Thermal conductivity of porous polycrystalline PbTe

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The efficiency of thermoelectric materials is enhanced by lowering their thermal conductivity. At intermediate temperatures, PbTe is one of the most promising materials. Grain boundaries can lower its inherently low thermal conductivity by scattering and confining phonons. Using a phase-field model parametrized by molecular dynamics, we find that in the porous material the thermal conductivity of PbTe is reduced by up to 35% at low temperatures. We observe that a phase transition at a finite density of voids governs the kinetics of impeding grain growth by Zener pinning.

Thermoelectric materials produce electrical energy from a temperature difference. Their efficiency is proportional to the figure of merit, $ZT = S^2\sigma T/\kappa T$, where $S$ is the Seebeck coefficient, $\sigma$ is the electrical conductivity, $T$ is the temperature, and $\kappa$ is the total thermal conductivity, comprising an electronic and a lattice contribution. However, efficiencies are often too low to compete with other forms of power generation and strategies to enhance the efficiency are crucial. The lattice thermal conductivity is the only quantity in $ZT$ that can be tuned independently, offering an avenue to improved efficiency.

PbTe is a leading thermoelectric material at intermediate temperatures, largely thanks to its low lattice thermal conductivity. The latter can be lowered by up to 35% at low temperatures. We observe that a phase transition at a finite density of voids governs the kinetics of impeding grain growth by Zener pinning.

In this Letter we implement a phase-field model to study the stability of small grains. We observe that voids are effective pinning particles that can stop grain growth in PbTe and find that the thermal conductivity of the porous material can be reduced by up to 35%.

The phase-field model is a framework to describe grain growth at the mesoscale, beyond the reach of molecular dynamics (MD). We consider the equations of motion for the concentration of Schottky defects, $c_v$, and for order parameters, $\eta_\alpha$, describing $N$ grain orientations under the constraint $\sum_\alpha^N \eta_\alpha = 1$:

$$\frac{\partial c_v}{\partial t} = \nabla \left( M \nabla \left( \frac{\partial f_{\text{local}}}{\partial c_v} - \kappa_v \nabla^2 c_v \right) \right) - s_v^{\text{GB}}(c_v - c_v^0) \left( 1 - \sum_\alpha \eta_\alpha^2 \right) - s_v^{\text{G}}(c_v - c_v^0) \left( \sum_\alpha \eta_\alpha^2 \right) + \zeta_c(T),$$

$$\frac{\partial \eta_\alpha}{\partial t} = - \frac{L}{V_m} \left( \frac{\partial f_{\text{local}}}{\partial \eta_\alpha} - \gamma \nabla^2 \eta_\alpha \right).$$

In Eqs. (1)-(2), $M$ is vacancy mobility, $L$ interface mobility, $V_m$ molar volume, $f_{\text{local}}$ local free energy, $\kappa_v$ and $\gamma$ are gradient energy coefficients, and $\zeta_c(T)$ represents Gaussian noise. The equations are coupled through the second and third terms in Eq. (1). The former accounts for annihilation of vacancies at the grain boundary, with rate $s_v^{\text{GB}}$: the vacancy concentration tries to reach its thermodynamic equilibrium value, $c_v^0$, with grain boundaries annihilating the excess. The third term in Eq. (1) accounts for the production of vacancies inside the grain, with rate $s_v^{\text{G}}$. $c_v^0$ is the vacancy concentration that the material tends to adopt far from grain boundaries due to external sources, such as radiation.

