PXO: Poly-XTAL operations V10.00. Free MATLAB codebase to generate and analyse complex 2D poly-crystalline grain structures

**INTRODUCTION AND FUNCTIONALITITES**

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**Author contributions**

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| Sunil Anandatheertha | Conceptualization, Software development and maintenance, documentation and manuscript preparation |

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## Highlights

* Free MATLAB codebase for researchers working on computational materials science, computational geology, dynamics of importance sampling Monte-Carlo schemes and graphenes.
* Make spatiotemporally gradient 2D grain structures and associate spatiotemporally gradient crystallographic texture to the grain structure
* Export ABAQUS input file for use in CPFEM
* Work with Ising model and Q-state Pott’s model simulation on square lattices
* Call MTEX libraries and mtex2gmsh

## Grain structures

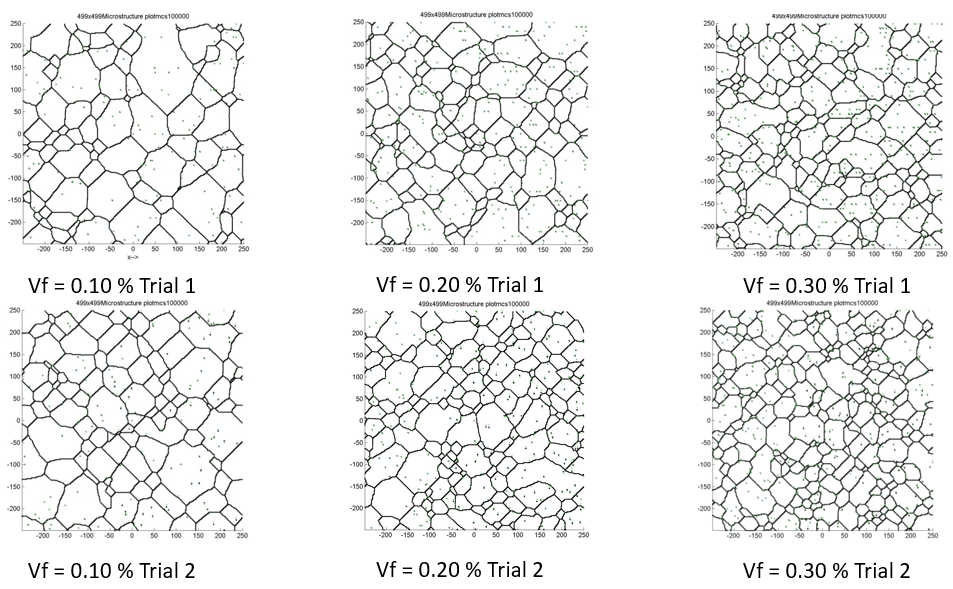
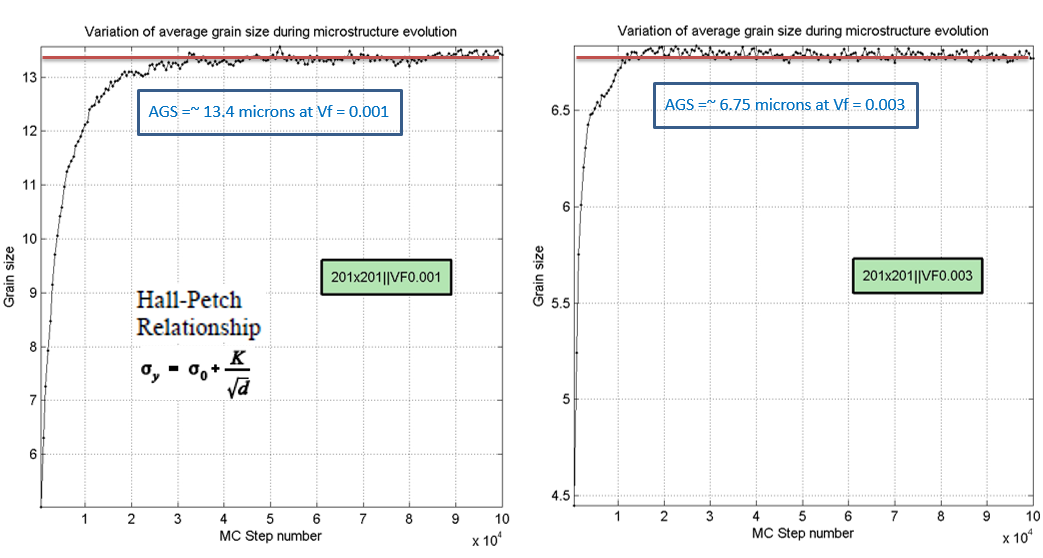
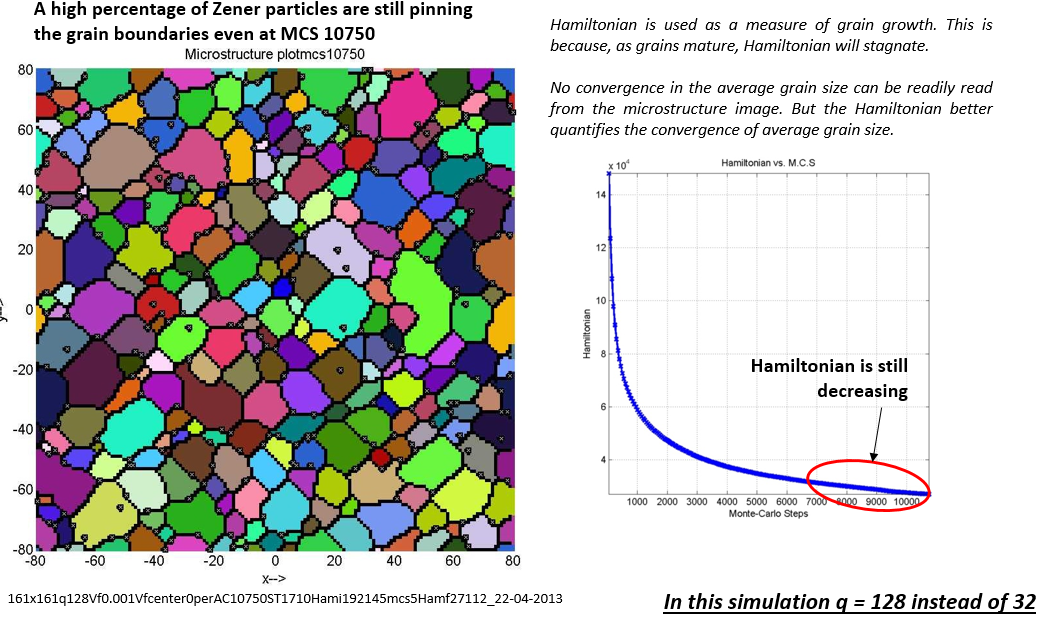
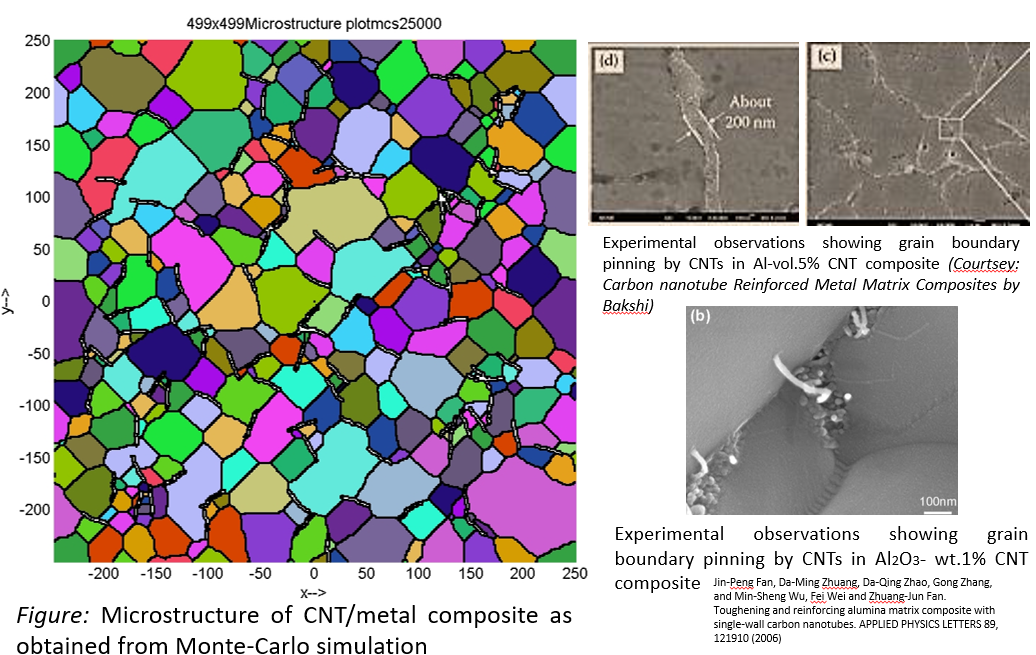


