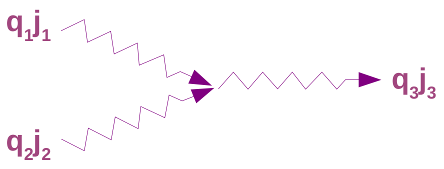

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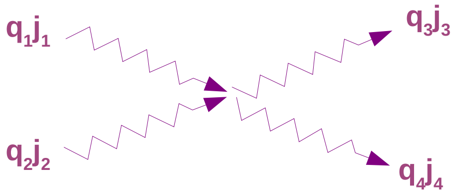

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Momentum conserving
Normal (N) - process

$$q_1 + q_2 = q_3$$

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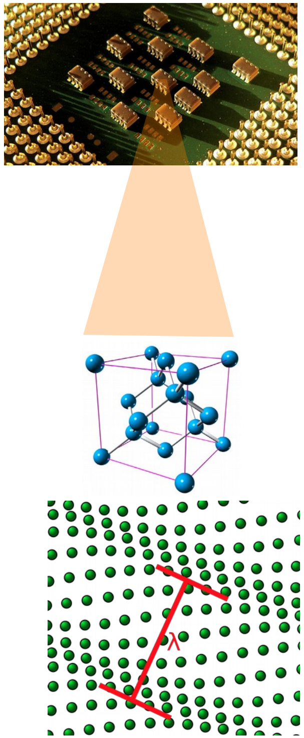

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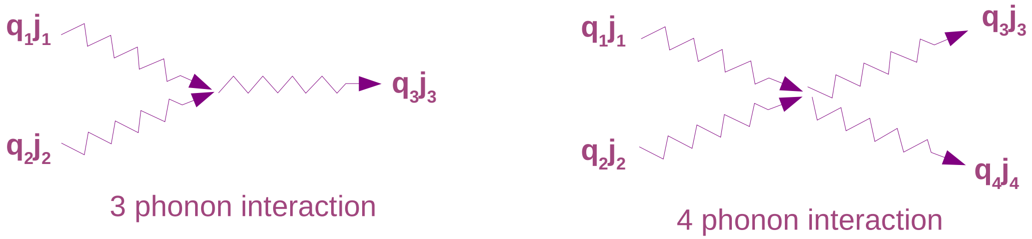

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Momentum dissipating
Umklapp (U) - process

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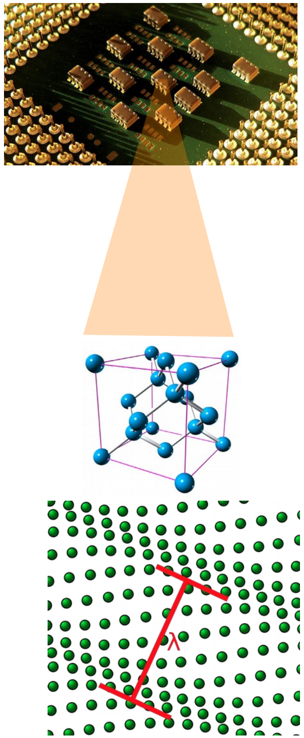

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Phonons : normal modes of lattice vibrations

Phonon scattering
(among themselves or boundaries, impurities and defects) > thermal resistance

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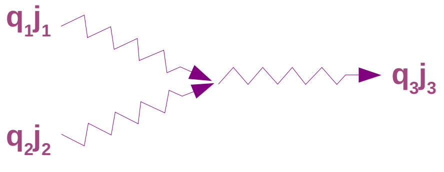

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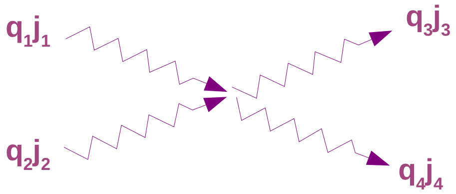

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$V_{\lambda\lambda_1\lambda_2}$ - Strength of phonon scattering

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$$n_\lambda^1 = n_\lambda^0 (1 + n_\lambda^0) \tilde{n}_\lambda^1$$

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$$n_\lambda^1 = n_\lambda^0(1 + n_\lambda^0)\tilde{n}_\lambda^1$$

n_λ^0 - Bose - Einstein distribution at local equilibrium
n_λ^1 - deviation from local equilibrium λ

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Approximate solution models

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Relaxation time approximation (RTA)

