

Initialize functions

```
(*Ensure that variables are defined globally*)
SetOptions[EvaluationNotebook[], CellContext -> "Global`"]
NotebookOpen[NotebookDirectory[] <> "GB-strain-scattering_init.nb"];
NotebookEvaluate[NotebookDirectory[] <> "GB-strain-scattering_init.nb"];
```

Define material values and phonon dispersion parameters

```
(*#####*)
(*### Material values for Si ###*)
(*#####*)

(*##### crystal properties #####*)
vs = 6084. (*[m/s] average speed of sound*);
V = 2 * 10-29 (*[m3] volume of atom*);
n = 2 (*# atoms per primitive unit cell (N in paper)*);
γ = 1 (*Gruneissen parameter*);
ν = 0.27 (*Poisson's ratio*);
kmax = k0[V * n] // N(*[m-1] edge of FBZ*);
ωD = vs kmax (*[s-1] Debye frequency*);
disp = "Debye";
ωk[k_] := vs k (*Debye dispersion relation*);
vg[k_] := vs (*phonon group velocity*);

(*##### phonon-phonon #####*)
C1 = 2.69 * 10-19 (*[s/K]*);
C2 = 167 (*[K]*);

(*##### point defect #####*)
C3 = 1.81 * 10-45 (*[s3]*);

(*##### microstructure #####*)
b = (V n)1/3 (*[m] Burger's vector*);
dGS = 350 * 10-9 (*[m] average grain size*);
n1D = 3 / dGS // N(*[m-1] number density of GBs *);
d = 3 * 10-9 (*[m] GB dislocation spacing (D in paper)*);
```

Diffraction peaks in $\Gamma_{\text{gb}}(\mathbf{k})$

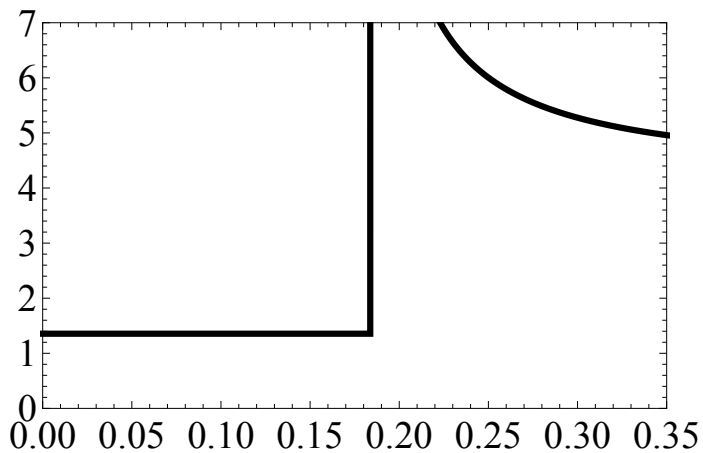
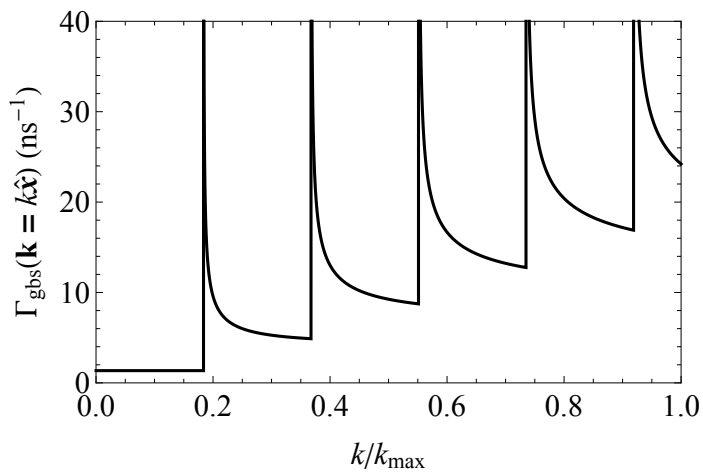
```

rMakeList[θ_, ϕ_] := Table[{ω/ωD, rGBS[ω/vs, θ, ϕ] * 10-9}, {ω, 0, ωD, 1010}]
(*θ=π/2 ϕ=0 is phonon incident normal to the GB.*)
rlistGBS = rMakeList[π/2, 0];

ListPlot[{rlistGBS},
  PlotStyle → {Black},
  PlotRange → {{0, 1}, {0, 40}},
  Joined → True,
  FrameLabel → {"k/kmax", "Γgbs(k = k $\hat{\mathbf{x}}$ ) (ns-1)"}]

ListPlot[{rlistGBS},
  Joined → True,
  FrameStyle → Directive[FontFamily → "Times New Roman", FontSize → 20, Black],
  PlotStyle → Directive[Black, Thickness[0.01]],
  PlotRange → {{0, 0.35}, {0, 7}}]

