Fully Atomistic Reactive Molecular Dynamics simulations of mechanical properties of Gold Nanotips Encapsulated with Carbon Nanocones

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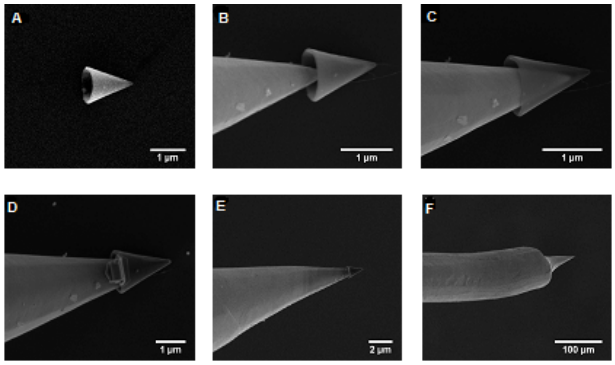
We have investigated the mechanical properties of gold nanotips encapsulated with Carbon Nanocones (MWNCs) through Raman experiments and fully atomistic molecular dynamics (MD) simulations. Our results show that when the gold tips are covered with MWNCs, the composite system presents an enhanced structural stability. The stress patterns extracted from MD simulations can explain the increased mechanical stability. We observed that besides protecting the gold tip from direct contact with the substrates/samples, the cones can be reversibly deformed while almost no structural damages are imposed to the internal Au tip. MWNCs can efficiently accumulate the strain/stress thus expanding the elastic regime of the gold tips and helping to maintain their physical integrity.

Introduction

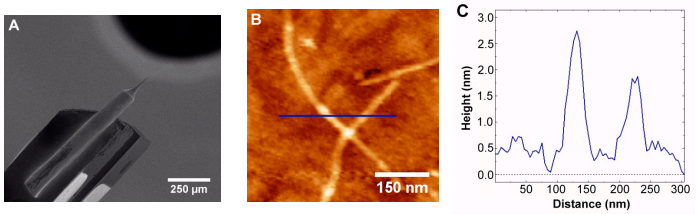
Gold use as nanotips in some applications is limited by its mechanical structural fragility. In order to overcome these difficulties, we have manipulated multiwalled carbon nanocones (MWNCs) to encapsulate chemically etched produced gold nanotips.



Encapsulation of a gold nanotip with a carbon nanocone. (A) One isolated MWCNC. (B-F) Moving, attaching and detaching a multiwalled carbon cone into a gold tip. In (F) the nanocone is no longer seen.

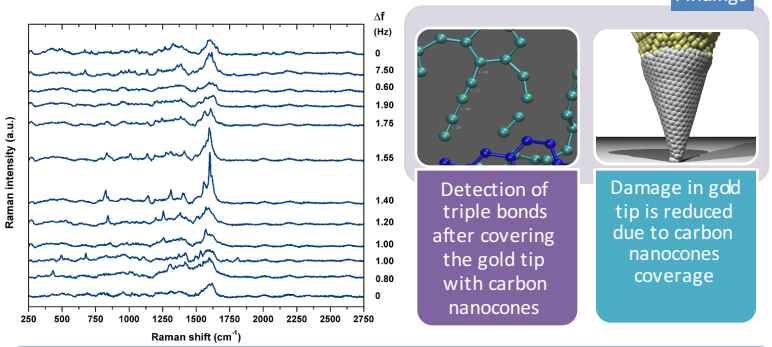
Experimental Results

Typically the composite tips can last up to one month of frequent use, much more than conventional non-modified gold tips and, more importantly, without losing image resolution and with great stability.



Atomic force microscopy (AFM) with the gold/carbon nanotip. (A) SEM image of an Au/cone tip glued on a tuning fork for SPM measurements. (B) AFM topography image of single wall carbon nanotubes on a glass cover slip. (C) Height profile at the blue line shown in (B).

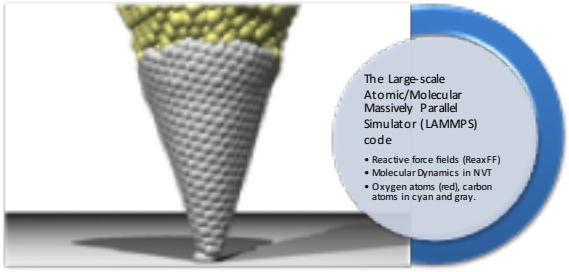
For more detailed structural information, we performed *in situ* Raman spectroscopy experiments, focusing on the MWCNT signals.



***In situ* Raman spectroscopy measurement of a Au tip modified with a MWNC under compression against a glass substrate.** The Raman spectra were obtained during the processes of pushing the tip against the substrates and retracting it.

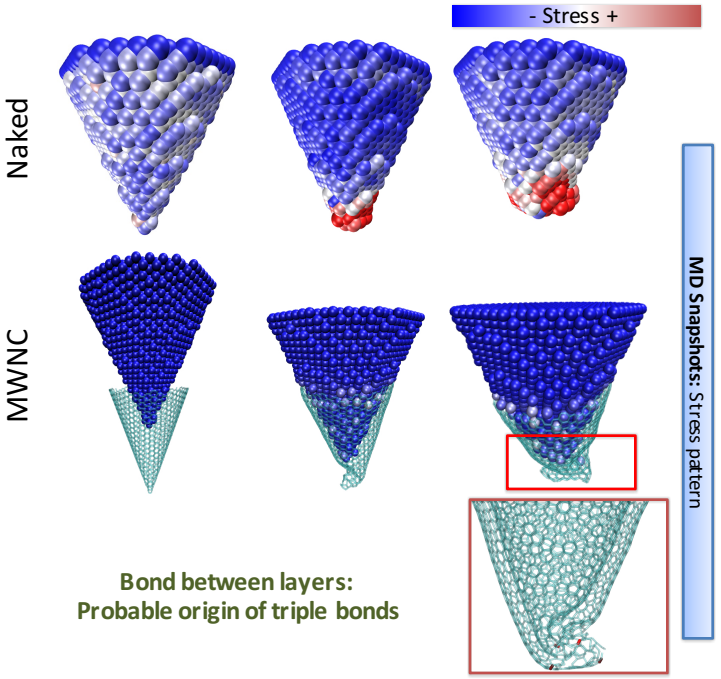
Theoretical Approach

Due to complexity of smashing processes and the existence of extensive deformations and/or mechanical fractures, sophisticated reactive molecular dynamics simulations are needed.

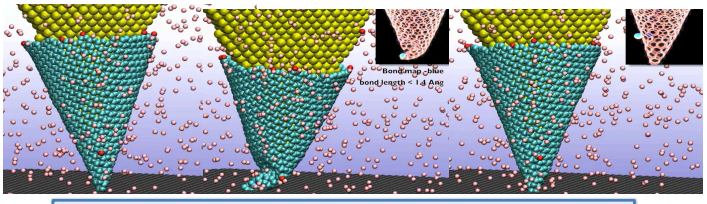


Theoretical Results

The MWNC encapsulations protects the gold tip against permanent deformations, because of the experienced lower levels of stress.



Smashing covered nanotip in gaseous atmospheres shows that the MWNCs are significantly resistant to chemical contamination.



MD Snapshots: Smashing in a gaseous atmosphere

Acknowledgements

Cano-Marquez, Abraham G., et al. *Scientific reports* 5 (2015).

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