Reliable force field potential for thermal transport in AlN

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Goal

Contribute to the atomistic understanding of the factors determining thermal transport in widely used semiconductors (e.g., AlN, GaN, AlGaN alloys). The method of choice to address this task is molecular dynamics, using so-called "force field potentials" (FFPs) for describing interatomic forces. As FFPs that correctly describe thermal transport are still scarce, here we propose an FFP capable of reliably describing the thermal transport properties of wurtzite AlN, an ideal substrate material in power and optoelectronics due to its large band gap, high thermal conductivity, low thermal expansion coefficient, and hardness.

Methodology

We used ab-initio data of the lattice and elastic constants, phonon band structure, and mode-Grüneisen parameters as reference data for fitting a Stillinger-Weber FFP for AlN.

Stillinger-Weber potential [1]

$$E = \sum_i \sum_{j>i} \Phi_2(r_{ij}) + \sum_i \sum_{j\neq i} \sum_{k>j} \Phi_3(r_{ij}, r_{ik}, \theta_{ijk})$$

$$\Phi_2(r_{ij}) = A_{ij}\epsilon_{ij}\left[B_{ij}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{p_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{q_{ij}}\right]\exp\left(\frac{\sigma_{ij}}{r_{ij}-a_{ij}\sigma_{ij}}\right)$$

$$\Phi_3(r_{ij}, r_{ik,ijk}) = \lambda_{ijk}\epsilon_{ijk}\left[\theta_{ijk}-\theta_{0,ijk}\right]^2 \cdot \exp\left(\frac{\gamma_{ij}\sigma_{ij}}{r_{ij}-\sigma_{ij}a_{ij}}\right)$$

Cost function:

The sum of relative errors between FFP and ab-initio results was used

$$S = \sum_i W_i S_i \quad , \quad S_i = \left\langle \left| \frac{f_i - f_{ab,i}}{f_{ab,i}} \right| \right\rangle$$

Results

Lattice Constants

	Exp	Ab-initio	FFP_{fitted}	$FFP_{Karaaslan}$ [3]	FFP_{Zhou} [4]
a (Å)	3.11	3.13 (+0.6)	3.14 (+1.0)	3.38 (+8.7)	3.08 (-1.0)
c (Å)	4.98	5.02 (+0.8)	5.10 (+2.4)	5.52 (+10.8)	5.03 (+1.0)

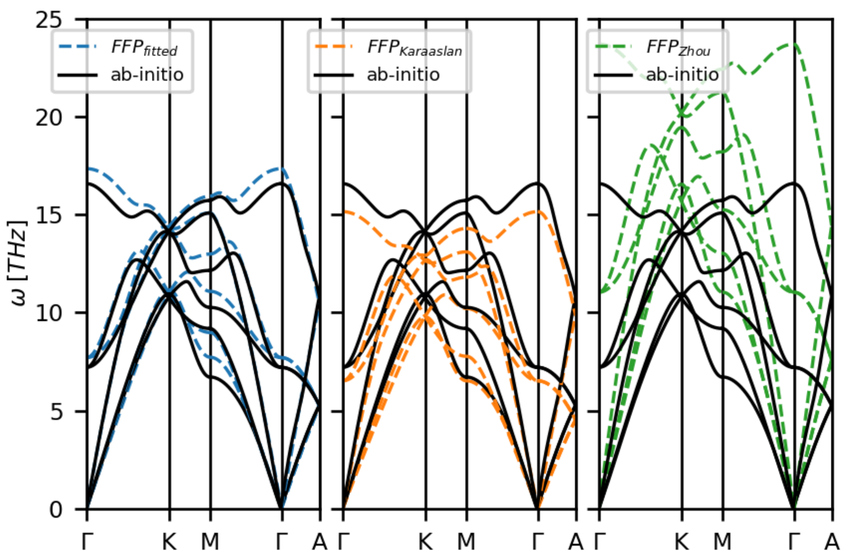
Values in parentheses: relative difference in percent compared to the experimental data.

Elastic constants

	Ab-initio			FFP		
	Lepkowski [2]	de Jong [6]	Ruiz [7]	FFP_{fitted}	$FFP_{Karaaslan}$ [3]	FFP_{Zhou} [4]
C_{11}	397	376	464	371 (-6.5, -1.3, -20.0)	289 (-27.2, -23.1, 37.8)	731 (+84.1, +94.4, +57.5)
C_{33}	372	353	409	390 (+4.8, +10.0, -4.6)	335 (-9.9, -5.1, 18.1)	764 (+105.4,+116.4,+86.8)
C_{44}	115	113	128	103 (-10.4, -9.7, -19.5)	75 (-34.8,-33.6,-41.4)	224 (+94.8,+98.2,+75.0)
C_{13}	115	98	116	127 (+10.4, +30, +9.5)	71 (-38.3, -27.6, -38.8)	207 (+80.0, +111.2, +78.4)
C_{12}	144	129	149	146 146 (+1.4, +13, -2)	116 (-19.4, -10.1, -22.1)	241 (+67.4,+86.8,+61.7)

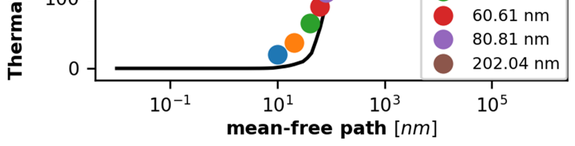
Values in parentheses are the relative differences from the available ab initio data in percent(Lepkowski [2], de Jong et al. [6], Ruiz et al. [7], respectively).

Phonon band structure



The fitted FFP accurately reproduces the used reference ab-initio phonon band structure (left panel).

Thermal Conductivity



- Values are in good agreement with the ab-initio and experimental data.
- Size effects are also accounted for by the fitted FFP.

Calculations were performed using non-equilibrium MD

References

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Outlook The fitted FFP provides an outstanding description of the elastic constants and harmonic phonon properties of AlN (much better than other FFPs reported in the literature). Moreover, it does an excellent job at reproducing the bulk and size-dependent thermal conductivity of AlN at 300 K. We are working on an improved FFP with a better description of anharmonicities and band structure. Moreover, the parametrization will be extended to encompass AlGaN alloys.

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