

Initialize plot formatting and set global variables

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SetOptions[{ListPlot, ListLogPlot, ListLogLogPlot, LogLogPlot},
  Frame → True,
  Axes → False,
  FrameStyle → Directive[Black, 16, FontFamily → "Times New Roman"],
  PlotStyle → Black];
```

Define functions and constants

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(*#####*)
(*##### Constants #####*)
(*#####*)
kB = 1.3806485 * 10-23 (*Boltzmann's cst (J K-1) *);
h = 6.6260696 * 10-34 (* Plank's cst (J s) *);
hbar = h / (2 π) (*Plank's cst (J s) *);

(*#####*)
(*#### Scattering off of an array of linear defects. #####*)
(*#####*)

qm[m_] :=  $\frac{2 \pi m}{d}$  (*d is D in paper*);

qxmσ[kx_, ky_, m_, sign_] := -kx + (sign) (kx2 + 2 ky qm[m] - qm[m]2)1/2;

(*Prefactor including forward scattering and Jacobian.*)
VpreSTGB[m_, kx_, ky_, sign_] :=

$$\frac{kx^2 - (\text{sign}) kx (kx^2 + 2 ky qm[m] - qm[m]^2)^{1/2} + ky qm[m]}{(kx^2 + 2 ky qm[m] - qm[m]^2)^{1/2}} // N;$$


TARRAY[kx_, ky_, kz_, V1Twidle2_] :=
Module[{k = (kx2 + ky2 + kz2)1/2, m, mmaxPos, mmaxNeg, sum = 0},
  mmaxPos = IntegerPart[ $\frac{d}{2 \pi} (ky + (kx^2 + ky^2)^{1/2})$ ];
  mmaxNeg = Abs[IntegerPart[ $\frac{d}{2 \pi} (ky - (kx^2 + ky^2)^{1/2})$ ]];
  (*Calculate m=0 term in the sum, the sum over σ=+- is built in.
    This term is present at all values of k.*/)
  sum = sum + (VpreSTGB[0, kx, ky, 1] V1Twidle2[-2 kx, -qm[0], k] +
    VpreSTGB[0, kx, ky, -1] V1Twidle2[-2 kx, -qm[0], k]);

  (*Calculate all m>0 terms in the sum, the sum over σ=+- is built in here.
    This limits the number of terms in the sum over m.*/)
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sum = sum + Sum[ ((VpreSTGB[m, kx, ky, 1] V1Twidle2[qxmσ[kx, ky, m, 1], -qm[m], k]) +
  (VpreSTGB[m, kx, ky, -1] V1Twidle2[qxmσ[kx, ky, m, -1], -qm[m], k])) ,
  {m, 1, mmaxPos, 1}];

(*Calculate all m<0 terms in the sum,
the sum over σ=+- is also built in here. Same criterion as above.*)
sum = sum + Sum[
  ((VpreSTGB[-m, kx, ky, 1] V1Twidle2[qxmσ[kx, ky, -m, 1], -qm[-m], k]) +
  (VpreSTGB[-m, kx, ky, -1] V1Twidle2[qxmσ[kx, ky, -m, -1], -qm[-m], k])) ,
  {m, 1, mmaxNeg, 1}];
(*Sums the terms calculated above and calculates a solution of τ-1*)

$$\frac{n1D}{d^2 k v g[k] \hbar^2} \text{sum}$$

]

(*#####
#####*)
(*##### Functions for calculating phonon scattering off of GB strain fields,
Γgbs #####*)
(*#####
#####*)
(*| $\tilde{V}_{1,\Delta}(qx, qy)$ |2, hydrostatic strain field from a STGB*)
V1Twidle2εΔ[qx_, qy_, k_] := Abs[hbar ωk[k] γ  $\frac{b(1-2\nu)}{(1-\nu)} \frac{qy}{qx^2 + qy^2}$ ]2 // N;

(*| $\tilde{V}_{1,s}(qx, qy)$ |2, pure shear strain field from a STGB*)
V1Twidle2εS[qx_, qy_, k_] := Abs[hbar ωk[k] γ  $\frac{b}{(1-\nu)} \frac{qx qy^2}{(qx^2 + qy^2)^2}$ ]2 // N;

(*| $\tilde{V}_{1,R}(qx, qy)$ |2, rotational distortion about the z-axis from a STGB*)
V1Twidle2εR[qx_, qy_, k_] := Abs[hbar ωk[k] γ  $b \frac{2 qx}{qx^2 + qy^2}$ ]2 // N;

(*Sum scattering rate from hydrostatic, shear, and rotational strain components,