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$$\frac{\partial n_\lambda}{\partial t} + \vec{\nu}_\lambda \cdot \vec{\nabla} n_\lambda = -\frac{n_\lambda - n_\lambda^0}{\tau_\lambda}$$

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τ_λ - phonon relaxation time

$\frac{1}{\tau_\lambda}$ - phonon scattering rate

Approximate solution models

Relaxation time approximation (RTA)

all phonons decay independently to local equilibrium

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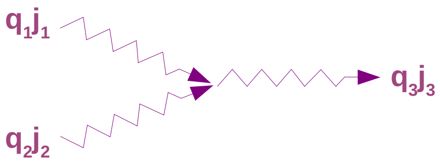

Normal Scattering

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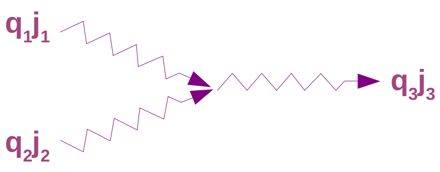

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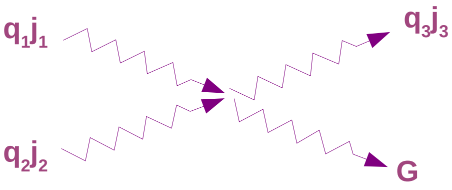

Umklapp Scattering

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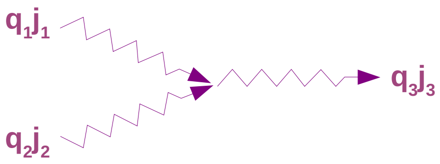

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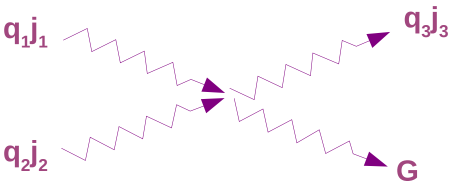

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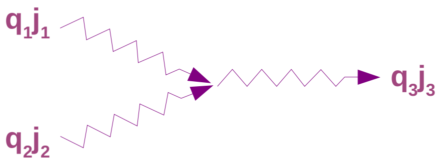

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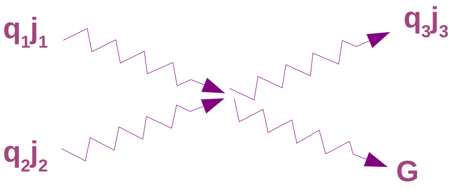

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$\frac{1}{\tau_\lambda^U}$ - Umklapp scattering rates

$\frac{1}{\tau_\lambda^N}$ - Normal scattering rates

$\frac{1}{\tau_\lambda^{defects}}$ - Scattering rates from defects

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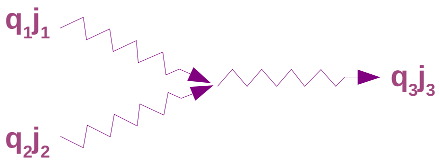

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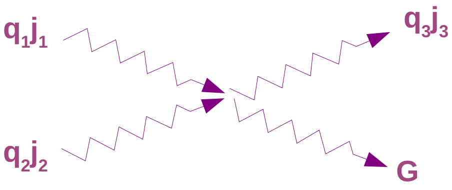

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$\frac{1}{\tau_\lambda^U}$ - Umklapp scattering rates

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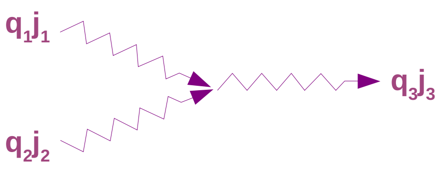

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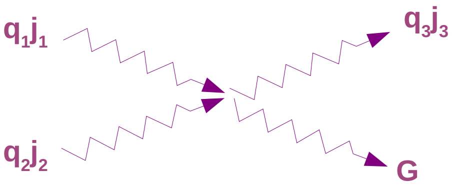

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$\frac{1}{\tau_\lambda^{defects}}$ - Scattering rates from defects

$$\kappa = \frac{1}{3} \sum_\lambda C_\lambda \nu_\lambda \Lambda_\lambda$$

κ : thermal conductivity

$C_\lambda = \frac{1}{\Omega} \hbar \omega_\lambda \frac{\partial n_\lambda^0}{\partial T}$: heat capacity