```



Calculating $\tau_{\text{gbs}}(\omega)^{-1}$

(*A convergence test was performed on δk by calculating κ_L at different δk . $\delta k = 2 \times 10^8$ was found to be fully converged. This calculation takes ~20 min on most personal computers*)

```
Clear[d]
τGBSList = {disp};
δk = 2. * 108;
For[d = 1.0 * 10-9, d ≤ 8.0 * 10-9, d = d * 2.0,
  Print[d];
  τGBSListd = Table[{ω / vs, τGBSθφIntegrate[ω / vs, 90]}, {ω, vs δk, ωD, vs δk}];
  AppendTo[τGBSList, {d, θcalc[b, d], τGBSListd}]
]
1. × 10-9
2. × 10-9
4. × 10-9
8. × 10-9

(*******)
(*#### Exports τGBS results ####*)
(*******)
Export[NotebookDirectory[] <> "../Results/tauSTGB_results.m", τGBSList]
/Users/rileyhanus/Desktop/Papers/Phonon_diffraction/Scripts/FOR_DISTRIBUTION/
Phonon-scattering-and-transport-in-polycrystals/core/../Results/tauSTGB_results.
m

(*******)
(*#### Imports the last exported τGBS result ####*)
(*******)
τGBSList = Import[NotebookDirectory[] <> "../Results/tauSTGB_results.m"];
```

