Lattice thermal conductivities (LTC) for a subset of polymer crystals from the Polymer Genome Library were investigated to explore high LTC polymer systems. We employed a first-principles approach to evaluating phonon lifetimes within the third-order perturbation theory combined with density functional theory, and then solved the linearized Boltzmann transport equation with single-mode relaxation time approximated by the computed lifetime. Typical high LTC polymer systems, polyethylene (PE) crystal and fiber, were benchmarked, which is reasonably consistent with previous references, validating our approach. We then applied it to not only typical polymer crystals, but also some selected ones having structural similarities to PE. Among the latter crystals, we discovered that beta phase of Poly(vinylidene fluoride) (PVF-β) crystal has higher LTC than PE at low temperature. Our detailed mode analysis revealed that the phonon lifetime of PVF-β is more locally distributed around lower frequency modes and four-times larger than that of PE. It was also found from a simple data analysis that the LTC relatively correlates with curvature of energy-volume plot. The curvature would be used as a descriptor for further exploration of high LTC polymer crystals by means of a data-driven approach beyond human-based one.

I. INTRODUCTION

High thermal conductivity (κ) realized by polymers attracts attentions mainly because it can reduce the weight of mobile devices with electrically insulating properties, not like metallic materials. [1] Though the conductivities of polymers are usually lower than those of metals, [2] they can be enhanced by making the ordering of the molecular’s orientations (crystallinity). It has been reported for polyethylene (PE) that the conductivity along the elongating direction of the molecules gets to be comparable to those of metals by increasing crystallinity. [3] High crystallinity is, however, known to be difficult to be achieved experimentally, leading lack of the contents of the database usable for the Materials Informatics (MI) [5], searching for such polymers with high thermal conductivities. Theoretical estimations of such conductivities would assist to provide data over a lot of polymers to screen out the synthesis targets.

Preceding theoretical works include several model analyses [6, 7] as well as those by empirical molecular dynamics. [8, 9] The predictions were, however, found to be seriously depending on the choice of empirical force fields [10]. Ab initio approaches [11, 12] are expected to exclude such ambiguity, and are getting to be feasible realized by the implementations of phonon analysis especially those beyond the harmonic approximation [13]. Such approaches have been applied to inorganic crystalline materials such as semiconductors, [13, 15] achieving the predictions fairly coinciding with experiments over the range, 1-10^5 W/mK. [13] For polymers, however, there has been little applications in spite of the industrial demands as described above, though there is a preceding work [10] applying the framework to evaluate the conductivity of PE as a typical prototype.

In this study, we evaluated the conductivity over such typical polymers for the exhaustive search for high κ, including PE, polyphenylene sulfide (PPS) and polyethylene terephthalate (PET). Those initial structures can be taken from the database of PolymerGenome project [16-18]. We began with the calibrating discussions on PE, verifying our implementations to check quantitative consistency with available experimental κ of crystalline and fiber PE. [4, 19] Confirming the fairly well coincidence on PE, we applied the framework to a couple of polymers with typical structures being different from each other in terms of the number of benzene rings. Finding the PE structure (zero benzene ring) being the best to achieve high κ, we concentrated on the polymer structure without ring. We took MI-like screening based on the cheaper calculations of bulk modulus to extract candidates for further evaluations of κ. (The candidates are listed in Table I.) We finally found that PVDF-beta polymer could achieve higher κ than that of PE below around 80 K.

II. MODEL AND METHODS

Heat carriers to contribute to κ include charged particles [20, 21], diffusing atoms [22], magnons [23], and phonons [20, 21, 23, 24]. The first three ingredients are excluded because the polymers considered here are insulating without any defects and non-magnetic. Only the phonons are

Ab initio search of polymer crystals with high thermal conductivity

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to be formulated for $\kappa$ of polymers, which is the Boltzmann equation applied to phonon flow.

The relaxation-time approximation \[13, 24\] of the Boltzmann equation leads to

$$\kappa = \frac{1}{NV_0} \sum_{\lambda} C_{\lambda} v_{\lambda}^2 \rho_{\lambda}^{\text{SMRT}}.$$  \hspace{1cm} (1)

Here, $N$ is the number of unitcells used for the simulation and $V_0$ is the volume of a unitcell. $C_{\lambda}$, $v_{\lambda}$, and $\tau_{\lambda}$ are the specific heat at constant volume, group velocity, and relaxation time of a phonon mode indexed by $\lambda$ (the upper index of $\tau_{\lambda}^{\text{SMRT}}$ stands for ‘Single-Mode Relaxation-Time’).

