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studies have demonstrated the computational costs associated with simulating 3-dimensional devices [19,22]. In one study [19], the simulation of a 3-dimensional toy device is far from steady-state but requires several hours using hundreds of CPU cores. Another simulation shows even larger computational costs [22]. Besides, many of these simulations rely on empirical models for the input material properties [17,19,25,26] and therefore cannot be used as a predictive tool for accurately simulating thermal transport.

In this study, we demonstrate a numerical method for nanoscale thermal simulations with the phonon BTE. The present method has the apply to simulation of many devices and materials [18,37]. For the band discretization, we first collect all phonon properties (including heat capacity , group velocity , and relaxation time from lattice dynamics calculations) and find the maximum mean free path Λ_{max} and minimum mean free path Λ_{min}. Then we divide the mean free path domain $[\Lambda_{min}, \Lambda_{max}]$ into several bins $[\Lambda_0, \dots, \Lambda\ ]$. For each bin, we obtain the representative phonon properties as

$$= \sum_{\Lambda=\Lambda_{n-1}}^{\Lambda_n} \Lambda$$

$$= \frac{\sum_{\Lambda=\Lambda_{n-1}}^{\Lambda_n} \Lambda \ \Lambda}{\sum_{\Lambda=\Lambda_{n-1}}^{\Lambda_n} \Lambda}$$

$$= \frac{\sum_{\Lambda=\Lambda_{n-1}}^{\Lambda_n} \Lambda \ \Lambda^2 \ \Lambda}{\sum_{\Lambda=\Lambda_{n-1}}^{\Lambda_n} \Lambda \ \Lambda} \qquad (\ )$$

The mode-level heat generation term depends on the type of heat generation. For example, the equilibrium mode-level heat generation term is proportional to the heat capacity of the phonon [29]. The mode-level heat generation originating from moving electrons through the electron-phonon interaction can be obtained from electron-phonon coupling calculations [38,39]. For each bin, we obtain the heat generation term for representative phonon the mode-level heat generation as

$$\dot{} = \sum_{\Lambda=\Lambda_{-1}}^{\Lambda} \dot{}_{\Lambda} \qquad (\ )$$

These formulas obey the additivity of energy, heat flux, and thermal conductivity. There are several integrations related to the phonon frequency and branch. The band discretization transforms the integration into summation:

$$\sum \int_{min}^{max} \frac{,\,,}{,} = \sum \sum \frac{,\,,}{,}$$

$$\sum \int_{min}^{max} \frac{,}{,} = \sum \sum \frac{,}{,}$$

$$\sum \int_{min}^{max} \ ,\ \ ,\,, = \sum \sum \ ,\ \ ,\,, \qquad (10)$$

There are also several integrations over the velocity directions. Directional discretization transforms those integrations into summations:

$$\int_{\Omega} \ ,\,, \ \Omega = \int_{min}^{max} \int_{min} \ ,\,, \ \sin$$

$$= \sum \sum \ ,\,,\,, \ \sin$$

$$\int_{\Omega} \ ,\,, \ \Omega = \int_{min}^{max} \int_{min} \ ,\,, \ \sin$$

$$= \sum \sum$$