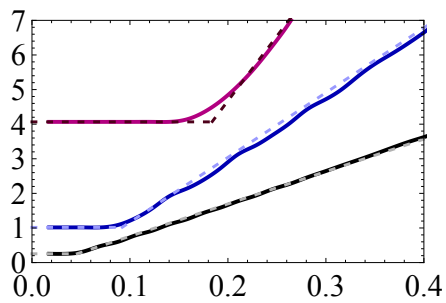
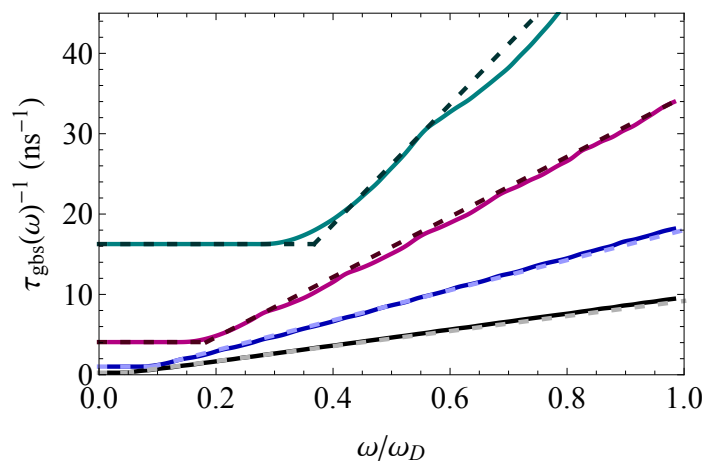
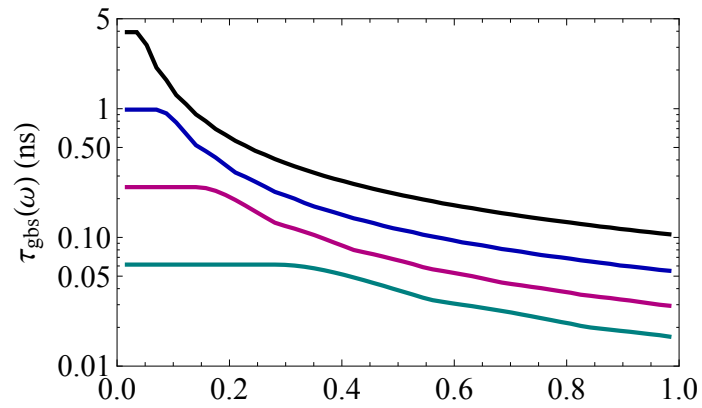
Plotting $\tau_{\text{gbs}}(\omega)$ for a STGB

```
"STGB"
Show[ListLogPlot[{τGBExtract[τGBSList, 2],
  τGBExtract[τGBSList, 3], τGBExtract[τGBSList, 4], τGBExtract[τGBSList, 5]},
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
    Directive[Black, Thickness[0.0075]]},
  FrameLabel -> {Style["", 16], Style["τgbs(ω) (ns)", 16]},
  PlotRange -> {{0, 1}, {0.01, 5}},
  Joined -> True,
  PlotRange -> All}]
Show[
  ListPlot[{τGBExtract[τGBSList, 2],
```

```

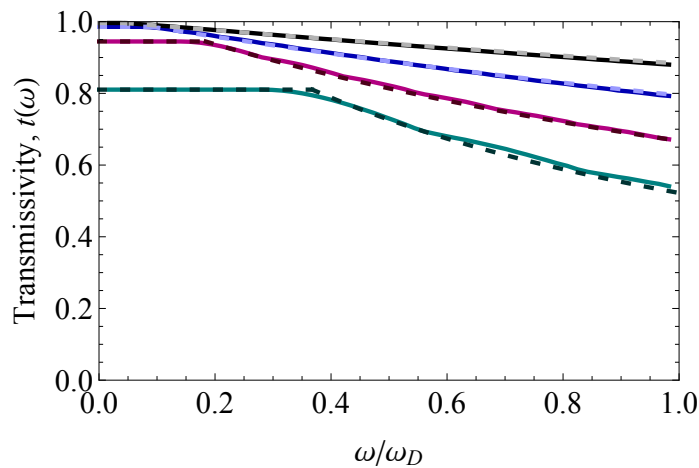
    RGBExtract[τGBSList, 3], RGBExtract[τGBSList, 4], RGBExtract[τGBSList, 5]],
    PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
      Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
      Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
      Directive[Black, Thickness[0.0075]]},
    FrameLabel -> {Style["ω/ωD", 16], Style["τgbs(ω)-1 (ns-1)", 16]},
    PlotRange -> {{0, 1}, {0, 45}},
    Joined -> True,
    InterpolationOrder -> 3,
    PlotRange -> All],
  Plot[{τinvEmp[ω * ωD, 1 * 10-9, b, n1D] * 10-9,
    τinvEmp[ω * ωD, 2 * 10-9, b, n1D] * 10-9, τinvEmp[ω * ωD, 4 * 10-9, b, n1D] * 10-9,
    τinvEmp[ω * ωD, 8 * 10-9, b, n1D] * 10-9}, {ω, 0, 1},
  PlotStyle -> {Directive[Dashing[{.01, 0.03}],
    RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}],
  Show[
    ListPlot[{RGBExtract[τGBSList, 2], RGBExtract[τGBSList, 3],
      RGBExtract[τGBSList, 4], RGBExtract[τGBSList, 5]},
    PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.01]],
      Directive[RGBColor[0.7, 0., 0.5], Thickness[0.01]],
      Directive[RGBColor[0., 0, 0.7], Thickness[0.01]],
      Directive[Black, Thickness[0.01]]},
    FrameLabel -> {Style["", 16], Style["", 16]},
    PlotRange -> {{0, 0.4}, {0, 7}},
    ImageSize -> 250,
    Joined -> True,
    InterpolationOrder -> 3,
    PlotRange -> All],
  Plot[{τinvEmp[ω * ωD, 1 * 10-9, b, n1D] * 10-9,
    τinvEmp[ω * ωD, 2 * 10-9, b, n1D] * 10-9, τinvEmp[ω * ωD, 4 * 10-9, b, n1D] * 10-9,
    τinvEmp[ω * ωD, 8 * 10-9, b, n1D] * 10-9}, {ω, 0, 1},
  PlotStyle -> {Directive[Dashing[{.01, 0.03}],
    RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}],
  STGB