Relaxation time, $\tau$, appearing in Eq. (1) is given by the inverse of the imaginary part of the self-energy of the phonon,

$$\Gamma_{\lambda} = \frac{18\pi}{\hbar^2} \sum_{\lambda', \lambda''} |\Phi_{-\lambda', \lambda''}|^2 \left\{ \left[ (n_{\lambda'} + n_{\lambda''} + 1) \delta(\omega - \omega_{\lambda'} - \omega_{\lambda''}) + (n_{\lambda'} - n_{\lambda''}) \left[ \delta(\omega + \omega_{\lambda'} - \omega_{\lambda''}) - \delta(\omega - \omega_{\lambda'} + \omega_{\lambda''}) \right] \right\},$$

as $\tau_{\lambda} = 1/2\Gamma_{\lambda} (\omega_{\lambda}).$ \[25, 26\] The analytic form of $\Gamma_{\lambda}$ is given by perturbation theories with respect to the electron-phonon interactions \[25, 26\]. To calculate $\Gamma_{\lambda}$ quantitatively, one requires to evaluate the lattice anharmonic contribution to the energy \[13\], which is feasible by ab initio methods. The anharmonic contribution \[27\] is essential to get finite conductivity because the harmonic approximation leads to the superposition of phonon motions, getting infinite conductivity without any collisions of phonons. A coefficient $b$ in an expansion of potential $U$ by an inter-atomic distance $u$:

$$U (u_0 + \tilde{u}) = U (u_0) + a\tilde{u}^2 + b\tilde{u}^3 + \cdots,$$ \hspace{1cm} (3)

is actually appearing in $\Gamma_{\lambda}$ because the term gives the scattering processes of phonon operators in the second quantization formalism when one substitute the operator representations of displacement, $u$.

The coefficients, $a$, $b$ are obtained by density functional theory (DFT): We used VASP \[28, 31\] and employed projector augmented waves (PAW) method. \[32\] We chose vdW-DF2 functional \[33\] in order to describe van der Waals forces well. We used phono3py package \[13\] to set up the calculations and compile up the ab initio results to obtain specific heat capacity, phonon lifetime, and thermal conductivity. The schematic diagram to obtain heat capacity is described in Fig. \[1\].

III. RESULTS AND DISCUSSION

A. Calibrations on Polyethylene

For PE, there are a lot of reference values of $\kappa$ available from both experiments \[4, 19, 34-41\] and ab initio calculations. \[10, 42\] Thus, we will check the reliability of our framework for the system as an example. The references include both those of ‘fibers’ and ‘crystals’ (the reason why we put apostrophe on it is explained below): A polymer’s crystal means the ordered stacking of 1-dim. fibers, that is quite difficult to be synthesized experimentally. Practical samples are actually the mixtures including disordered 1-dim. fibers as well as fragments of crystals in a polycrystalline manner. The experimental reference values of ‘1-dim. fibers’ mean the extrapolation of the observed values towards the limit by increasing the order of orientations of fibers. For PE, such extrapolations are performed by controlling the volume fraction. \[4\] Values of ‘crystals’ are obtained by some model formulae such as that by Halpin-Tsai.\[43\] By putting values observed for the mixture of fibers as well those of amorphous, the formulae give the estimations for crystals. \[44, 45\]

Our estimation of the specific heat at constant volume of PE gets $C_v = 1.653$ [Jg$^{-1}$K$^{-1}$] at $T = 310.15$ [K] obtained by phonopy package \[46\], being in fairly agreement with the experimental value at the same temperature, 1.479 [Jg$^{-1}$K$^{-1}$] \[47\]. The coincidence would ensure that our framework works quantitatively well at least up to the extent of the harmonic approximation. Fig. \[2\] shows the comparisons of thermal conductivities ($\kappa(T)$) of our estimations and preceding theoretical/experimental values for ‘crystals’ and fibers. Quantitative coincidence seem fairly well, especially reproducing the difference by an order between crystal and fiber. Though that is consistent within the theoretical works between ours and preceding works \[10\], the temperature dependences seem to behave in quite different way when we compare with experimental ones. To discuss the difference, we would like to concentrate only on fiber cases. For ‘crystals’, the analysis gets to be too complicated because the consequences come from behind the empirical model formulae as we explained above, inherently including many ambiguities (sample qualities, model approximations etc). Furthermore on crystals, the

FIG. 1. This is the workflow to evaluate thermal conductivity based on ab initio calculations. The harmonic and anharmonic coefficients $a$, $b$ are obtained by ab initio calculations. The thermal conductivity is evaluated from the coefficients by solving a Boltzmann equation under relaxation-time approximation \[13\].

\[
E(u) = au^2 + bu^3 + \cdots
\]
consistency within theoretical studies would support the justification of the present work.

