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The effect of microstructure on lattice thermal conductivity of ScN thin films

Sit Kerdsonpanya¹, Olle Hellman^{1,2}, Bo Sun³, Yee Kan Koh³, Ngo Van Nong,⁴ Jun Lu¹, Sergei I. Simak¹, Björn Alling^{1,5}, Per Eklund¹

¹ Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden

² Department of Applied Physics and Materials Science, California Institute of Technology, Pasadena, California 91125, USA

³ Block EA, 9 Engineering Drive 1, #07-08, 117576 Singapore

⁴ Dept. of Energy Conversion and Storage, Technical University of Denmark, Risø Campus, Frederiksborgvej 399, Building 779, 4000 Roskilde, Denmark

⁵ Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

*e-mail of presenting author: sitke@ifm.liu.se

Thermoelectric applications require materials with low lattice thermal conductivity. Thus the knowledge of lattice thermal conductivity of materials under realistic conditions is vitally important. Here we have studied the effect of microstructure on lattice thermal conductivity of ScN thin films using a theoretical model based on a new *ab initio* description that includes the temperature dependence of the interatomic force constants, and treats anharmonic lattice vibrations [1-3]. We compare the results with the experimental data by Time Domain Thermoreflectance (TDTR). ScN is selected as a model system because its power factor is large ($2.5 \times 10^{-3} \text{ Wm}^{-1}\text{K}^{-2}$ at 800K) while the thermal conductivity is high, yielding low thermoelectric figure of merit (ZT) of about 0.2 [4]. Thus, reduction of the lattice thermal conductivity is needed. Our results show a trend of reduction in lattice thermal conductivity with decreasing grain size, with good agreement between the theoretical model and experimental data. Therefore we suggest a possibility to control thermal conductivity by tailoring the microstructure of ScN. More importantly, we provide a mathematical tool to predict the effect of the microstructure on the lattice thermal conductivity of materials based on first-principles calculations.

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