```



Convert $\tau(\omega)$ to $t(\omega)$ and plot

```
Show[ListPlot[{tGBExtract[τGBSList, 2], tGBExtract[τGBSList, 3],
  tGBExtract[τGBSList, 4], tGBExtract[τGBSList, 5]},
  PlotRange -> {{0, 1}, {0., 1}},
  FrameLabel -> {"ω/ωD", "Transmissivity, t(ω)"},
  Joined -> True,
  PlotStyle -> {Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]],
    Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
    Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
    Directive[Black, Thickness[0.0075]]}],
  Plot[{tEmp[ω * ωD, 1 * 10-9, b, n1D], tEmp[ω * ωD, 2 * 10-9, b, n1D],
    tEmp[ω * ωD, 4 * 10-9, b, n1D], tEmp[ω * ωD, 8 * 10-9, b, n1D]}, {ω, 0, 1},
  PlotStyle -> {Directive[Dashing[{.01, 0.03}],
    RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
    Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}]]
```



Calculating κ_L

```
Timing[
  κTList = {disp};
  For[i = 2, i ≤ 5, i++,
    Print[τGBSList[[i, 1]] // N];
    κT = {};
    For[T = 5, T ≤ 500, T = T * 1.1,
      AppendTo[κT, {T, κLCalc[τTotCalc[τGBSList[[i, 3]], T], T}]]];
    AppendTo[κTList, {τGBSList[[i, 1]] // N, τGBSList[[i, 2]], κT}]]]
```

