Synthesis of Nonlinear Optical Material $Ag_5PS_4Cl_2$ Crystals

Kyra Bergman, Vivian Nguyen, and Jian Wang
Department of Chemistry and Biochemistry, Wichita State University, Wichita, KS

With the use of an infrared (IR) laser, nonlinear optical materials produce new photons via second harmonic generation (SHG) process. Properties of good nonlinear optical materials include crystallization in the noncentrosymmetric (NCS) space group, significant second harmonic generation (SHG) coefficient, high tolerance to laser damage (laser damage threshold), phase-matching behavior, and resistance to chemical change[1]. Thus, second harmonic generation only occurs in noncentrosymmetric (NCS) crystals. Pentasilver Tetrathiophosphate Dichloride ($Ag_5PS_4Cl_2$) crystallizes in NCS structure without any property investigation. Here we study synthesis methods to grow $Ag_5PS_4Cl_2$ and measure its optical properties. We found that the percentage weight of the compound, the compound mass to AgCl flux ratio, and the temperature profile primarily affected the synthesis of Pentasilver Tetrathiophosphate Dichloride. Ideally, a two to one ratio of compound mass to flux mass synthesized at 800°C, dwelling for 120 hours and cooling to 25°C for 48 hours, resulted in the closest phase match for $Ag_5PS_4Cl_2$. Our findings lead to additional synthesis of $Ag_5PS_4Cl_2$ at the specified conditions, introducing a second step. Further research will be done to remove the flux from the $Ag_5PS_4Cl_2$ crystal with additional flux, high temperature synthesis, and centrifuging.

Reference:

[1] Aslam, H. Z.; Doane, J. T.; Yeung, M. T.; Akopov, G. Advances in Solid-State Nonlinear Optical Materials: From Fundamentals to Applications. ***ACS Applied Optical Materials*** **2023**, *1* (12), 1898–1921. DOI:10.1021/acsaom.3c00352.