$\Lambda_\lambda = \tau_\lambda \nu_\lambda$: Mean free path

Approximate solution model 1 - RTA

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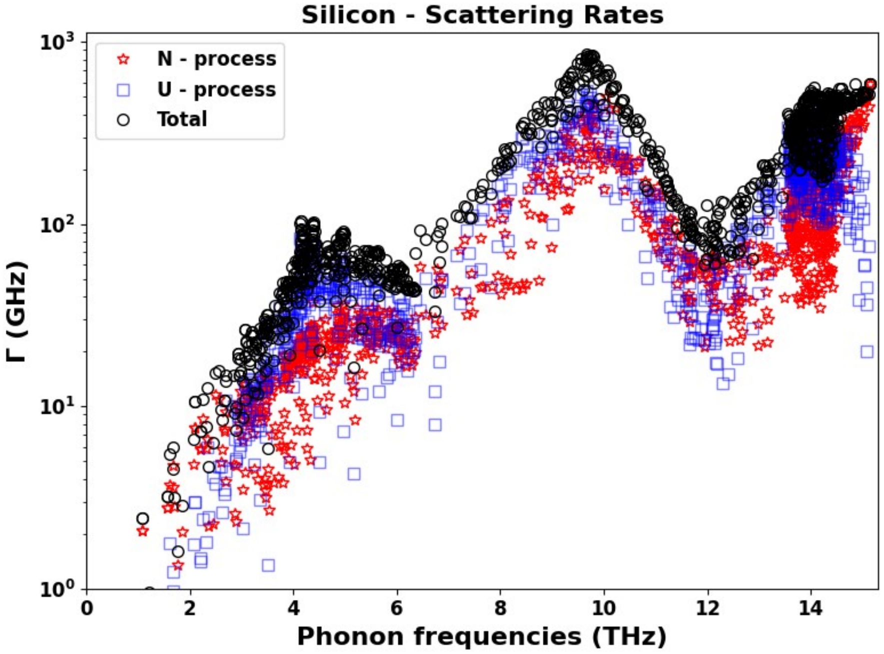
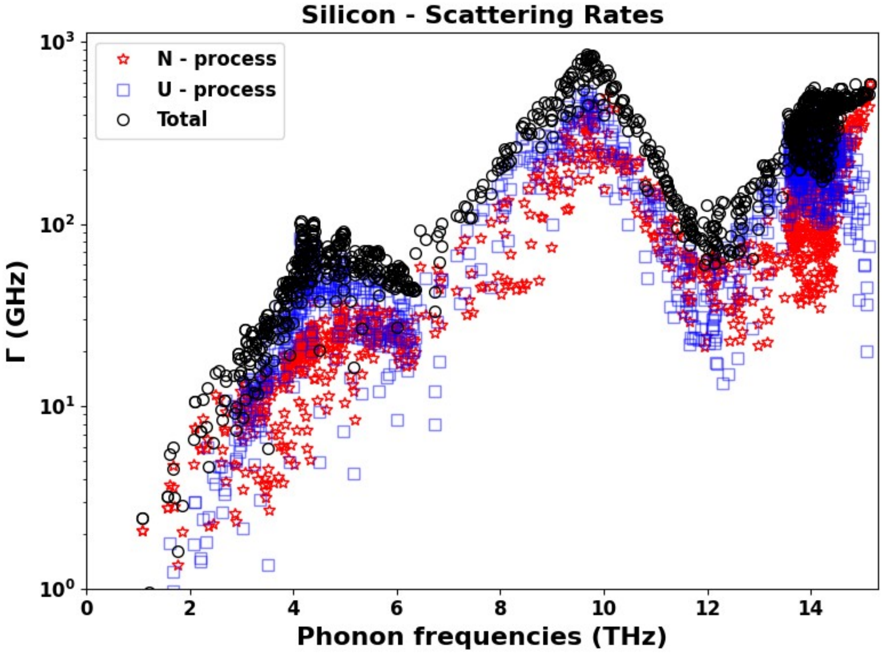


Figure: Scattering rates of Silicon at 300K
(^{28}Si – 92.22%, ^{29}Si – 4.68%, ^{30}Si – 3.09%)