Grain boundary energies and mobilities, and vacancy diffusion coefficients were calculated via MD using the force field of Ref. [12]. Vacancy mobility is characterized through the diffusion coefficient, $D_v$, calculated from the mean square displacement in MD, $M = D_v c_v / RT$. Interface mobility and the gradient coefficient for order parameters, which are related to the grain boundary mobility, $m$, and energy, $\sigma$, respectively, were obtained from MD through $L = \pi^2 m / 48 \Delta x$ and $\gamma = 48 \sigma \Delta x V_m / \pi^2$, where $\Delta x$ is the grid spacing. The grain boundary energy was calculated from the excess free energy due to grain boundaries. Grain boundary mobility was obtained from the velocity of a moving grain boundary when an artificial potential was applied to an adjacent grain to increase the free energy on one side of the interface [13]. The grain boundary energy and mobility show anisotropic behaviour as predicted by Dislocation Theory [14–16].
We analyzed grain growth at different void fractions, $d_v$, at 500 K with constant void radius, $r_v = 45$ nm, at the steady state regime where Eq. 4 is valid. The void fraction is defined as the percentage of grid points occupied by voids and the vacancy concentration in bulk is $c_v = 10^{-4}$. Lines correspond to Eq. 4. Inset: the exponent $n$ (Eq. 4) depends on $d_v$ and shows a transition from the regime where voids are sufficiently separated ($\lesssim 2\%$) to a regime where the spacing between voids becomes comparable to grain size ($\gtrsim 5\%$). The dependence of $n$ on $d_v$ is the same at 300 (blue squares) and 500 K (red dots).

We analyzed grain growth at different void fractions, $d_v$, in polycrystalline PbTe using phase-field simulations at 500 K and 300 K. We found that $n$ is 1.94 in void-free polycrystalline PbTe ($d_v = 0$), with $k$ following Arrhenius law in temperature [20]. Grain size follows Hillert’s distribution [21] in the steady-state regime. At bulk vacancy concentrations above the equilibrium concentration, $n$ remains constant and grain growth does not stop. Voids are effective pinning particles for grain wall motion so we investigate if they can stabilize polycrystalline PbTe. We observe that the exponent $n$ in Eq. 4 depends on void fraction, as can be seen in Fig. 1 for a fixed void size of 45 nm. For void fractions $d_v = 0 - 1.2\%$, grain growth does not differ from the void-free system and $n = 1.94$ is the best fit in Eq. 4. However, $n$ increases with void fraction for $2\% < d_v < 5\%$, asymptotically reaching $n \to 3$ for the largest $d_v$; we found $n = 2.77$ for $d_v = 8\%$. The same dependence is found for 300 K. Furthermore, as the exponent changes the mean grain size distribution shifts from Hillert’s distribution when $n \approx 2$ to a log-normal distribution at $n \approx 3$. Since Hillert’s distribution was derived assuming that it converges to a self-similar fixed point, this departure signals a characteristic size in the higher $d_v$ regime. The power-law growth in time, observed upon scale-invariant phase-field simulations, can be associated with the universal exponent $\nu = 1/n$. Therefore, Fig. 1 reveals a change in critical exponent from $\nu = 1/2$, characteristic of a Gaussian fixed point, towards an interacting theory with $\nu \approx 1/3$. This implies a finite void-void interaction in the high-$d_v$ fixed point. By Widom-Rushbrooke scaling relations we expect all other critical exponents to be modified and other measurable quantities, e.g. thermal conductivity, to be affected. Most importantly, a change in $n$ highlights that the kinetics of impeding grain growth by Zener pinning is a collective phenomenon governed by a phase transition. The existence of a tentative critical point suggests that this mechanism may be at play in more general situations, and sheds light into the question of why polycrystals are so abundant in nature [17].

The change of exponent in Fig. 1 is related to a new fixed point where a characteristic length scale emerges.

\[ f_{\text{local}} = f(c_v, T) + \sum_{\alpha \neq \beta} W_{\alpha \beta}r_{\alpha \beta}, \]

with

\[ f(c_v, T) = h_v c_v + f_2 c_v^2 + f_3 c_v^3 + f_4 c_v^4 + \frac{RT}{c_v} \ln c_v + \frac{1}{c_v} \ln (1 - c_v), \]

where $W_{\alpha \beta} = 2\sigma V_m/3\Delta x$ is the excess free energy between grains $\alpha$ and $\beta$, $h_v$ is the formation enthalpy and $f_2, f_3, f_4$ are mixing terms such that a void-free system and a system with voids are equally stable. Voids are defined as regions with $c_v = 0.999$ and they hinder grain boundary motion. The gradient coefficient for vacancies is linked to the mixing energy: $c_v = f_2 l_v^2/2$ where $l_v$ is the typical distance between vacancies.

