Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Theoretical study of interfacial thermal conductance for β-HMX/PVDF interface[1] HANG FAN, School of Mechatronical Engineering, Beijing Institute of Technology, Beijing 100081, P. R. China, FUDE NIE, Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621900, P. R. China, PENGWAN CHEN, School of Mechatronical Engineering, Beijing Institute of Technology, Beijing 100081, P. R. China — The heat conduction across the heterogeneous interface between β-HMX and PVDF is investigated. We use the diffuse mismatch model incorporating exact phonon dispersion and polarization to predict the interfacial thermal conductance. Based on lattice dynamics, the phonon dispersion relation is calculated from 2nd order interatomic force constants under harmonic approximation. Phonon density of states contributation is analysed from the view of assigned phonon mode. The calculated interface phonon transmission indicates that low frequency phonon modes dominant the interface thermal transport, while energy conducted by frquency mismatch phonon mode is refected by the interface. The interfacial thermal conductance as a function of temperature and accumulated interfacial thermal conductance are also calculated. Combined with the calculated thermal conductivity of β-HMX and PVDF by equlibrium molecular dynamics, the thermal conductivity of mixture β-HMX/PVDF system is analysed with simple series model. Particle size effect is also analysed.

[1]This work was supported by NSAF (Grant No. U1530262 and No. U1330202) and President Foundation of CAEP (Grant No. YZJJLX2016005)

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Date submitted: 15 Feb 2019 Electronic form version 1.4