Figure 1:





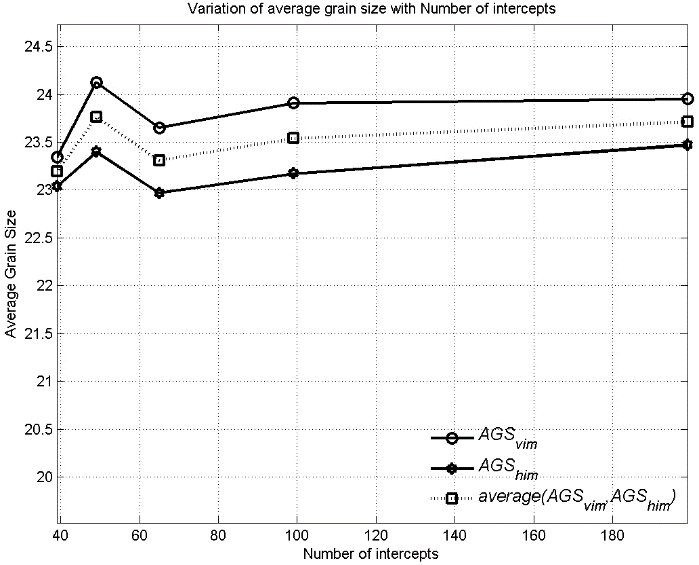


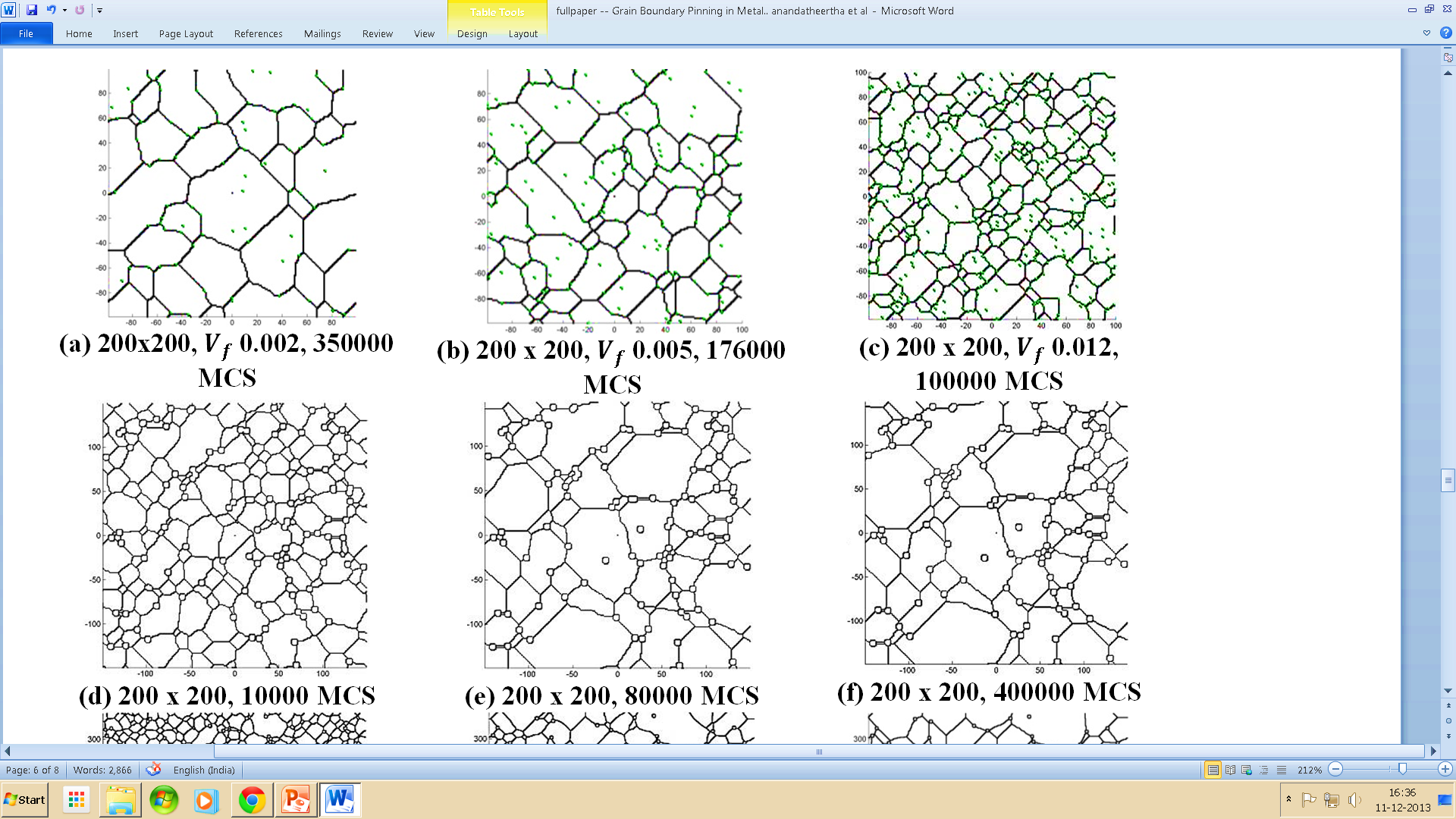
Experimental observations showing grain boundary pinning by CNTs in Al-vol.5% CNT composite *(Courtsey: Carbon nanotube Reinforced Metal Matrix Composites by Bakshi)*