Curvature-driven grain growth due to the excess free energy at the grain boundary is studied with Eqs. 1–4. The underlying assumption of phase-field models is scale invariance and so growth is described by a general scaling equation for the mean grain size, $\langle r(t) \rangle$ [18]:

\[ \frac{d\langle r(t) \rangle}{dt} = \frac{k}{n\langle r(t) \rangle^{n-1}}, \]

where $k$ is the kinetic coefficient and depends on the material and temperature. The exponent $n$ depends on the material and is around 2 in pure materials [18–19]. According to this equation, the mean grain size grows until the single crystal is reached:

\[ \langle r(t) \rangle^n - \langle r(t_0) \rangle^n = k(t - t_0). \]

FIG. 1. Evolution of the mean grain size over time at different void fractions, $d_v$, at 500 K with constant void radius, $r_v = 45$ nm, at the steady state regime where Eq. 4 is valid. The void fraction is defined as the percentage of grid points occupied by voids and the vacancy concentration in bulk is $c_v = 10^{-4}$. Lines correspond to Eq. 4. Inset: the exponent $n$ (Eq. 4) depends on $d_v$ and shows a transition from the regime where voids are sufficiently separated ($\lesssim 2\%$) to a regime where the spacing between voids becomes comparable to grain size ($\gtrsim 5\%$). The dependence of $n$ on $d_v$ is the same at 300 (blue squares) and 500 K (red dots).

The numerical values of the coefficients in the phase-field model for PbTe are: $D_v = 1.14 \cdot 10^{-7}$ cm$^2$/s, $h_v = 1.21$ eV, $f_2 = 0.07$ eV, $f_3 = -3.47$ eV, $f_4 = 2.19$ eV, $\sigma_0 = 2410$ mJ/m$^2$, $m = 0.8$ m s$^{-1}$ MPa$^{-1}$. 

$\nu = 1/n$. Therefore, Fig. 1 reveals a change in critical exponent from $\nu = 1/2$, characteristic of a Gaussian fixed point, towards an interacting theory with $\nu \approx 1/3$. This implies a finite void-void interaction in the high-$d_v$ fixed point. By Widom-Rushbrooke scaling relations we expect all other critical exponents to be modified and other measurable quantities, e.g. thermal conductivity, to be affected. Most importantly, a change in $n$ highlights that the kinetics of impeding grain growth by Zener pinning is a collective phenomenon governed by a phase transition. The existence of a tentative critical point suggests that this mechanism may be at play in more general situations, and sheds light into the question of why polycrystals are so abundant in nature [17].

The change of exponent in Fig. 1 is related to a new fixed point where a characteristic length scale emerges.
We now investigate how voids can stop grain growth in the saturated system, in which the curvature of the grain boundaries is affected by voids, inter-void distance is small, and void size and the local grain boundary radius of curvature are comparable \cite{22,23}. We consider the equation of motion for grain growth. If \( p_Z \) is the reduced pinning pressure exerted by Zener particles, in the presence of voids, Eq. \( 6 \) becomes \cite{24}

\[
\frac{d(r(t))}{dt} = k \left( \frac{1}{2r(t)} - p_Z \right). \tag{7}
\]

The first term corresponds to Eq. \( 3 \) with \( n = 2 \). The Zener pressure reads

\[
p_Z = \frac{3d_v \sigma_{Zv}}{2v}, \tag{8}
\]

with \( r_v \) void radius. The exponent \( a(d_v) \) changes from \( a(d_v) = 1 \) at low \( d_v \) (where voids act as independent scattering centres) to \( a(d_v) = 1/3 \) at high \( d_v \) (where voids act collectively). Replacing \( p_Z \) into Eq. \( 7 \) grain growth slows down until the RHS vanishes. The grain radius \( R_Z \) in the saturation limit is

\[
R_Z = \frac{\alpha r_v}{3d_v \sigma_{Zv}}, \tag{9}
\]

where \( \alpha \) is a constant that accounts for deviations in experiments.

We analyzed grain growth under high void fractions in PbTe for different void sizes using phase-field simulations. According to Fig. \( 2 \) grain growth occurs following Eq. \( 7 \) (dashed red line) until the limiting \( R_Z \) is reached. Limiting sizes of \( R_Z \approx 180 \) and \( R_Z \approx 155 \) nm are obtained for void radii \( r_v = 32 \) and \( r_v = 26 \) nm, respectively. Fig. \( 2 \) also shows that the limiting grain size is roughly independent of temperature, in agreement with Eq. \( 9 \).

