

## 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"];
```

## Import data

```
(*Si, pc: Wang 2011 (Figure 2 550(99%)), sc: Glassbrenner 1964*)
κLdataSipc = Import[NotebookDirectory[] <> "/ExpData/Si-pc_Wang-Fig2.csv", "CSV"];
κLdataSisc =
  Import[NotebookDirectory[] <> "/ExpData/Si-sc_Glassbrenner.csv", "CSV"];
κLdataSisc = Table[{κLdataSisc[[i, 1]],  $\frac{100}{\kappa LdataSisc[[i, 2]]}$ },
  {i, 2, Length[κLdataSisc]}];

(*AlN, Watari 2002 (Figure 2, ceramic B and pure single crystal)*)
κLdataAlNpc =
  Import[NotebookDirectory[] <> "/ExpData/AlN-pc_Watari-Fig3.csv", "CSV"];
κLdataAlNsc = Import[NotebookDirectory[] <>
  "/ExpData/AlN-sc_Watari-Fig3.csv", "CSV"];

(*Al2O3, pc: Berman 1952 (Figure 1, sintered alumina),
sc: Berman 1951 (Figure 5, artificial sapphire)*)
κLdataAl2O3pc =
  Import[NotebookDirectory[] <> "/ExpData/Al2O3-pc_Berman-1952.csv", "CSV"];
κLdataAl2O3pc = Table[{κLdataAl2O3pc[[i, 1]], 100 * κLdataAl2O3pc[[i, 2]]},
  {i, 1, Length[κLdataAl2O3pc]}];
κLdataAl2O3sc = Import[NotebookDirectory[] <>
  "/ExpData/Al2O3-sc_Berman-1951.csv", "CSV"];
κLdataAl2O3sc = Table[{κLdataAl2O3sc[[i, 1]], 100 * κLdataAl2O3sc[[i, 2]]},
  {i, 1, Length[κLdataAl2O3sc]}];
```

## Modeling polycrystalline Si

```
(*#####*)
(*#### 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(*Grun parameter*);
```

```

v = 0.27(*Poisson's ratio*);
kmax = k0[V*n] // N(*[m-1] edge of FBZ*);
ωD = vs kmax (*[s-1] Debye frequency*);
ωmax = ω0[vs, V*n] (*[s-1] max frequency for BvK*);

(*##### phonon-phonon (from Wang et al.)#####)
C1 = 2.69 * 10-19 (*[s/K]*);
C1BvK = 1.53 * 10-19 (*[s/K]*);
C2 = 167 (*[K]*);
C2BvK = 140 (*[K]*);

(*##### point defect (from Wang et al.)#####)
C3 = 1.81 * 10-45 (*[s3]*);
C3BvK = 1.69 * 10-45 (*[s3]*);

(*##### microstructure #####)
b = (V n)1/3 (*[m] Burger's vector (bGB in paper)*);
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)*);

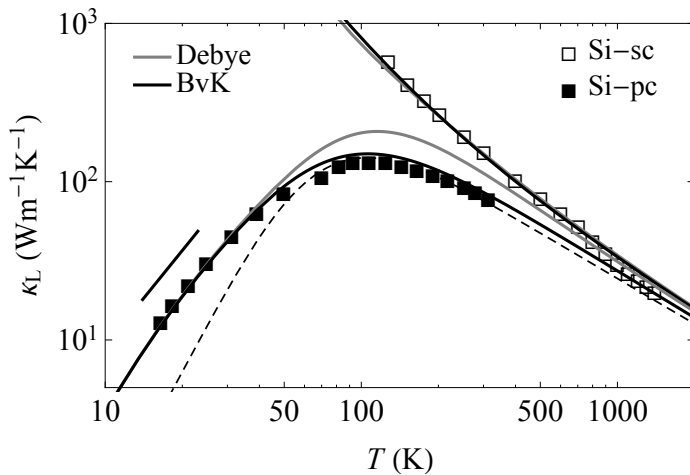
Show[ListLogLogPlot[{κLdataSisc, κLdataSipc},
  PlotRange → {{10, 2000}, {5, 1000}},
  FrameTicks → {{Table[{10k, Superscript[10, k]}, {k, 0, 3}], Automatic},
    {Automatic, Automatic}},
  FrameLabel → {Style["T (K)", SingleLetterItalics → False], Style["κL (Wm-1K-1)", SingleLetterItalics → False]},
  PlotMarkers → {{□, 18}, {■, 18}},
  PlotLegends → Placed[
    PointLegend[{Style["Si-sc", 15, FontFamily → "Times New Roman"], Style["Si-pc",
      15, FontFamily → "Times New Roman"]}, Spacings → 0.1], {0.85, 0.87}]],
LogLogPlot[{κL[T, (τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1, vs, ω / vs, {ω, 0, ωD}],
  κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 + τPD[ω, C3BvK]-1)-1,
    vGBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}],
  κL[T, (τinvEmp[ω, d, b, n1D] + τppModel[ω, T, C1, C2]-1 + τPD[ω, C3]-1)-1,
    vs, ω / vs, {ω, 0, ωD}],
  κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 + τinvEmp[ω, d, b, n1D] + τPD[ω, C3BvK]-1)-1,
    vGBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}],
  κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 + τPD[ω, C3BvK]-1 +
    