Approximate solution model 1 - RTA



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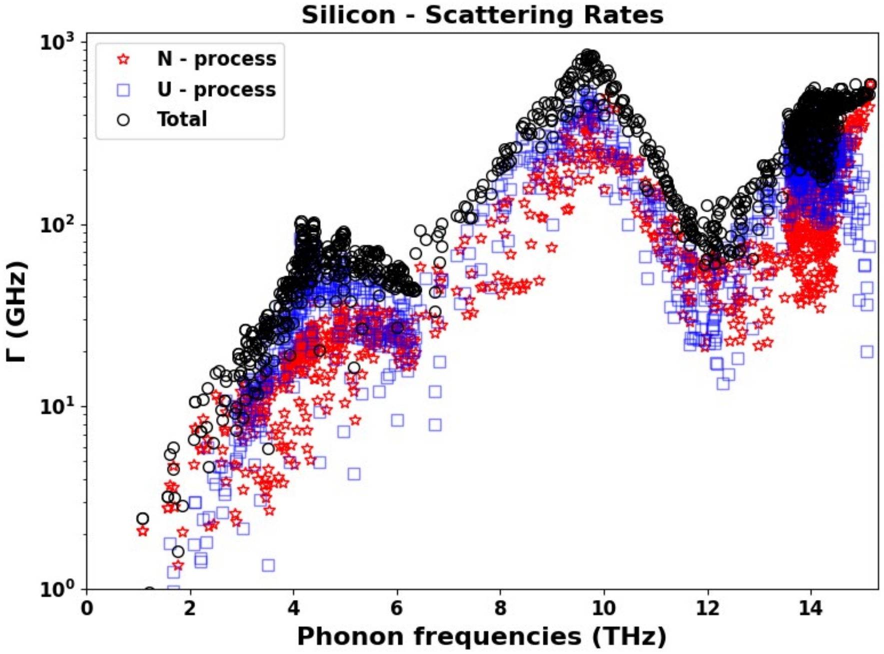
Both N and U scattering are of comparable strength

Approximate solution model 1 - RTA



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(^{28}Si – 92.22%, ^{29}Si – 4.68%, ^{30}Si – 3.09%)

Both N and U scattering are of comparable strength

Thermal conductivity of Silicon
(17^3 q-grid, including phonon – isotope scattering)

RTA prediction : 122.5735 W/m-K
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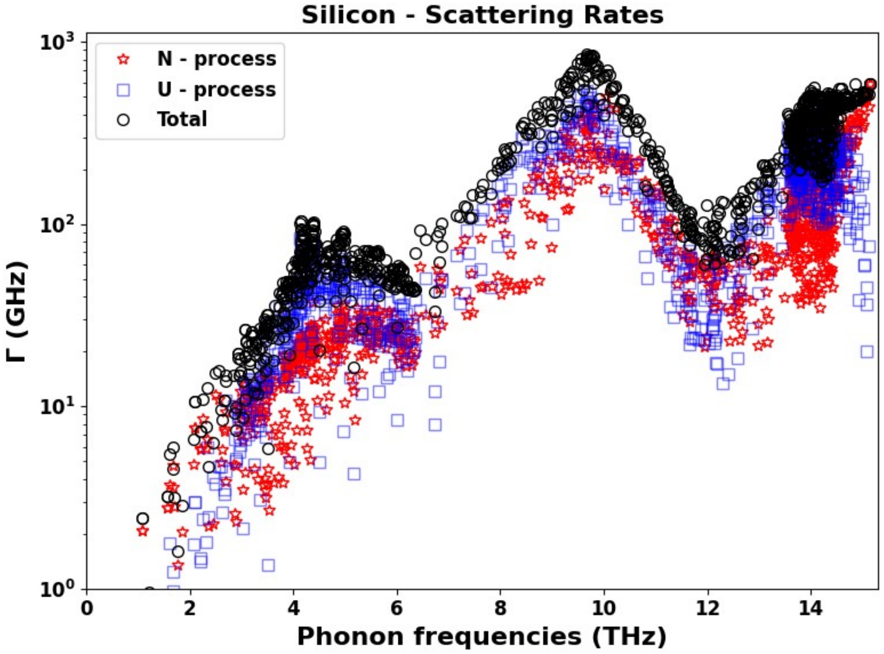
Approximate solution model 1 - RTA



