

# ΕΥΡΩΠΑΪΚΟ ΚΟΙΝΩΝΙΚΟ ΤΑΜΕΙΟ

## Επιχειρησιακό Πρόγραμμα

Ανάπτυξη Ανθρώπινου Δυναμικού, Εκπαίδευση & Δια Βίου Μάθηση

ΕΙΔΙΚΟΣ ΛΟΓΑΡΙΑΣΜΟΣ ΚΟΝΔΥΛΙΩΝ  
ΕΡΕΥΝΑΣ ΑΡΙΣΤΟΤΕΛΕΙΟΥ  
ΠΑΝΕΠΙΣΤΗΜΙΟΥ ΘΕΣΣΑΛΟΝΙΚΗΣ

ΑΡΙΣΤΟΤΕΛΕΙΟ ΠΑΝΕΠΙΣΤΗΜΙΟ  
ΘΕΣΣΑΛΟΝΙΚΗΣ

**ΕΔΒΜ34 Project 95370**  
**MIS 5005134**

**Νανο-χημο-μηχανική  
στην Παραμόρφωση και  
Θραύση: Θεωρία  
και Εφαρμογές σε LIB @  
SGS**



Ευρωπαϊκή Ένωση  
Ευρωπαϊκό Κοινωνικό Ταμείο

• Με τη συγχρηματοδότηση της Ελλάδας και της Ευρωπαϊκής Ένωσης

• Στοιχεία επικοινωνίας: E.C Aifantis, Lab of Mechanics and Materials, mom@mom.gen.auth.gr





# Νανο-χημο-μηχανική στην Παραμόρφωση και Θραύση: Θεωρία και Εφαρμογές σε LiB & SGS [ΕΔΒΜ34 MIS 5005134]

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## Summary

The classical laws for Hookean deformation and Fickian transport are modified to include extra Laplacian terms and corresponding internal lengths modeling nonlocal chemomechanical interactions with emphasis at the nanoscale. Then, special cases are considered to describe deformation and fracture aspects of new energy materials; namely Li-ion battery (LIB) nanostructured anodes for energy storage and disclinated metallic microcrystals including icosahedral small particles (ISP) for catalysis applications.

## Benchmark Results

### • LIBs

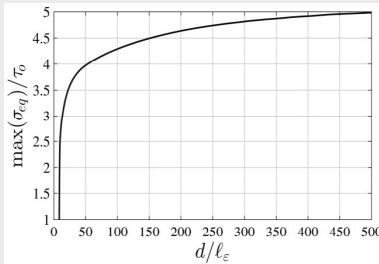


Figure 1 Size effect exhibited by the global maximum  $\max(\sigma_{eq})$  that appears over the entire lithiation process.

### • ISPs

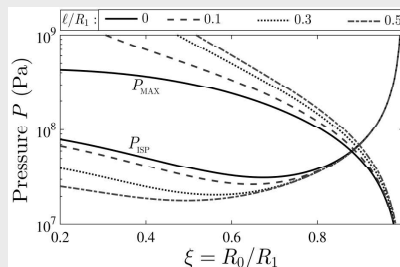


Figure 2: Stress gradient effects on the functions  $P_{ISP}(\xi)$  and  $P_{MAX}(\xi)$  for a hollow ISP

## Deliverables

### A. Journal Publications

- I. Tsagrakis, I. Konstantopoulos, A. Sidiropoulos and E.C. Aifantis, *On Certain Applications of Gradient Nanochemomechanics: Deformation and Fracture of LIB and SGS*, *J. Mech. Beh. Mat.* **28**, 74-80, 2019

### B. Conference/Proceedings Presentations

- E.C. Aifantis, I. Tsagrakis, I. Konstantopoulos and A. Sidiropoulos, *Nonsingular Gradient and Fractional Fracture Mechanics*, MSMF9, Brno, 26-28 June 2019. [PLENARY]
  - E.C. Aifantis, I. Tsagrakis, I. Konstantopoulos and A. Sidiropoulos, *Gradient & Fractional/Fractal Models for Elasticity, Diffusion, Plasticity and Dislocations: Applications to LIBs and DMCs*, APM 2019, St Petersburg, 24-28 June 2019. [PLENARY]
  - E.C. Aifantis, I. Tsagrakis, I. Konstantopoulos and A. Sidiropoulos, *Gradient Theory in Small Scales*, MS&T 2018, Columbus, 14-18 Oct 2018. [INVITED]
- ### C. Workshops/Symposia
- C. Tsallis Mini-Symposium Sept 21, 2018
  - Shechtman-Suresh Honorary Symposium Nov 30- Dec 2, 2018.

## Conclusions

Coupled nano-chemo-mechanical models have been developed to be used in current energy storage and catalysis technologies. The focus was on nanostructured LIB anodes and ISP objects with pentagonal symmetry. The results indicate that such models can capture size effects that are observed in these components and can potentially lead to protocols and design criteria to prevent failure and optimize their performance in related applications.