and convert to spherical coordinates.*)
ΓGBS[k_, θ_, ϕ_] :=
  (ΓARRAY[k Sin[θ] Cos[ϕ] // N, k Sin[θ] Sin[ϕ] // N, k Cos[θ] // N, V1Twidle2εΔ] +
  ΓARRAY[k Sin[θ] Cos[ϕ] // N, k Sin[θ] Sin[ϕ] // N, k Cos[θ] // N, V1Twidle2εS] +
  ΓARRAY[k Sin[θ] Cos[ϕ] // N, k Sin[θ] Sin[ϕ] // N, k Cos[θ] // N, V1Twidle2εR]);

(*Creates an array for the polar plots of τgbs*)
τPolarPlot[k_] := Module[{τϕlist},
  τϕlist = Table[{ΓGBS[k, π/2, ϕ]-1 Cos[ϕ] * 109,

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rGBS[k,  $\pi/2$ ,  $\phi$ ]-1 Sin[ $\phi$ ] * 109}, { $\phi$ , 0, 2  $\pi$ , 0.005}];
ListPlot[ $\tau\phi$ list,
  FrameStyle → Directive[Black, 16, FontFamily → "Times New Roman"],
  PlotMarkers → {•, 5};
  PlotRange → {{-1.7, 1.7}, {-1, 1}},
  Joined → True,
  AspectRatio → 1,
  FrameLabel → {" $\tau_{\text{gbs}} \cos(\phi)$  (ns)", " $\tau_{\text{gbs}} \sin(\phi)$  (ns)"}];

(*Numerically integrate  $\tau_{\text{gbs}}[k, \theta, \phi]$  over  $\theta$  and  $\phi$  to get  $\tau_{\text{gbs}}[k]$  which can be
related to  $t[k]$ . ( $\theta=0$ ) and ( $\phi=\pi/2$ ) are omitted from the integral since the
integrand is indeterminate at those locations. The  $(\text{Sin}[\theta]\text{Cos}[\phi])^2$  are present
because we are concerned with transport normal to the plane (kx direction). The
additional Sin[ $\theta$ ] is from converting to spherical coordinates.*)
 $\tau_{\text{GBS}}\theta\phi\text{Integrate}[k_, n_] := \text{Module}[\{\text{integrand}, \theta, \phi, \Delta\},
  \Delta = \left(\frac{\pi}{2.0}\right)/n;$ 
  integrand = 0;
  For[ $\theta = \Delta$ ,  $\theta \leq \frac{\pi}{2}$ ,  $\theta = \theta + \Delta$ ,
    For[ $\phi = \Delta$ ,  $\phi < \frac{\pi}{2}$ ,  $\phi = \phi + \Delta$ ,
      integrand = integrand +  $\frac{\text{Sin}[\theta - \frac{\Delta}{2}]^3 \text{Cos}[\phi - \frac{\Delta}{2}]^2}{\text{rGBS}[k, \theta - \frac{\Delta}{2}, \phi - \frac{\Delta}{2}]}$ ];
    8 * integrand *  $\Delta * \Delta * \left(\frac{3}{4\pi}\right)$ 

  (*#####*)
  (*##### Calculate  $\kappa_L$  from a discrete list of values #####*)
  (*#####*)

  (*Performing the  $\theta$  and  $\phi$  integration for  $\tau^{-1} = \Gamma_{\text{gbs}} + \tau_{\text{p-p}}^{-1}$ *)
   $\tau\theta\phi\text{Integrate}[k_, T_, n_] := \text{Module}[\{\text{integrand}, \theta, \phi, \Delta\},
    \Delta = \left(\frac{\pi}{2.0}\right)/n;$ 
    integrand = 0;
    For[ $\theta = \Delta$ ,  $\theta \leq \frac{\pi}{2}$ ,  $\theta = \theta + \Delta$ ,
      For[ $\phi = \Delta$ ,  $\phi < \frac{\pi}{2}$ ,  $\phi = \phi + \Delta$ ,
        integrand = integrand +  $\frac{\text{Sin}[\theta - \frac{\Delta}{2}]^3 \text{Cos}[\phi - \frac{\Delta}{2}]^2}{\text{rGBS}[k, \theta - \frac{\Delta}{2}, \phi - \frac{\Delta}{2}] + \tau_{\text{ppModel}}[k, T, C1, C2]^{-1}}$ ];

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8 * integrand * Δ * Δ *  $\left(\frac{3}{4\pi}\right)$ ]

(*The total relaxation time, including phonon-phonon,
and phonon-GB scattering calculated via Matthiessen's rule.
