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[] <> "../Literature_Data/Si-pc_Wang-Fig2.csv", "CSV"];
κLdataSisc = Import[NotebookDirectory[] <>
     "../Literature_Data/Si-sc_Glassbrenner.csv", "CSV"];
```

$$\kappa LdataSisc = Table\left[\left\{\kappa LdataSisc[[i, 1]], \frac{100}{\kappa LdataSisc[[i, 2]]}\right\},\right.$$

```
   {i, 2, Length[κLdataSisc]}];


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


(*Al2O3, pc: Berman 1952 (Figure 1, sintered alumina),
sc: Berman 1951 (Figure 5, artificial sapphire)*)
κLdataAl2O3pc = Import[
    NotebookDirectory[] <> "../Literature_Data/Al2O3-pc_Berman-1952.csv", "CSV"];
κLdataAl2O3pc = Table[{κLdataAl2O3pc[[i, 1]], 100 * κLdataAl2O3pc[[i, 2]]},
    {i, 1, Length[κLdataAl2O3pc]}];
κLdataAl2O3sc = Import[NotebookDirectory[] <>
     "../Literature_Data/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 (*[m^3] volume of atom*);
n = 2(*# atoms per primitive unit cell (N in paper)*);
```

```
γ = 1(*Grun parameter*);
ν = 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[{10^k, Superscript[10, k]}, {k, 0, 3}], Automatic},
    {Automatic, Automatic}},
  FrameLabel → {Style["T (K)"], 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 +

     vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax]
     ────────────────────────────────────────────)⁻¹,
            0.7 * 10⁻⁶

    vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax],
```
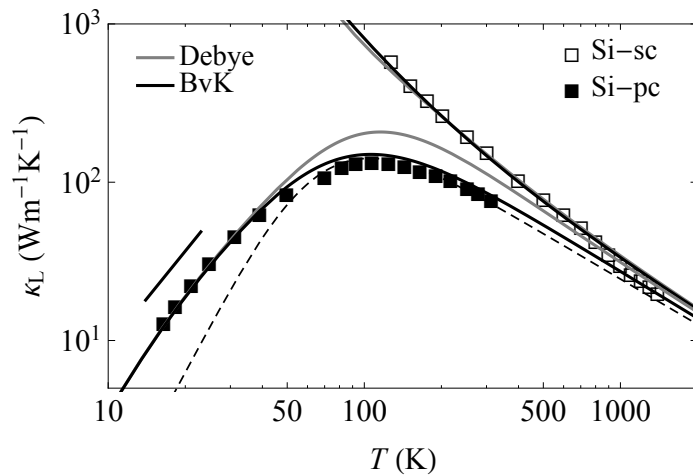
```
      {ω, 0, ωmax}]}, {T, 1, 5000},
   PlotStyle → {Gray, Black, Gray, Black,
      Directive[Dashed, Black, Thickness → 0.003]},
   PlotLegends → Placed[LineLegend[
      {Style["Debye", 15, FontFamily → "Times New Roman"], Style["BvK", 15,
        FontFamily → "Times New Roman"]}, Spacings → 0.2], {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 * 10^5}},
  FrameTicks → {{Table[10^k, Superscript[10, k]}, {k, 0, 5}], Automatic},
    {Automatic, Automatic}},
  FrameLabel → {Style["T (K)"], Style["κL (Wm^-1K^-1)", SingleLetterItalics → False]},
  PlotMarkers → {{△, 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 + vs/Casmir)^-1, vs, ω / vs, {ω, 0, ωD}],
   κL[T, (τppModel[ω, T, C1BvK, C2BvK]^-1 + 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 + 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]]
```
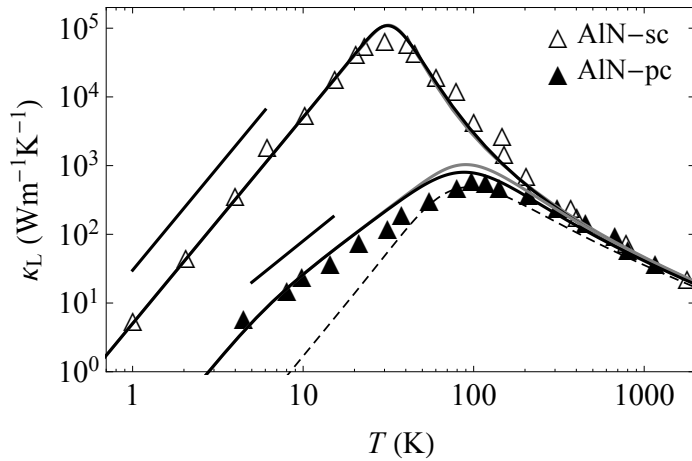
Modeling polycrystalline Al$_2$O$_3$

```
(*##############################*)
(*#### 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;
```

```mathematica
d = 5.5 * 10^-9;
```

```mathematica
Show[ListLogLogPlot[{κLdataAl2O3sc, κLdataAl2O3pc},
  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["κL (Wm^-1K^-1)", SingleLetterItalics → False]},
  PlotMarkers → {{○, 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[{κL[T, (τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1 + vs/Casmir)^-1,
     vs, ω/vs, {ω, 0, ωD}], κL[T, (τppModel[ω, T, C1BvK, C2BvK]^-1 +
       τPD[ω, C3BvK]^-1 + (vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax])/Casmir)^-1,
    vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax], kωBvK[ω, ωmax, kmax], {ω, 0, ωmax}],
   κL[T, (τppModel[ω, T, C1, C2]^-1 + τPD[ω, C3]^-1 + τinvEmp[ω, d, b, n1D])^-1,
    vs, ω/vs, {ω, 0, ωD}],
   κL[T, (τppModel[ω, T, C1BvK, C2BvK]^-1 + τPD[ω, C3BvK]^-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 + τPD[ω, C3BvK]^-1 +
       (vgBvK[kωBvK[ω, ωmax, kmax], ωmax, kmax])/(1.5 * 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]}],
 ListLogLogPlot[{T2[15, {Tref, 9, 35}], T3[40, {Tref, 2, 6}]}, Joined → True]]
```