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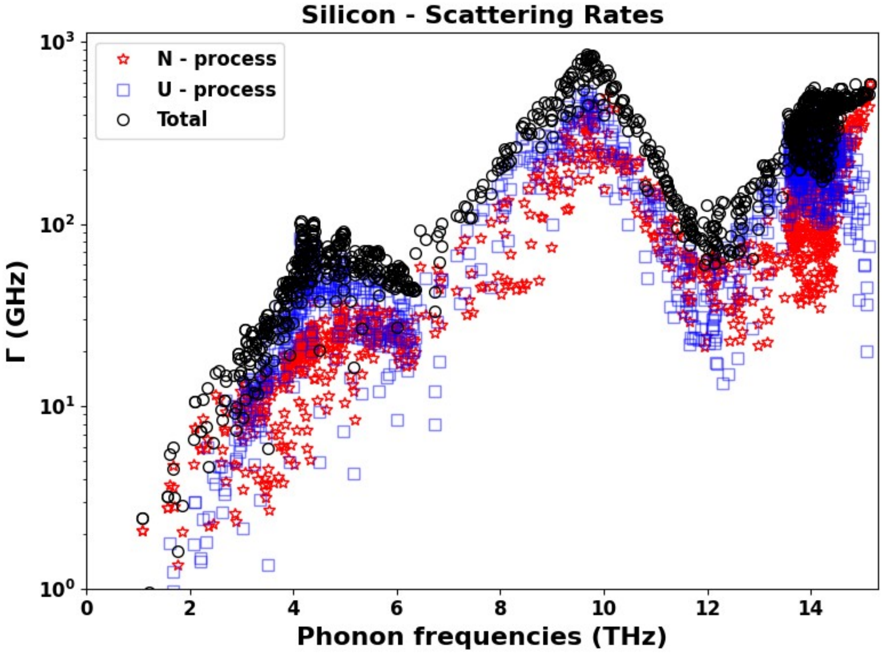

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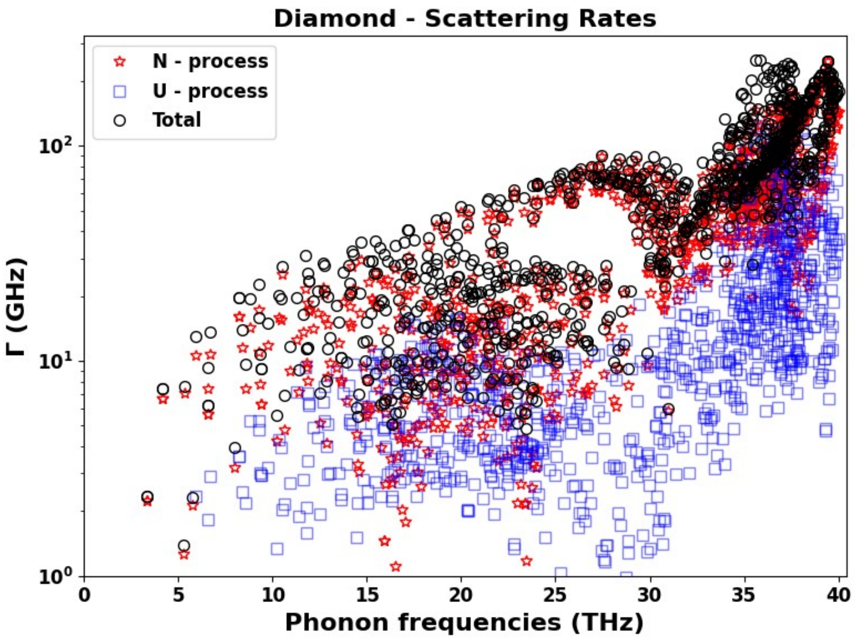

