Calculating and analyzing the relationship between thermal conductivity and microstructure in rare-earth doped fluoride crystals

Kexin Liu, [a, b] Dapeng Jiang, [a, b] Gang Bian, [a, b] and Liangbi Su,*[a, b, c]

[a]*State Key Laboratory of High Performance Ceramics and Superfine Microstructure, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai 201899, China*

[b]*Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China*

[c]*suliangbi@mail.sic.ac.cn*

The raw materials for preparing RE-ion doped fluoride crystals are mainly high-purity rare earth fluoride powder and calcium/strontium/barium fluoride powder, in which the purity of the powder needs to be verified and purified. Bridgman method was used to grow single crystal samples with a diameter of less than 10mm in multichannel graphite crucibles under inert atmospheres. Reasonable control of drawing speed, temperature gradient, and other parameters. The absolute stationary method of longitudinal heat flux is used to measure the thermal conductivity (50-300K) of RE ion- doped fluoride crystals. The test error of thermal conductivity is less than 5%[1-3].

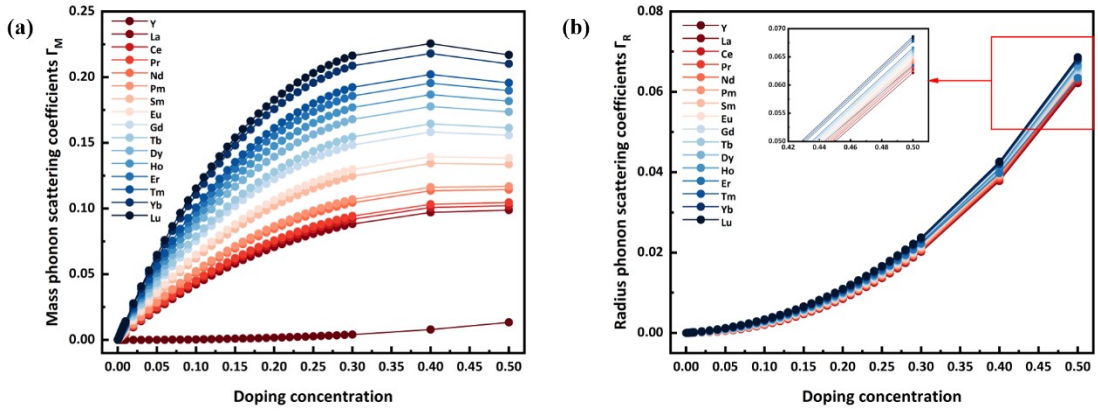

Fig.S1 (a)Mass phonon scattering coefficients of RE:SrF_2 crystals with low doping concentration; (b)Radius phonon scattering coefficients of RE:SrF_2 crystals with low doping concentration.

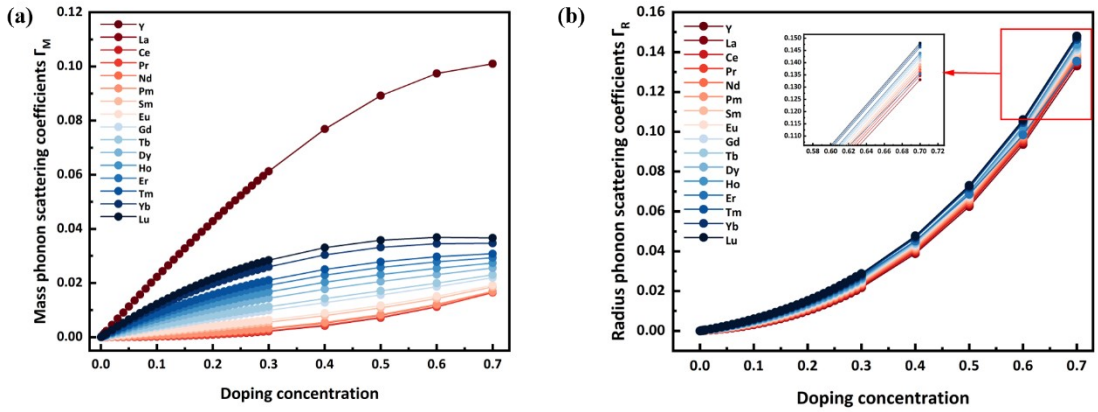

Fig.S2 (a)Mass phonon scattering coefficients of RE:BaF_2 crystals with low doping concentration; (b)Radius phonon scattering coefficients of RE:BaF_2 crystals with low doping concentration.