$$\frac{vGBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax]}{0.7 * 10^{-6}})^{-1},
    vGBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax],
    {ω, 0, ωmax}]], {T, 1, 5000},$$

```

```

PlotStyle → {Gray, Black, Gray, Black,
  Directive[Dashed, Black, Thickness → 0.003]},
PlotLegends → Placed[LineLegend[
  {Style["Debye", 15, FontFamily → "Times New Roman"], Style["BvK", 15,
    FontFamily → "Times New Roman"]}, Spacings → 0.2], {0.15, 0.87}],
ListLogLogPlot[{T2[18, {Tref, 14, 23}]}], Joined → True]]

```



## Modeling polycrystalline AlN

```

(*******)
(****** values for AlN ******)
(*******)

(****** crystal parameters ******)
vs = 6976. ;
V = 1.04 * 10-29 ;
n = 4;
kmax = k0[V * n] // N;
ωD = vs kmax;
ωmax = ω0[vs, V * n];
γ = 1.1;
ν = 0.2 ;

(****** phonon-phonon scattering ******)
C1 = 2.2 * 10-19;
C1BvK = 1.3 * 10-19;
C2 = 270;
C2BvK = 250;

(****** microstructure ******)
Casmir = 6 * 10-3;

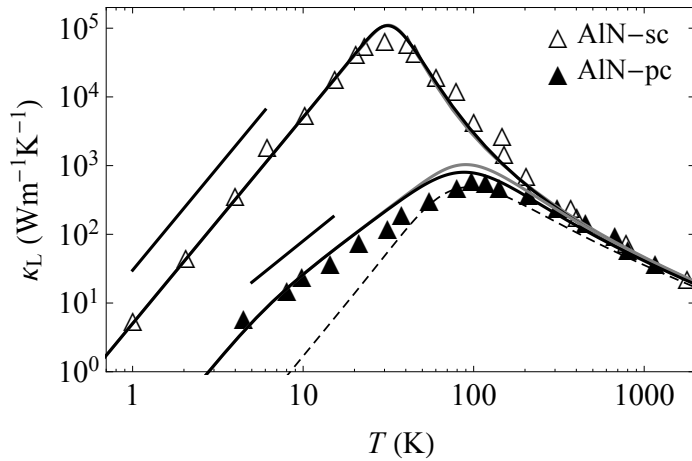
```

```

dGS = 1. * 10-6;
n1D = 3 / dGS // N;
d = 8. * 10-9;
b = (V * n)1/3;

Show[ListLogLogPlot[{κLdataAlNsc, κLdataAlNpc},
  PlotRange → {{0.7, 2000}, {1, 2 * 105}},
  FrameTicks → {{Table[{10k, Superscript[10, k]}, {k, 0, 5}], Automatic},
    {Automatic, Automatic}},
  FrameLabel → {Style["T (K)", SingleLetterItalics → False], Style["κL (Wm-1K-1)", SingleLetterItalics → False]},
  PlotMarkers → {{Δ, 18}, {▲, 18}},
  PlotLegends →
    Placed[PointLegend[{Style["AlN-sc", 15, FontFamily → "Times New Roman"],
      Style["AlN-pc", 15, FontFamily → "Times New Roman"]},
      Spacings → 0.1], {0.85, 0.87}],
  LogLogPlot[{κL[T, (τppModel[ω, T, C1, C2]-1 +  $\frac{vs}{Casmir}$ )-1, vs, ω / vs, {ω, 0, ωD}],
    κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 +  $\frac{vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax]}{Casmir}$ )-1,
      vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax],
      kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}], {T, .1, 5000},
    PlotStyle → {Gray, Black}],
  LogLogPlot[
    {κL[T, (τinvEmp[ω, d, b, n1D] + τppModel[ω, T, C1, C2]-1)-1, vs, ω / vs, {ω, 0, ωD}],
      κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 + τinvEmp[ω, d, b, n1D])-1,
        vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}],
      κL[T, (τppModel[ω, T, C1BvK, C2BvK]-1 +  $\frac{vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax]}{2 * 10^{-6}}$ )-1,
        vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax],
        kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}], {T, .1, 5000},
    PlotStyle → {Gray, Black, Directive[Dashed, Black, Thickness → 0.003]}],
  ListLogLogPlot[{T2[20, {Tref, 5, 15}], T3[30, {Tref, 1, 6}]}, Joined → True]]

```



## Modeling polycrystalline $\text{Al}_2\text{O}_3$

