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ANALYSIS OF CHARACTERISTICS OF RANDOM MICRO STRUCTURES OF NANOMATERIALS

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A thesis submitted to the Faculty of Engineering and the Built Environment, University of the Witwatersrand, Johannesburg, in fulfilment of the requirements for the degree of Doctor of Philosophy.

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DECLARATION

I declare that this thesis is my own unaided work. It is being submitted to the Degree of Doctor of Philosophy to the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination to any other University.

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(Signature of Candidate)

…….. day of …….. year…….

day month year

ABSTRACT

Predicting and manipulating materials macroscopic properties from the knowledge of their microstructure characteristics are attracting significant attention in the field of Materials Science and Engineering. Nowadays, Nanoscience and Nanotechnology are engaged in these studies. Nanomaterials constituents, called herein unambiguously microstructures, have inherently random features/characteristics. In the research reported in this thesis the tools of stochastic processes and stochastic differential equations theory have been used as they offer a sound approach to understanding and analysing microstructures characteristics. This research adopts the approach of first delineating the necessary mathematical formulations, followed by their applications.

Substantial number of atoms at nanomaterial Grain Boundaries, GBs, lowers the material thermal stability leading to grain growth. The growth of individual grain size, ***d***, in a nanomaterial is apprehended to be jointly caused by Grain Boundary Migration, GBM, and Grain Rotation-Coalescence, GRC, mechanisms. A model is established that includes the previously ignored GRC in the expression for increment of ***d*** and, further, considering the fact that the energy required to activate GBM increases during grain growth. The stochastic counterpart of the expression is obtained by adding two fluctuation terms; to account for the random fluctuations in ***d*** caused by GBM and GRC. Results show that nanomaterials low stabilities are also due to their grains' high rotational mobilities at low grain size dispersion, CV(d). Using information about microstructure size evolution, its probability density function, pdf, is determined using the generalised Fokker-Planck-Kolmogorov equation. Results demonstrate that the type of scaling state pdf depends on the nature of the fluctuation terms. Grain growth parameters are calibrated in such a way that the pdf evolves lognormally throughout.

Microstructure-property dependence has for long been given by the Hall-Petch to Reverse Hall-Petch relationship, HP-RHPR, (a relationship between mechanical property and mean grain size, E(d), only). A modified model for this dependence is established using complete information about microstructure size distribution. Results suggest that both E(d) and CV(d) are central in designing materials with required properties. Reasons for conventional, homologous and anomalous temperature dependences of yield stress are revealed.

Thus, implementing desired stochastic "properties" of microstructures entails designing required

materials mechanical properties.

To my father

Ba Jacob Tengen

and my mother

Na Nahbula Prescila Kontan

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