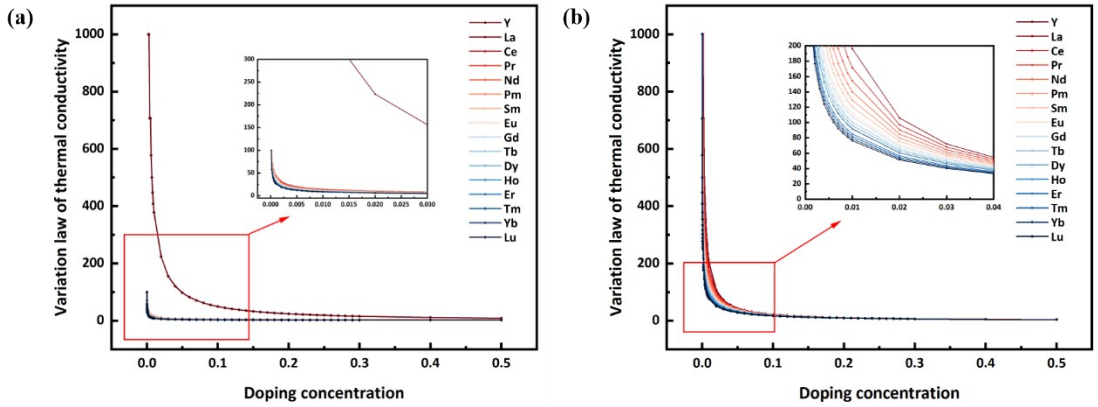

Fig.S3 (a) Variation law of thermal conductivity of RE:SrF_2 crystals in mass phonon scattering coefficients with low doping concentration; (b) Variation law of thermal conductivity of RE:SrF_2 crystals in radius phonon scattering coefficients with low doping concentration.

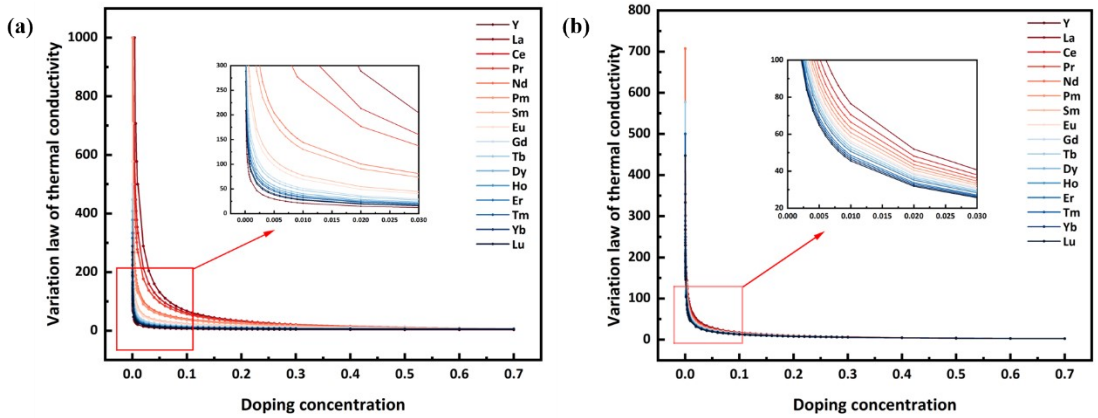

Fig.S4 (a) Variation law of thermal conductivity of RE:BaF_2 crystals in mass phonon scattering coefficients with low doping concentration; (b) Variation law of thermal

conductivity of RE:BaF_2 crystals in radius phonon scattering coefficients with low doping concentration.

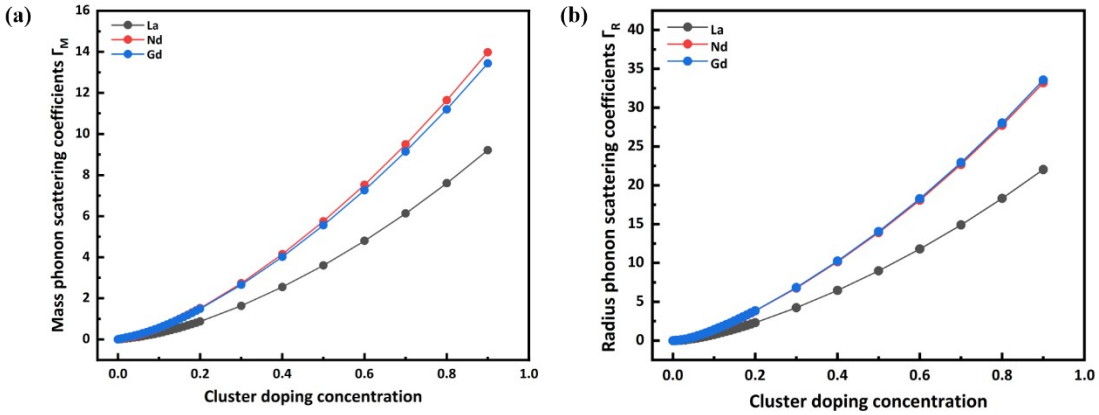

Fig.S5 (a)Mass phonon scattering coefficients of RE:SrF_2 crystals with high doping concentration; (b)Radius phonon scattering coefficients of RE:SrF_2 crystals with high doping concentration.

Reference

1. P. A. Popov, P. P. Fedorov and V. A. Konyushkin, *Crystallography Reports*, 2015, **60**, 744-748.
2. P. A. Popov, P. P. Fedorov, S. V. Kuznetsov, V. A. Konyushkin, V. V. Osiko and T. T. Basiev, *Doklady Physics*, 2008, **53**, 198-200.
3. P. A. Popov, P. P. Fedorov and V. V. Osiko, *Doklady Physics*, 2014, **59**, 199-202.