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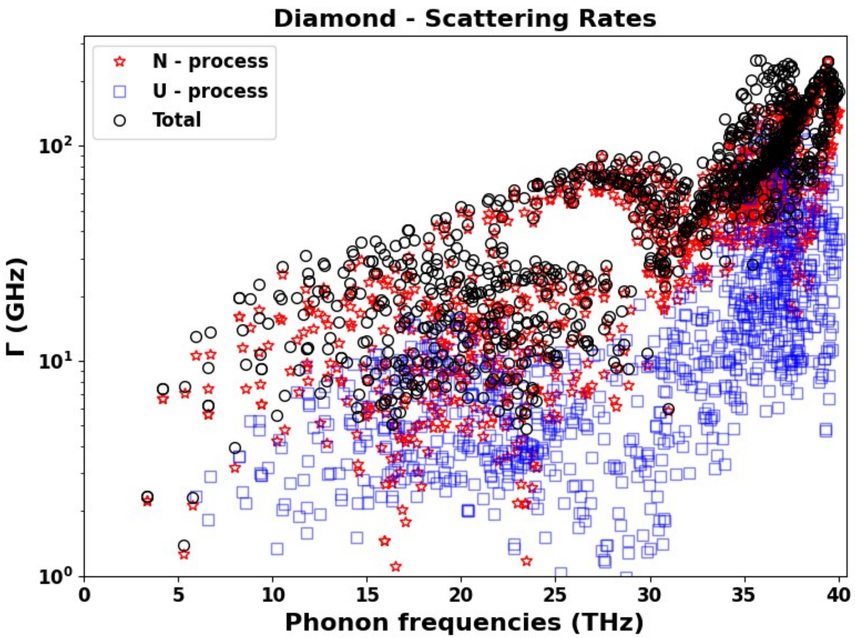

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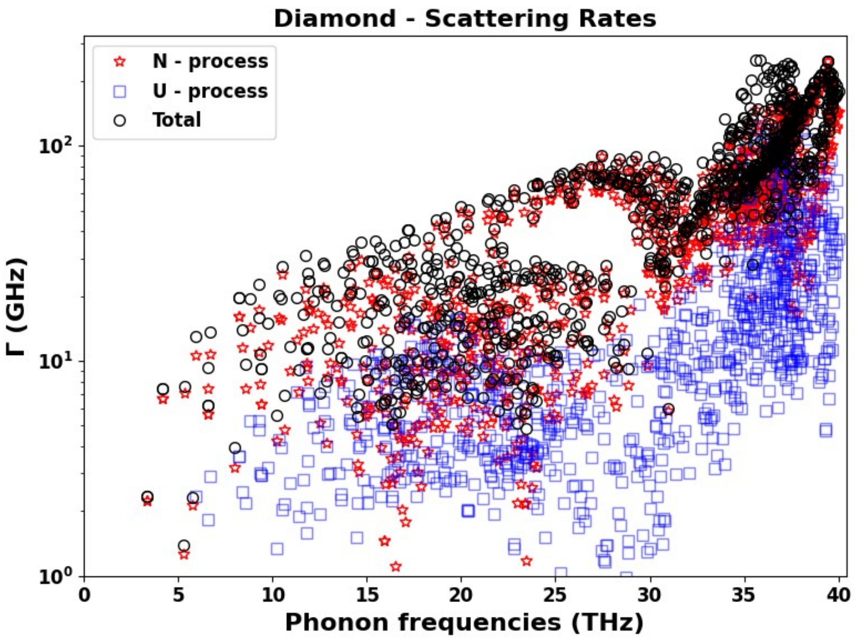

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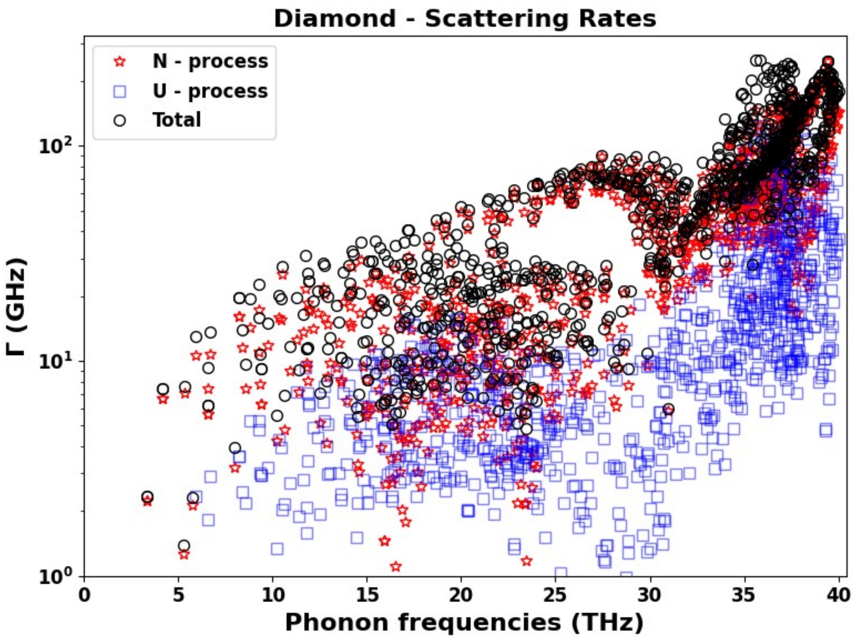