Small grain sizes are associated with lower thermal conductivities and higher efficiencies. According to Eq. \( 9 \), small grain sizes would be effectively pinned by sufficiently small voids. However, small voids are not stable and dissolve at finite temperatures. According to classical nucleation theory (CNT), if a void is smaller than a critical size, it shrinks and disappears, while it keeps growing if it is larger. This critical size depends on temperature and vacancy concentration. An approximation can be obtained from CNT, in which the free energy change to form a spherical void is given by \cite{25}:

\[
\Delta G^{vd}_V = 4\pi r_v^2 \sigma_v - \frac{4\pi r_v^3}{32} k_B T \ln \left( \frac{C_V}{C_{V}^{eq}} \right), \tag{10}
\]

where \( \sigma_v \) is the void-solid interfacial energy, \( \Omega \) is the atomic volume, \( C_V \) is the total vacancy concentration and \( C_{V}^{eq} \) is the equilibrium value at temperature \( T \). \( C_V \) includes vacancies in bulk and vacancies forming voids. If the simulation box is large enough, \( C_V \) can be approximated by the vacancy concentration in bulk. In Eq. \( 10 \),

![FIG. 2. Evolution of the mean grain size over time at constant void fraction, \( d_v = 8 \% \), at different void radii at 500, 700 and 900 K in the steady-state regime. The vacancy concentration in bulk is \( c_v = 10^{-4} \). All curves would converge at sufficiently long times. Dashed brown line corresponds to Eq. \( 7 \) where \( k \) and \( p_Z \) are fitting parameters.](image-url)

the first term corresponds to the increase in energy due to the formation of the void-solid interface and the second term is related to the free-energy change to relocate vacancies inside a void. The critical void size is reached when \( d(\Delta G_V)/dr_v = 0 \):

\[
r_v^{cr} = \frac{2\Omega \sigma_v}{k_B T \ln \left( \frac{C_V}{C_{V}^{eq}} \right)}. \tag{11}
\]

To determine the critical void size we solved numerically Eq. \( 1 \) with a void in the center of the simulation box. Simulations were run at different temperatures (300 – 900 K) and for \( c_v = 0.1, 0.05, 0.01 \). We observed that voids are stable at intermediate temperatures but not at high temperatures because high vacancy mobilities promote diffusion and destabilize voids. At low temperatures the mobility is low and vacancies take longer to find each other. Instead, a higher density of small vacancy clusters is observed. On the other hand, if the number of vacancies is small, void formation is more difficult and their cutoff radius is larger. Assuming that the simulation box is large enough, we first determined critical void sizes by analyzing the stability limit, and then from Eq. \( 11 \) obtained \( \sigma_v \). The time required to equilibrate voids under small vacancy concentrations can be hours to days, which is not accessible to simulation. Therefore, we determined the critical void size for higher concentrations and extrapolated, using Eq. \( 11 \), to \( c_v^{bulk} = 10^{-4} \), which was the concentration used in the study of Zener pinning. At 500 K, the critical void size is around 5 nm.
interaction through elastic energy that should scale like \( \gamma_r r_v^4 \). An analysis of entropic effects leads to the same scaling. Therefore, both effects are accounted for by an additional phenomenological term in the free energy:

\[
\Delta G_{V} = 2 \cdot 4 \pi r_v^2 \sigma_v - 2 \cdot 4 \pi r_v^3 k_B T \ln \left( \frac{C_V}{C_V^0} \right) + \gamma_r r_v^4,
\]

with \( \gamma_v \) and \( s \) constants. The first two terms are the same as in Eq. (10). Terms like the last one in Eq. (12) have been proposed for other systems exhibiting nucleation of secondary particles \cite{20, 23}. They allow for metastable nuclei, as found in experiments. Here we use \( s = 4 \), which best reproduces the entropy. If \( \gamma_v \) is chosen such that a second minimum with \( \Delta G_{V} = 0 \) exists, then systems containing no voids and systems containing voids of metastable size are equally favourable. Experimental studies confirm the presence of such metastable void sizes in actual PbTe samples \cite{8}.

