Estimation of enantiomeric excess using tunable spin-phase gradient beam

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Abstract: A novel method of using angle-cut uniaxial crystal is used to generate and tune the spin-phase gradient in the beam cross-section. The beam is used to measure ultra-small optical rotation angle with variable sensitivity and is extended to distinguish between the sense of rotation of the chiral molecules. The proposed method can measure the enantiomeric excess in a chiral mixture and can be used to monitor asymmetric reactions in real-time.

1. Introduction

In a sample containing enantiomeric mixture of chiral molecule it is important to quantify the purity of one of the enantiomers with respect to the other as their bio-chemical activities vary widely [1]. Though recent advances in asymmetric synthesis are designed to efficiently obtain one preferred enantiomer over the other it is necessary to monitor the process as the methods involve chiral catalysts and auxiliaries [1]. The enantiomeric excess (*ee*) is commonly used to quantify the asymmetric synthesis efficiency. A wide variety of techniques are currently used including mass spectrometry, circular dichroism and its variations, chiral chromatography and NMR spectroscopy. Despite these advances, optical differentiation of molecular chirality and quantitative *ee* determination has the potential for high-throughput and real-time screening of the synthesis [1]. Here we propose and demonstrate a novel method of using inhomogeneously polarized optical beam with tunable spin-phase gradient [2, 3], biased suitably to sensitively distinguish between the enantiomers of chiral molecule.

2. Experiment and results

The tailored optical beam is generated by passing laser beam through an angle cut uniaxial KTP crystal which is oriented such that the phase gradient within the beam cross-section is in opposite direction with reference to the beam center. Performing a weak projection measurement on the output beam, after passing through QWP and chiral solution provides a sensitive way to differentiate between the enantiomers, determined from the shift direction of the beam centroid. Schematic of the experimental setup is shown in Figure 1 (a).

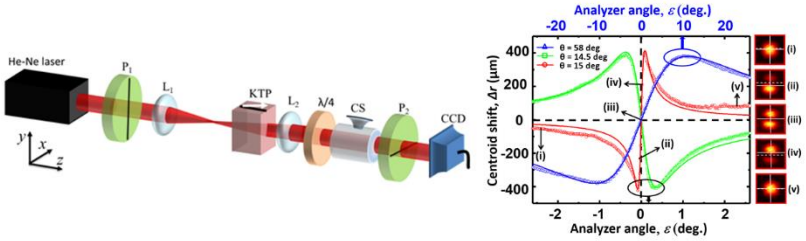

Fig. 1. (a) Schematic of the experimental setup and (b) Centroid shift as a function of analyzer angle for different orientation of the crystal.

The calibration measurement of beam centroid shift versus analyzer angle (Fig. 1 (b)), without the chiral solution, shows that the phase gradient in the linear region of the graph can be adjusted depending on the orientation angle (θ) of the crystal. Orienting the crystal to obtain the highest slope differentiates between the enantiomers with maximum sensitivity, as now the line will either rotate to the left (-θ) or to the right (+θ) depending on the *ee* of the solution. Details of our measurement will be presented at the conference.

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4. References

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