FIG. 2. [pe_chain] (a:10, b:4) Thermal conductivities of the polyethylene in the 3-dim. crystal and the 1-dim. chain, as a function of the temperature, compared with experiments and other preceding works. The present study fairly reproduces the quantitative difference by an order between those in crystals and fibres observed experimentally. Though the temperature dependence differs from the experimental 'crystal' case significantly, it fairly coincides with the preceding ab initio study. We note that the experimental data provided as 'crystal' is not taken from true crystals, but estimated by extrapolations from the data of fibre data.

Fig. 3 shows the detailed comparison of the temperature dependence, $\kappa(T)$, between our simulation (red) and the experiment (blue)[4]. The difference between experiments and the simulation would be attributed to the dimensionality. While the simulation treats an isolated 1-dim. fiber, the practical experiments treat the bunch of fibers which includes inter-fiber contributions. Since the contribution is also included in the crystal case, the comparison between the fiber and the crystal within our simulation would help to understand why the $T$-dependence between red and blue plots in Fig. 3 differs each other. In Eq. (1), we can decompose $\kappa(T)$ into the mode contributions under the summation over the mode index, $\lambda = (b, q)$, where $b$ and $q$ denote the indices for band and wave vector, respectively. Since in the simulation there is no $T$-dependence of $v'_1$ (group velocity), the dependence of $\kappa(T)$ is determined by those of $C(T)$ and $\tau(T)$. Fig. 5 and 4 show the distributions of the mode contributions for the relaxation time and the specific heat, respectively, shown as the intensity on the $(b, q)$-plane. The brighter region corresponds to the 'active range', where the larger contributions distribute. We can find in Fig. 5 that the active range gets to be largely restricted for the fiber case when compared to crystal case. This difference would be attributed to the difference in the $T$-dependences on Fig. 3. When we force the modes activated by hand artificially so that their distributions for fibers can get to the same as those of crystal, the $T$-dependence gets to be closer to the experimental case in lower temperature range, as shown by the black plots in Fig. 5. This would support that the $T$-dependence is dominated by the dimensionality, since the difference of the distributions for fiber and crystal cases reflects their difference in the dimensionality, namely whether the inter-fiber transportation exists or not.

It is interesting that $\kappa(T)$ of PE fiber looks changing in proportion to $\sim T^3$, although the sample size effect [19, 48] does not exist in the simulation. This fact indicates that the change ratio of $\tau(T)$ for temperature is much smaller than that of $C(T)$. This apparently contradicts that phonon life time diverges towards infinity when temperature decreasing in general. However, our system is a fiber and the phonons could be scattered on the wall of fiber. This could restrict the divergence of $\tau(T)$ and let $\kappa(T)$ follow $\sim T^3$.

FIG. 3. [fig.results.pe_chain.pe_chain.1] (b:4) Temperature dependences of the thermal conductivity, $\kappa(T)$, of polyethylene fibers. The blue plot represents experimental data, while the red does our theoretical results for an isolated 1-dim. fiber. The black plot corresponds to the case with the artificially modified distribution of the mode contributions (see text).

FIG. 4. These graphs show $C_v$ of each phonon mode designated by indices of $q$-point and ones of phonon band, for PE 3-dim. crystal (upper) and 1-dim. fiber (lower) under different temperatures: $T$=50, 170, 300 K.
These graphs show relaxation-time of each phonon mode designated by indices of q-point and ones of phonon band, for PE 3-dim. crystal (upper) and 1-dim. fiber (lower) under different temperatures: T=50, 170, 300 K.

The magnitude relationship between experiments (blue) and simulations (red) in Fig. 3 turns from 'exp.> sim.' to 'exp.< sim.' and again to 'exp.> sim.' as T increases. The more active range of τ(T) for crystal (a model for experiments with larger dimensionality), as explained above, would be the plausible reason at the lower T range. In the 1-dim. fiber case, the modes within the narrow active range have remarkably large relaxation time while in the crystal case the wider range consists of those with moderately large relaxation time, just like a 'conservation rule', as we found by carefully inspections of τ for both cases. C(b, q; T), shown in Fig. 4, plays as the 'mask' put over the distribution of τ(b, q; T), by forming a product to give κ. The mask gets to have the weight around the active range of τ by increasing C(T) at the mode around there, especially around T ∼ 170 K. This leads to the overtaking to get 'exp.< sim.' at the middle range of T. Generally speaking, κ(T) should decay at the high temperature range due to the increasing of the phonon scattering. Simulation results (red) surely follows this consequence but the experimental ones (blue) does not meanwhile, which leads to 'exp.> sim' again. The difference would explained by the dimensionality: There are more number of phonon paths in the experimental situation than in the simulation, owing to the thermal transport among fibers. The extra paths could help for phonons to avoid colliding each other and suppress phonon scattering.