Calculating τTotal(ω) this way and plugging the result
in to the isotropic Callaway model gives the same result as
using Mattiessen's rule inside of the integral over θ and φ.*)
τTotCalc[τGBlist_, T_] := Table[{τGBlist[[i, 1]],
  (τppModel[ωk[τGBlist[[i, 1]]], T, C1, C2]⁻¹ + τPD[ωk[τGBlist[[i, 1]]], C3]⁻¹ +
  τGBlist[[i, 2]]⁻¹)⁻¹}, {i, 1, Length[τGBlist]}];
(*Kernal of the spectral heat capacity.*)
cvkern[T_, ωfunc_] := kB  $\frac{\left(\frac{\hbar \omega \text{func}}{k_B T}\right)^2 \text{Exp}\left[\frac{\hbar \omega \text{func}}{k_B T}\right]}{\left(\text{Exp}\left[\frac{\hbar \omega \text{func}}{k_B T}\right] - 1\right)^2}$ ;

(*Calculate κL,xx,
where we have taken the single isotropic phonon mode approximation.
Input an array for τtot and calculates lattice thermal conductivity.*)
κLCalc[τTotList_, T_] := Module[{integrand, i, Δk, ki},
  Δk = τTotList[[2, 1]] - τTotList[[1, 1]];
  integrand = 0;

  For[i = 1, i ≤ Length[τTotList], i++,
    ki = τTotList[[i, 1]];
    integrand = integrand + cvkern[T, ωk[ki]] * vg[ki]² * τTotList[[i, 2]] * ki²];
   $\frac{1}{2\pi^2}$  integrand * Δk]

(*#####*)
(*##### Semi-empirical formulas for τgbs(ω) and t(ω) #####*)
(*#####*)
τinvEmp[ω_, d_, b_, n1D_] :=
 $\frac{8}{3} n1D \text{vs} \gamma^2 \left(\frac{b}{d}\right)^2 +$ 
 $0.93 \left(1 + \frac{(1 - 2\gamma)^2}{4(1 - \gamma)^2} + \frac{1}{32(1 - \gamma)^2}\right) n1D \gamma^2 \left(\frac{b^2}{d}\right) \left(\omega - \frac{4\pi \text{vs}}{3d}\right) \text{HeavisideTheta}\left[\omega - \frac{4\pi \text{vs}}{3d}\right];$ 
τinvEmpHigh[ω_, d_, b_, n1D_] :=  $\left(1 + \frac{(1 - 2\gamma)^2}{4(1 - \gamma)^2} + \frac{1}{32(1 - \gamma)^2}\right) n1D \gamma^2 \left(\frac{b^2}{d}\right) (\omega)$ ;
tEmp[ω_, d_, b_, n1D_] :=  $\frac{4 n1D \text{vs} \tau_{\text{invEmp}}[\omega, d, b, n1D]^{-1}}{3 + 4 n1D \text{vs} \tau_{\text{invEmp}}[\omega, d, b, n1D]^{-1}}$ ;
tGen[ω_, α_] :=  $\left(1 + \frac{\alpha \omega}{\omega D}\right)^{-1}$ ;

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(*******)
(****** Fuctions for calculating  $\kappa_L$  from semi-empirical expression ******)
(*******)

(****** calculate kmax from volume of PUC, vPUC ******)
k0[vPUC_] :=  $\left(6 \frac{\pi^2}{vPUC}\right)^{1/3}$ ;

(****** BvK dispersion for transport modeling ******)
 $\omega_0[vS_, vPUC_] := \frac{2}{\pi} vS \left(6 \frac{\pi^2}{vPUC}\right)^{1/3}$ ;

 $\omega_{kBvK}[k_, \omega_{max}_, k_{max}_] := \omega_{max} \sin\left[\frac{\pi k}{2 k_{max}}\right]$ ;

