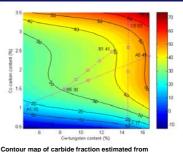
## **MODELLING AT NANO- & MICRO- SCALES**

# **Role of Structure Property Relationships**

### Dr Rehan Ahmed





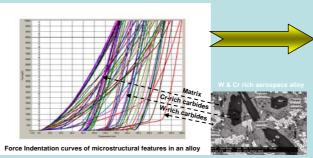
Contour map of carbide fraction estimated from mathematical model of W and C content

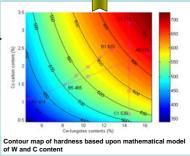
#### INTRODUCTION

CHALLENGES of modelling at nano- and micro-scales are due to the changes in dominant physical mechanisms which dictate the performance of miniature devices.

PERFORMANCE of bulk materials is less relevant in comparison to their near-surface properties which is dominated by the microstructural features.

MODELLING the mechanical and physical behaviour at these scale requires an understanding of structure property relationships which are surface dominated and governed by forces which are generally considered negligible at macro-scale



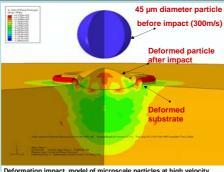


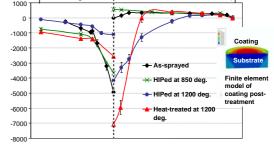
#### **NON-LINEAR MODELLING at MICRO-SCALE**

IMPACT resistance models at micro-scale are complex due to contact and high strain rate non-linearity. Influence of surface roughness, relative velocity, and frictional properties for micro-devices can hence be better understood through these models.

MECHANICAL properties of individual particles at nanoand micro-scale via experimental techniques provide the input data for numerical models.

NEUTRON diffraction, Raman Spectrometry and nanoindentation techniques are adapted to validate the





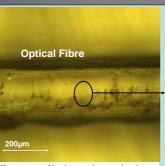
Deformation impact model of microscale particles at high velocity

Residual stress measurement via neutron diffraction in 300µm thick coatings

#### **MODELLING POLYMERIC MATERIALS** (Creep and Stress Relaxation modulus)

CREEP and stress relaxation mechanisms at micro- and nano-scales provide an understanding of their performance in an engineering application. Mechanical properties of these materials can therefore vary with time, temperature and humidity.

**MEAUREMENT** of near surface properties is critical to incorporate more reliable and accurate material parameters in the design process.



Measurement of hardness and creep relaxation at nano-scale

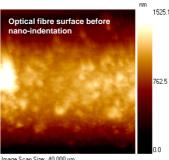
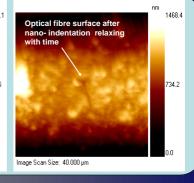


Image Scan Size: 40.000 μm

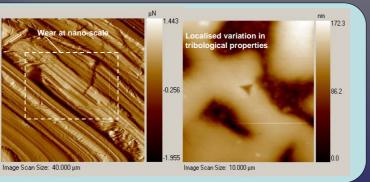


**SUMMARY** 

#### NANO-TRIBOLOGY

FRICTIONAL mechanisms at nano-scale are dominated by atomic, capillary, Vander-wall and electrostatic forces. Measurement of these forces is essential to ensure the durability of engineering design of micro devices, as conventional tribological models are not accurate at these scales due to large surface volume ratio and changes in lubrication mechanism.

WEAR mechanisms are dominated by real area contact at asperity level and is influenced by both frictional and lubrication mechanisms operational at this scale.



### **Principal Collaborators**















Interlinking molecular dynamics, meso-scale and continuum models