### B. Screening for high κ polymers

Fig. 7 compares the calculated κ(T) for the chosen polymers. The filled points corresponds to the results for the typical polymers, PE, PPS, and PET, where PE has much higher κ(T) than the others. This would be because only PE does not include benzene rings, which is why we intensively surveyed κ(T) of the six linear polymers. Among them, PVDF-beta and PVFP has comparatively high thermal conductivity. It is further surprising that the κ(T) of PVDF-beta is superior to that of PE below ~80 K. It is explained from the difference of the mappings of phonon relaxation time: Fig. 9 represents that the phonon modes having long relaxation time are concentrated in the low eigen energy region in the case of PVDF-beta crystal at 50 K. Conversely, the left upper figure of fig. 5 represents that such modes are distributed in a wide range of eigen energy in the case of PE crystal. Under low temperature, only phonon modes with low eigen energy have high C_v, so PVDF-beta crystal has higher thermal conductivity. On the other hand, when the temperature increases, the C_v of phonon modes with middle to high eigen energy get increased and PE crystal has higher thermal conductivity eventually.

Though we performed eventually the evaluations of κ for all the cases, it is quite expensive to perform it for the entire possible structures of polymers in general. It is therefore desirable to establish the way of the screening for the higher κ with cheaper computational costs. Since for κ the anharmonicity matters, the trend of the magnitude of it would be captured by the Gruneisen parameter, being a typical measure for the anharmonicity. The parameter relates to the bulk modulus, and hence the trend is expected to be captured by the quantity, for which the required computational cost gets to be saved a lot. Fig. 6 corresponds to the estimations of the bulk modulus, and we clearly see that the trend of the modulus, namely the curvatures of E(V) well correlates with that of κ given in Fig. 7 (the lower the modulus, the higher the κ, as expected from the relation (50)).

Fig. 6. The dependence of the ground state energies on the volume, E(V). The plots are given as a function of ϵ, where $V = (1 + \epsilon)^3 V_0$ with the equilibrium volume, $V_0$.

Fig. 8 proves that the modulus (curvature) would be a good descriptor for the κ for the polymers, achieving the correlation coefficient ~0.9045.
TABLE I. Our target polymers are listed in this table with their abbreviations.

| Name                         | Abbreviation |
|------------------------------|--------------|
| Poly(ethylene)               | PE           |
| Poly(phenylene sulfide)      | PPS          |
| Poly(ethylene) terephthalate | PET          |
| Poly(vinylidene fluoride)-delta | PVDF-delta  |
| Poly(vinylidene fluoride)-beta | PVDF-beta   |
| Poly-trifluoroethylene       | PTrFE        |
| Poly(tetrafluoroethylene-alt-ethylene) | ETFE      |
| Polycrylonitrile             | PAN          |
| Poly(vinyl fluoride)         | PVF          |

FIG. 7. This figure compares crystalline thermal conductivity of the selected polymers. The linear polymers without benzene rings tend to have higher thermal conductivity than PET and PPS. PVDF-beta and PVF have impressively high thermal conductivity comparable with PE.

FIG. 8. This figure maps thermal conductivity and bulk modulus \((\partial^2 E/\partial \varepsilon^2)^{-2}\) for crystals of the selected polymers (\(\varepsilon\) is defined in Fig. 9). A linear relationship is observed clearly between both quantities, where the fitting line is given by least-square method and its formula is \(y = 1.137 \times 10^7 x - 9.075\).

FIG. 9. This graph maps the relaxation time of each phonon mode for PVDF-beta crystal at 50 K. The horizontal axis represents the indices of \(q\)-point and the vertical axis does those of phonon band.

IV. CONCLUSION

Thermal conductivity of polymer crystals have almost not been studied because of the difficulty of synthesis \([4, 19]\). We investigated thermal conductivity for some polymer crystals by first principles calculations \([13]\). Our calculation successfully reproduced that PE crystal has higher thermal conductivity by one digit than its fiber \([4]\). On the other hand, the predicted temperature dependence of thermal conductivity of fibers is qualitatively different from the experimental ones \([4]\). This is because the thermal conduction among fibers are not excluded in the experiments unlike the simulations. According to the ab initio predictions for PE, PPS, and PET crystals, it is established that PE crystal has much higher thermal conductivity than the others. Therefore we surveyed thermal conductivities of the six polymer crystals similar to PE in addition, and we revealed that PVDF-beta and PVF crystals have comparatively high thermal conductivities with PE crystal. We have also found out an interesting law: The predicted thermal conductivities are clearly in proportion to the curvature of energy-volume curve. Since it is much cheaper to predict the latter value, this law would be useful to discovery a new polymer crystal having further high thermal conductivity.

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