 $k_{\omega BvK}[\omega_, \omega_{max}_, k_{max}_] := \frac{2 k_{max}}{\pi} \text{ArcSin}\left[\frac{\omega}{\omega_{max}}\right]$ 

(*k as a function of  $\omega$  in BvK*);
vgBvK[k_,  $\omega_0$ _, k0_] :=  $\frac{\pi \omega_0}{2 k_0} \cos\left[\frac{k \pi}{2 k_0}\right]$ ;

(****** Phonon-phonon scattering function. ******)
 $\tau_{ppModel}[\omega_, T_, B1_, B2_] := (B1 \omega^2 T \text{Exp}[-B2/T])^{-1}$ 
(****** Point defect scattering function. ******)
 $\tau_{PD}[\omega_, DPD_] := (DPD \omega^4)^{-1}$ ;

(******  $\kappa_L$  functions ******)

 $Cs[\omega_, kfunc_, vgfunc_, T_] := \frac{3 \hbar^2}{2 \pi^2 k_B T^2} \frac{\omega^2 kfunc^2 \text{Exp}\left[\frac{\hbar \omega}{k_B T}\right]}{vgfunc \left(\text{Exp}\left[\frac{\hbar \omega}{k_B T}\right] - 1\right)^2}$ ;

 $\kappa_L[T_, \taufunc_, vgfunc_, kfunc_, intllimits_] :=$ 
 $\frac{1}{3} N \text{Integrate}[Cs[\omega, kfunc, vgfunc, T] vgfunc^2 \taufunc, intlimits];$ 

 $\kappa_L[\omega_, T_, \taufunc_, vgfunc_, kfunc_] := \frac{1}{3} Cs[\omega, kfunc, vgfunc, T] vgfunc^2 \taufunc;$ 

(*******)
(****** Misc. Functions ******)
(*******)

(****** Readies data for plotting ******)
 $\tau_{GBExtract}[\tau_{GBList}_, n_] :=$ 
 $\text{Table}\left[\{\tau_{GBList}[[n, 3, i, 1]] vs/\omega D, \tau_{GBList}[[n, 3, i, 2]] * 10^9\},\right.$ 
 $\left.\{i, 1, \text{Length}[\tau_{GBList}[[n, 3]]]\}\right];$ 
 $\tau_{GBExtract}[\tau_{GBList}_, n_] := \text{Table}\left[\{\tau_{GBList}[[n, 3, i, 1]] vs/\omega D,$ 
 $\left(\tau_{GBList}[[n, 3, i, 2]] * 10^9\right)^{-1}\}, \{i, 1, \text{Length}[\tau_{GBList}[[n, 3]]]\}\right];$ 

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tGBExtract[τGBList_, n_] := Table[{τGBList[[n, 3, i, 1]] vs / ωD,
  
$$\frac{4 n1D \text{ vs } \tau GBList[[n, 3, i, 2]]}{3 + 4 n1D \text{ vs } \tau GBList[[n, 3, i, 2]]}$$
, {i, 1, Length[τGBList[[n, 3]]]}];
```

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(*##### Power law reference lines #####*)
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T2[norm_, Trange_] := Table[{Tref,  $\frac{Tref^2}{Trange[[2]]^2}$  norm // N}, Trange];
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```
T3[norm_, Trange_] := Table[{Tref,  $\frac{Tref^3}{Trange[[2]]^3}$  norm // N}, Trange];
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(*##### Calculates the GB angle from the
  burgers vector and the dislocation spacing. #####*)
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θcalc[b_, s_] := 2 ArcTan[ $\left(\frac{b}{2 s}\right)$ ] (180. / π);
```