$1. \times 10^{-9}$

$2. \times 10^{-9}$

$4. \times 10^{-9}$

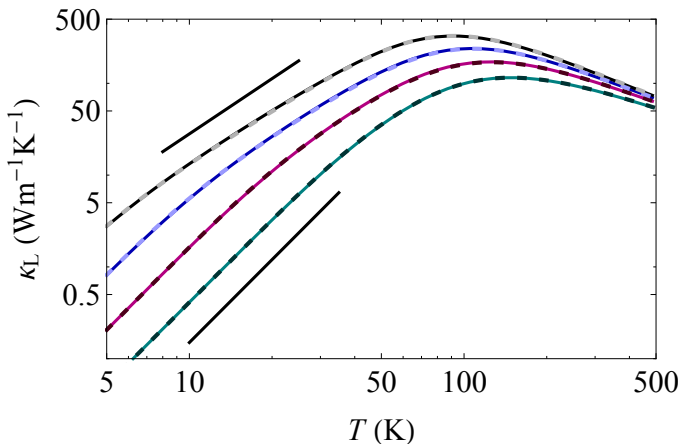
$8. \times 10^{-9}$

{0.28003, Null}

Show[

```
ListLogLogPlot[{κTLList[[2, 3]], κTLList[[3, 3]], κTLList[[4, 3]], κTLList[[5, 3]]},
  FrameLabel → {Style["T (K)", Black], Style["κL (Wm-1K-1", SingleLetterItalics → False]}},
  FrameTicks → Automatic,
  Joined → True,
  PlotStyle →
    {RGBColor[0., 0.5, 0.5], RGBColor[0.7, 0., 0.5], RGBColor[0., 0, 0.7], Black},
  PlotRange → {{5, 500}, {0.1, 500}},
  ImageSize → 350],
```

```
LogLogPlot[
  {κL[T, (τinvEmp[ω, 1 * 10-9, b, n1D] + τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1,
    vs, ω / vs, {ω, 0, ωD}],
  κL[T, (τinvEmp[ω, 2 * 10-9, b, n1D] + τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1,
    vs, ω / vs, {ω, 0, ωD}],
  κL[T, (τinvEmp[ω, 4 * 10-9, b, n1D] + τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1,
    vs, ω / vs, {ω, 0, ωD}],
  κL[T, (τinvEmp[ω, 8 * 10-9, b, n1D] + τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1,
    vs, ω / vs, {ω, 0, ωD}]], {T, 5, 500},
  PlotStyle → {Directive[Dashing[{.01, 0.03}],
    RGBColor[0, 0.2, 0.2], Thickness[0.0075]],
  Directive[Dashing[{.01, 0.03}], RGBColor[0.3, 0., 0.1], Thickness[0.0075]],
  Directive[Dashing[{.01, 0.03}], RGBColor[0.6, 0.6, 1], Thickness[0.0075]],
  Directive[Dashing[{.01, 0.03}], GrayLevel[0.7], Thickness[0.0075]]}],
  ListLogLogPlot[{T2[18, {Tref, 8, 25}], T3[0.15, {Tref, 10, 35}]], Joined → True]
```



```

LineLegend[{Directive[Black, Thickness[0.0075]],
  Directive[RGBColor[0., 0, 0.7], Thickness[0.0075]],
  Directive[RGBColor[0.7, 0., 0.5], Thickness[0.0075]],
  Directive[RGBColor[0., 0.5, 0.5], Thickness[0.0075]]},
{Style["      8      2", FontFamily → "Times New Roman", 18],
  Style["      4      5", FontFamily → "Times New Roman", 18],
  Style["      2     10", FontFamily → "Times New Roman", 18],
  Style["      1     19", FontFamily → "Times New Roman", 18]}, Spacings → 0.3]

