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Supporting Information

Optical Quality Tetragonal Phase Single-Crystal Fiber of Potassium Di-hydrogen Phosphate With Efficient Second-Harmonic Generation

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Materials and Methods

The materials used are ultra-high purity KDP microcrystals for growing high-quality single crystal products for extremely-high-power laser applications, which undergoes constant and stringent purity monitoring by employing ICP (Inductively Coupled Plasma) mass spectroscopic analysis.

The X-ray diffraction (XRD) data of tetragonal-shaped KDP single crystal microstructures were collected at 3W1A beamline in Beijing Synchrotron Radiation Facility. The molecular structures and packing arrangements are obtained by direct computation methods and then refined by full-matrix least-squares technique on F^2 using SHELX algorithm. For the purpose of comparison, XRD spectra of fine-ground KDP bulk crystals and a single-crystal KDP fiber were recorded using another commercial polycrystalline X-ray diffractometer equipped with a diffracted beam monochromator set for Cu KR radiation (λ = 1.54056 Å) in the 2θ range from 10 ^{0} to 90 ^{0} with a step size of 0.0216048 ^{0} and scan speed of 10 ^{0}/min.

SEM image of the tetragonal microstructures taken with a Hitachi S-4800 ultrahigh resolution field-emission scanning electron microscope at an accelerating voltage of 5.0 kV and the samples were Au-sputtered.

To investigate the SHG of the tetragonal KDP microstructures, 1-W CW 1064 nm Nd:YAG laser was used as the pump source (Maxphotonics Co., Ltd.). The output of the laser has a diameter of 2 mm. The pump light was first purified by a broadband polarizing beam splitter (PBS) cubes and then injected into a 100 X microscope objective which launches the pump field through the entrance facet of the micro-structure under investigation. Both the entrance and exit facets of the microstructures were not polished, and this resulted in less than a 20% coupling efficiency at each facet(a rough estimate). At the exit of the microstructure a laser-grade 1064 nm locking filter stops the residual pump laser and the SHG light was collected and focused onto a CCD camera by a microscope objective (40 X). The estimate of SHG efficiency is using the method reported before.[1]

Reference

1 Y. Ren, X. Zhao, L. Deng and E. W. Hagley, *Sci. Adv.*, 2016, **2**, e1600404.