The study of Eq. (12) at different temperatures is shown in Fig. 3 for a bulk vacancy concentration \( c_v = 10^{-4} \). These metastable sizes correspond to \( \Delta G_{V} = 0 \). A strong dependence of the metastable size on temperature is observed. Inserting it into Eq. (9) leads to our main result: how the typical size of the crystal grain depends on the temperature, \( T_{CR} \), in which the sample has been coarsened (inset of Fig. 3).

To obtain a soluble model we assume that \( r_v \) and \( d_v \) retain their values at \( T_{CR} \) and that the majority of voids are at grain boundaries. From our phase-field model we obtain not only \( r(t) \), but also the distribution of grain sizes, \( \omega(d_i/d_v; T_{CR}) \), which follows a log-normal law. This enables us to compute the effective lattice thermal conductivity, \( \kappa_{eff} \), of porous polycrystalline PbTe.

\[\text{FIG. 3. Free energy of a system containing two voids of radius } r_v \text{ at different temperatures according to Eq. (12). Inset: evolution of the metastable void size with temperature.}\]

Assuming phonon confinement and averaging over grain sizes, the effective \( \kappa_{eff} \) of the ensemble is given by

\[
\kappa_{eff}(T; \chi_v; T_{CR})^{-1} = \sum_i \omega \left( \frac{d_i}{d_v}; T_{CR} \right) \left[ \frac{1}{d_i + \delta_{gb}(T)} \kappa_b(T) + \frac{1}{d_i} \right],
\]

where \( \kappa_b(T) \) is the thermal conductivity of the pure material, \( d \) is grain diameter, \( \langle d \rangle (T_{CR}) \) is mean grain size, \( \delta_{gb} \) is grain boundary width, \( R_K \) is the Kapitza resistance, and \( \omega \) is the log-normal weight for grain size \( d_i \). \( \langle d \rangle (T_{CR}) \) has memory as it depends on the thermal history of the sample. Given the metastable void size, \( r_v \), from Fig. 3 at temperature \( T \), the limiting grain diameter can be calculated by Eq. (10), \( d = 2 R_Z \). Above we consider the general case where the grain size distribution is determined by some \( T_{CR} \) not necessarily equal to the thermodynamic temperature in a thermoelectric device.

The grain boundary width \( \delta_{gb} \) and Kapitza resistance \( R_K \) were studied using MD by the direct method with voids at the grain boundary \cite{12, 29}. \( \delta_{gb} \) increases with temperature as \( \delta_{gb} = \delta_0 (T_m - T)^{-1/2} \), where \( T_m = 924^\circ C \) is the melting temperature \cite{30} and \( \delta_0 = 289 \text{ nm K}^{1/2} \) is a fitting parameter for data collected from Ref. \cite{12}. \( R_K \) is inversely proportional to the heat capacity and is constant above the Debye temperature \cite{31}. MD simulations show that \( R_K \) in the presence of voids at the grain boundary depends on void coverage, \( \chi_v \), as \( R_K = R_K^0 (1 - \chi_v)^{-1} \) where \( R_K^0 \) refers to the void-free case.

We plot the result of Eq. (13) in Fig. 4 at \( d_v = 8\% \). We show a family of curves \( \kappa_{eff}(T) \) for different thermal...
coarsening temperatures $T_{CR}$. This provides information about thermal conductivity necessary to design thermoelectric devices. A comparison between curves shows the effect of nanostructuring. The lattice thermal conductivity can be reduced nearly in half by grain boundaries pinned by voids. $\kappa_{eff}(T)$ increases slower than in bulk, so the differences are largest at the lowest temperatures.

In conclusion, by combining MD simulations with a phase-field model, we determine the lattice thermal conductivity of porous polycrystalline PbTe. It can be reduced by 35% by anisotropic grain boundaries pinned by voids. The reduction in conductivity is larger when the sample has not first been heated at higher temperatures, thus questioning the usefulness of nanostructuring for thermoelectric efficiency at high temperatures. Furthermore, although the increase in void content reduces lattice conductivity, high void fractions can result in loss of plasticity and other undesirable effects [32, 33].

This study sheds light into the general question of the metastability of polycrystalline samples against the single crystal. We have shown that grain growth is arrested by voids pinned at grain boundaries, with the size of voids and grains being determined by vacancy concentration and temperature. A similar phenomenon may be induced by impurities, instead of or in addition to voids [24].

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