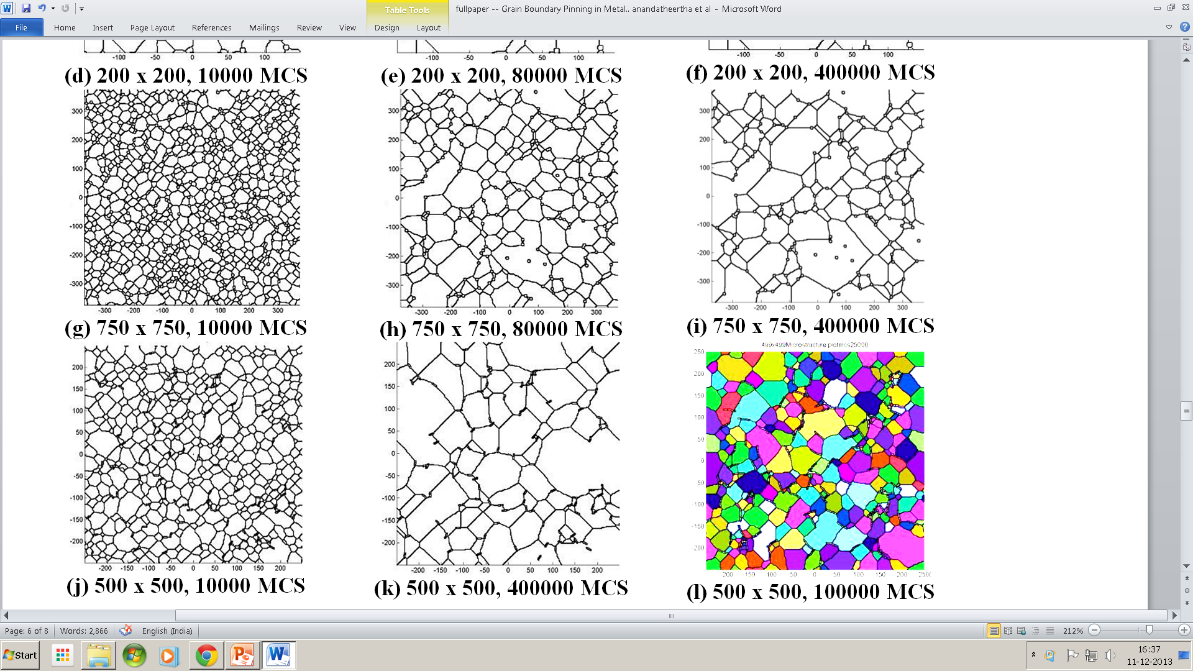
*Experimental observations showing grain boundary pinning by CNTs in Al2O3- wt.1% CNT composite*

Jin-Peng Fan, Da-Ming Zhuang, Da-Qing Zhao, Gong Zhang, and Min-Sheng Wu, Fei Wei and Zhuang-Jun Fan. Toughening and reinforcing alumina matrix composite with single-wall carbon nanotubes. APPLIED PHYSICS LETTERS 89, 121910 (2006)









## Kernel function parameters for POTTS grain structures

Refer “*PXO\_test\_cases-POTTS\_Kernels\_V1.0.xlxs*” for values and the corresponding grain structure snapshots that are produced.

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