ME – PhD Thesis Colloquium

IN-SITU TRIBOLOGICAL EXPERIMENTS TO STUDY THE EFFECT OF CONTACT STRESSES ON RAMAN SCATTERING

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ABSTRACT

This thesis presents the design, development, and validation of novel instruments that enable in situ micro-Raman spectroscopic measurements at mechanically loaded interfaces: an indentation apparatus for static loading and a reciprocating tribometer for dynamic sliding contact studies. These instruments address fundamental challenges in tribology and contact mechanics by providing unprecedented experimental access to "hidden interfaces" where critical mechanical interactions occur. Traditional approaches to investigating contact interfaces rely predominantly on theoretical models that assume idealized conditions, limiting our understanding of actual mechanical behavior. The quantitative measurement of local pressure distributions has remained challenging due to limitations in experimental techniques capable of probing mechanically loaded interfaces without disrupting the interactions being studied. This research addresses this methodological gap through the innovative integration of mechanical testing with in situ Raman spectroscopy. Raman spectroscopy offers unique capabilities for probing mechanical deformation through k the analysis of vibrational modes within molecular structures. The stress-induced shifts in Raman spectral features provide direct indicators of material response to applied loads, with the magnitude of these shifts quantitatively correlated with local stress states. This research specifically examines the stress dependency of Raman spectra associated with optical phonons at $k = 0$, allowing the calculation of phenomenological coefficients that characterize changes in interatomic forces under mechanical loading. Both instruments utilize dual double cantilever flexure (DDCF) mechanisms for precise normal load application and double cantilever flexure (DCF) systems for accurate shear force measurements, creating stable mechanical loading conditions while maintaining optical access for spectroscopic analysis. The DDCF mechanism enables for precise normal load application with exceptional stability and minimal parasitic motion, maintaining the optical path integrity essential for spectroscopic measurements. The DCF system provides accurate shear force measurements during sliding contact experiments while maintaining the structural integrity of the overall instrument. The indentation apparatus enables for controlled normal loading with minimal lateral displacement, ensuring stable optical alignment throughout spectroscopic measurements. The reciprocating tribometer addresses the challenge of accessing interfaces during sliding contact through the incorporation of optically transparent elements, enabling direct spectroscopic access to the sliding interface without disrupting natural tribological processes. Both instruments seamlessly interface with a Micro-Raman spectroscopic system that combines micrometer-scale spatial resolution to map spectral responses across contact regions. The research employed diverse materials carefully selected to represent both crystalline and polymeric structures with distinct Raman-active vibrational modes. Crystalline silicon served as a model material due to its well-characterized Raman response to mechanical stress, providing validation for the experimental methodology. Polymeric materials such as polydimethylsiloxane (PDMS), polytetrafluoroethylene (PTFE), and hydrogel offered complementary insights into the behavior of viscoelastic materials under similar loading conditions. The experimental results revealed clear correlations between mechanical loading and Raman spectral shifts across all materials studied. In crystalline silicon, the characteristic Raman peak exhibited systematic shifts toward lower wave numbers with increasing indentation load, enabling quantitative calculation of local stress values based on established stress-shift coefficients. Polymeric materials displayed more complex spectroscopic responses reflecting their heterogeneous structures and viscoelastic properties. Particularly significant findings emerged from the reciprocating tribometer experiments, where spectra acquired during sliding showed distinctive differences compared to static loading, including peak broadening and the emergence of new spectral features associated with molecular reorientation and mechanochemical effects. Comparative studies between dry and lubricated contacts revealed the formation of ordered molecular structures within the lubricant layers, correlating with the reduced friction coefficients and suggesting direct mechanistic links between molecular organization and macroscale tribological performance. This research advances the measurement science for contact mechanics by establishing robust methodologies to directly observe and quantify interfacial phenomena at previously inaccessible scales. The experimental results validate certain aspects of established contact theories while challenging others. Furthermore, spectroscopic analysis of lubricated interfaces provides unprecedented molecular-level insights into lubrication mechanisms, with potentially significant implications for rational lubricant design. The instruments developed in this research create new opportunities for studying dynamic processes at mechanically loaded interfaces in various applications and material systems. Future work could expand the scope of the material to include emerging engineering materials, incorporate complementary spectroscopic techniques, investigate time-dependent phenomena, and integrate temperature control systems for thermomechanical behavior studies.

ABOUT THE SPEAKER

Mahesh Kumar Singh is currently working as Scientist at Applied Materials, India, with where he works at the intersection of mechanical and materials engineering with the focus on Optical Metrology. He has registered for his doctoral studies in the Department of Mechanical Engineering at the Indian Institute of Science, Bangalore with Prof. M. S. Bobji in August, 2014. His research focuses on probing mechanical-induced deformation at contact interfaces using micro-Raman spectroscopy.