

**Project Title:**

**FINITE ELEMENT SIMULATIONS OF TIP-ENHANCED RAMAN SPECTROSCOPY AND MICROSCOPY**

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Tip-enhanced Raman spectroscopy (TERS) uses a sharpened metallic tip to identify and characterize the physical and chemical properties of various materials with true nanometer resolution. It has become the tool of choice for nondestructive spectroscopic and nanoscopic studies of carbon nanomaterials and of today's electronic devices. In this work, we will optimize all the parameters needed to obtain high near field signal in TERS. We introduce a thermally assisted tip-enhanced Raman spectroscopy using the heat generated from the enhanced electromagnetic field at the tip apex that is transferred to the sample by conduction and radiation. This technique can be used to characterize various materials where a nanometer-sized heat source of variable temperature range is required. The goal is to obtain the optimum parameters such as tip size and geometry, tip and sample optical properties, experimental configurations including wavelength and polarization of incident light. The parameters will be obtained for both air and aqueous environment under different temperature and bias conditions.

The project will be using Finite Element Method (ANSYS Multiphysics). The research requires a 3D model which will make the calculation a bit higher (20mins/job).

Initial results show that the TERS enhancement factor is dependent on the temperature of the tip/sample and environment arising from increasing

laser power. This is due to changes in the optical properties of the tip/sample at elevated temperature.

With this initial result, further studies are still necessary to study the dependence on other factors such as tip geometry and experimental configurations.

The project is still in its early stage (started Nov 2009) and this is the main reason why no publications have been made. However, initial results are promising.

**Reference:**

**A. Tarun**, N. Hayazawa, and S. Kawata, "Tip-enhanced Raman Spectroscopy for Nanoscale Strain Characterization," *Anal. Bioanal. Chem.* 394, 1775-1785 (2009).

N. Hayazawa, **A. Tarun**, A. Taguchi, and S. Kawata, "Development of Tip-enhanced Near-field Optical Spectroscopy and Microscopy" *Jpn. J. Appl. Phys.* 48 (2009).

A. Tarun, N. Hayazawa, and S. Kawata, "Site-Selective Cutting of Carbon Nanotubes by Laser Heated Silicon Tip," *Jpn. J. Appl. Phys.* 49, 025003 (2010).