```

```

— 8 2
— 4 5
— 2 10
— 1 19

```

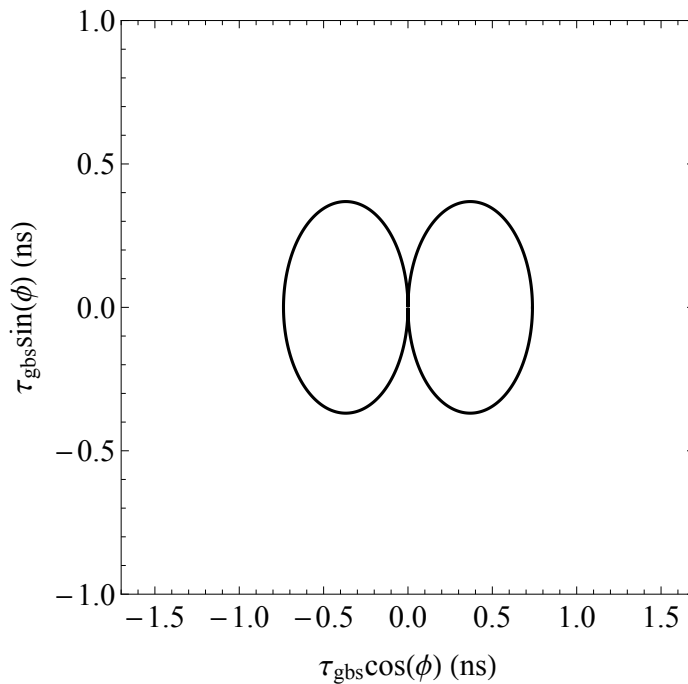
Supplemental: Pole plots of $\Gamma^{-1}(\mathbf{k})$

```

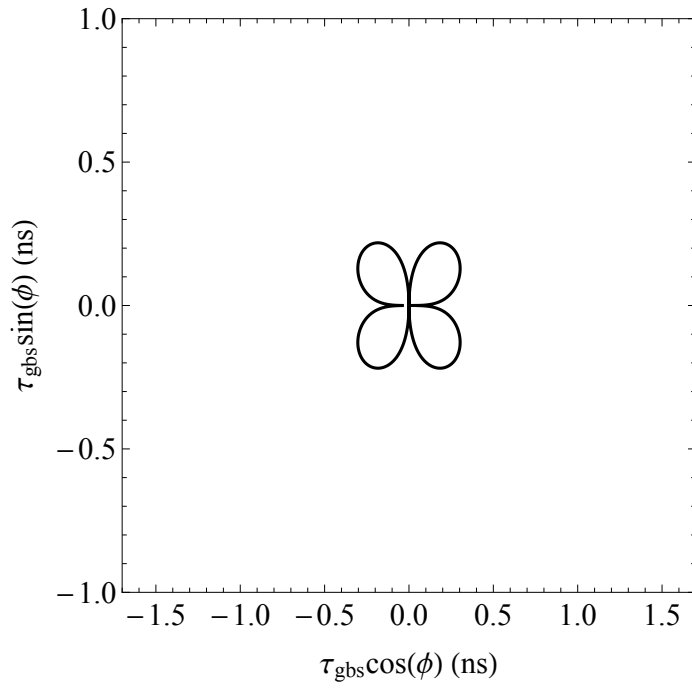
d = 3 * 10-9;
For[i = 1, i ≤ 4, i++,
  Print["k=" <> ToString[i] <> " $\frac{\pi}{d}$ "];
  Print[τPolarPlot[i π/d]]]

```

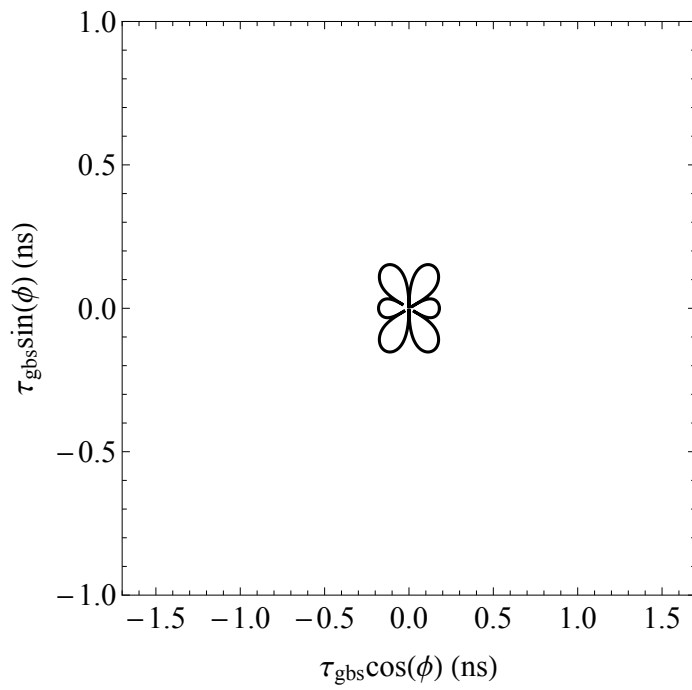
$k=1 \frac{\pi}{d}$



$k=2 \frac{\pi}{d}$



$$k=3 \frac{\pi}{d}$$



$$k=4 \frac{\pi}{d}$$