```
(*#####*)
(*##### values for Al2O3 #####*)
(*#####*)

(*##### crystal properties #####*)
vs = 7011. ;
V = 8.5 * 10^-30 ;
n = 10;
kmax = k0[V * n] // N;
ωD = vs kmax;
ωmax = ω0[vs, V * n];
γ = 1.3;
ν = 0.23;

(*##### phonon-phonon #####*)
C1 = 30 * 10^-19 ;
C1BvK = 15 * 10^-19;
C2 = 350 ;
C2BvK = 320;

(*##### point defect #####*)
C3 = 1 * 10^-45;
C3BvK = 1 * 10^-45;

(*##### microstructure #####*)
b = (V * n)^(1/3);
Casmir = 2.4 * 10^-3;
dGS = 1 * 10^-6;
n1D = 3 / dGS // N;
```

$d = 5.5 \cdot 10^{-9}$ ;

```
Show[ListLogLogPlot[{ $\kappa_L$ dataAl203sc,  $\kappa_L$ dataAl203pc},
  PlotRange → {{1, 500}, { $10^{-1}$ ,  $10^4$ }},
  FrameTicks → {{Table[{ $10^k$ , Superscript[10, k]}, {k, -1, 4}], Automatic},
    {Automatic, Automatic}},
  FrameLabel → {Style["T (K)"], Style[" $\kappa_L$  (Wm-1K-1)", SingleLetterItalics → False]},
  PlotMarkers → {{o, 18}, {•, 18}},
  PlotLegends →
    Placed[PointLegend[{Style["Al2O3-sc", 15, FontFamily → "Times New Roman",
      SingleLetterItalics → False], Style["Al2O3-pc", 15,
        FontFamily → "Times New Roman", SingleLetterItalics → False]},
      Spacings → 0.1], {0.82, 0.15}],
  LogLogPlot[{ $\kappa_L$ [T, ( $\tau_{ppModel}[\omega, T, C1, C2]^{-1} + \tau_{PD}[\omega, C3]^{-1} + \frac{vs}{Casmir}$ )-1,
    vs,  $\omega$  / vs, { $\omega$ , 0,  $\omega D$ }],  $\kappa_L$ [T, ( $\tau_{ppModel}[\omega, T, C1BvK, C2BvK]^{-1} +$ 
       $\tau_{PD}[\omega, C3BvK]^{-1} + \frac{vgBvK[k\omega BvK[\omega, \omega max, kmax], \omega max, kmax]}{Casmir}$ )-1,
       $vgBvK[k\omega BvK[\omega, \omega max, kmax], \omega max, kmax], k\omega BvK[\omega, \omega max, kmax], \{\omega, 0, \omega max\}$ ],
     $\kappa_L$ [T, ( $\tau_{ppModel}[\omega, T, C1, C2]^{-1} + \tau_{PD}[\omega, C3]^{-1} + \tau_{invEmp}[\omega, d, b, n1D]$ )-1,
      vs,  $\omega$  / vs, { $\omega$ , 0,  $\omega D$ }],
     $\kappa_L$ [T, ( $\tau_{ppModel}[\omega, T, C1BvK, C2BvK]^{-1} + \tau_{PD}[\omega, C3BvK]^{-1} + \tau_{invEmp}[\omega, d, b, n1D]$ )-1,
       $vgBvK[k\omega BvK[\omega, \omega max, kmax], \omega max, kmax], k\omega BvK[\omega, \omega max, kmax], \{\omega, 0, \omega max\}$ ],
     $\kappa_L$ [T, ( $\tau_{ppModel}[\omega, T, C1BvK, C2BvK]^{-1} + \tau_{PD}[\omega, C3BvK]^{-1} +$ 
       $\frac{vgBvK[k\omega BvK[\omega, \omega max, kmax], \omega max, kmax]}{1.5 \cdot 10^{-6}}$ )-1,  $vgBvK[k\omega BvK[\omega, \omega max, kmax],$ 
       $\omega max, kmax], k\omega BvK[\omega, \omega max, kmax], \{\omega, 0, \omega max\}$ ]}], {T, 1, 5000},
  PlotStyle → {Gray, Black, Gray, Black, Directive[Dashed,
    Black, Thickness → 0.003]}],
  ListLogLogPlot[{T2[15, {Tref, 9, 35}], T3[40, {Tref, 2, 6}]}, Joined → True]
```