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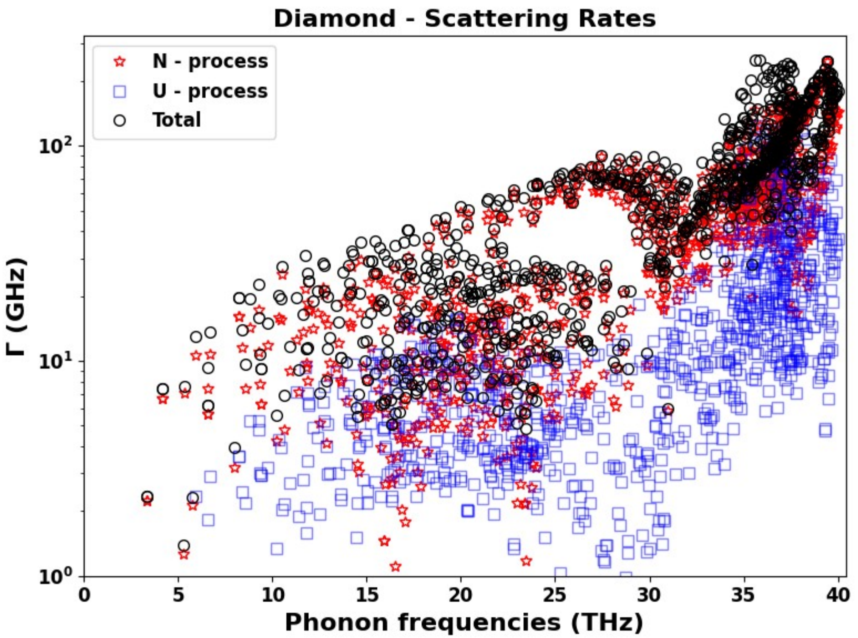

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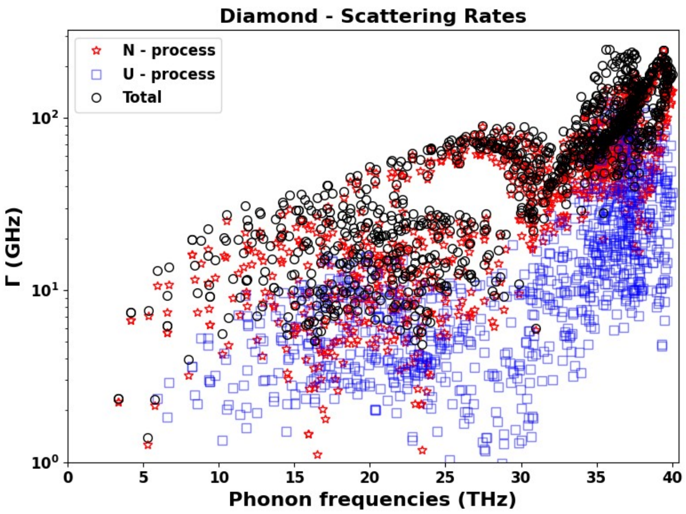

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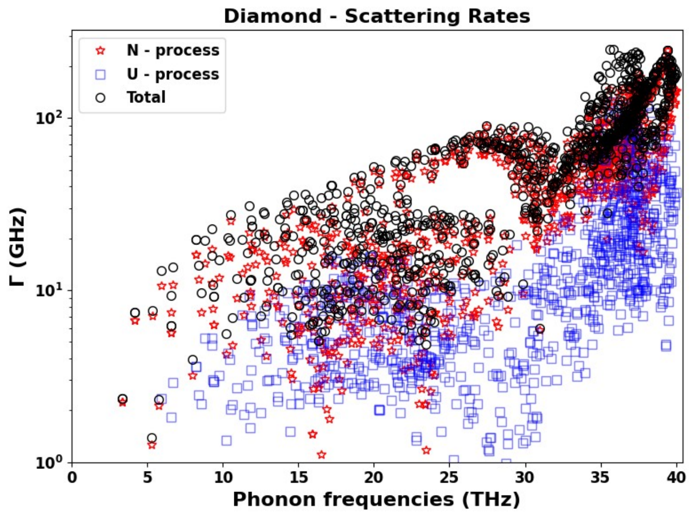

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