

Alexander Cheng, Alain Kassab, Ernian Pan and Benny Hon, Preface, Engineering Analysis with Boundary Elements, Volume 31, Issue 5, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Page 387.

(<http://www.sciencedirect.com/science/article/B6V2N-4N5KXTB-1/2/b1ba3dc9bec7e2ad030d7958da0d1dd3>)

Jianming Zhang and Masataka Tanaka, Systematic study of thermal properties of CNT composites by the fast multipole hybrid boundary node method, Engineering Analysis with Boundary Elements, Volume 31, Issue 5, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Pages 388-401.

(<http://www.sciencedirect.com/science/article/B6V2N-4N14D46-1/2/29c0d69c0a3fdc589bd0a9c2bd6a9400>)

Abstract: Carbon nanotubes (CNTs) are predicted to possess superior heat conductivity, which makes the CNTs promising in development of fundamentally new composite material. With the current advancement in nanotechnology, it is possible to design materials with desired properties for specific applications. On the other hand, the overall properties of CNT composites are usually evaluated using a representative volume element (RVE) with a number of CNTs embedded. For realistic modeling, an RVE including a large number of CNTs, for example, tens or hundreds, is necessary. However, analysis of such an RVE using standard numerical methods faces two severe difficulties: discretization of the geometry into elements and the very large computational scale. In this paper, the first difficulty is alleviated by developing the hybrid boundary node method (HdBNM), which is a boundary-type meshless method. To overcome the second difficulty, a simplified mathematical model for thermal analysis of CNT analysis is first proposed, by which the size of the linear system can be reduced by nearly half. Then, the HdBNM is combined with the Fast Multipole Method (FMM) based on the model to further reduce the computational scale. A variety of RVEs containing different numbers of CNTs, from small to large scales, have been studied in an attempt to investigate the influence of CNT length, distribution, orientation and volume fraction on the overall thermal properties of the composites. Insights have been gained into the thermal behavior of the CNT composite material.

Keywords: Carbon nanotube; Nanocomposites; Heat conductivity; Hybrid boundary node method; Simplified model; Fast Multipole Method

Zhenyu Yang and Ya-Pu Zhao, Adsorption of His-tagged peptide to Ni, Cu and Au (1 0 0) surfaces: Molecular dynamics simulation, Engineering Analysis with Boundary Elements, Volume 31, Issue 5, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Pages 402-409.

(<http://www.sciencedirect.com/science/article/B6V2N-4N2M6CK-1/2/f7518fc2cfa205db97df5685b8466eda>)

Abstract: Molecular dynamics (MD) simulations are performed to study the interaction of His-tagged peptide with three different metal surfaces in explicit water. The equilibrium properties are analyzed by using pair correlation functions (PCF) to give an insight into the behavior of the peptide adsorption to metal surfaces in water solvent. The intermolecular interactions between peptide residues and the metal surfaces are evaluated. By pulling the peptide away from the peptide in the presence of solvent water, peeling forces are obtained and reveal the binding strength of peptide adsorption on nickel, copper and gold. From the analysis of the dynamics properties of the peptide interaction with the metal surfaces, it is shown that the affinity of peptide to Ni surface is the strongest, while on Cu and Au the affinity is a little weaker. In MD simulations including metals, the His-tagged region interacts with the substrate to an extent

greater than the other regions. The work presented here reveals various interactions between His-tagged peptide and Ni/Cu/Au surfaces. The interesting affinities and dynamical properties of the peptide are also derived. The results give predictions for the structure of His-tagged peptide adsorbing on three different metal surfaces and show the different affinities between them, which assist the understanding of how peptides behave on metal surfaces and of how designers select amino sequences in molecule devices design.

Keywords: Molecular dynamics; Adsorption; His-tagged peptide; Pair correlation function; Root mean square displacement/deviation; Nanotechnology

S.Yu. Reutskiy, The method of approximate fundamental solutions for axisymmetric problems with Laplace operator, *Engineering Analysis with Boundary Elements*, Volume 31, Issue 5, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, May 2007, Pages 410-415.

(<http://www.sciencedirect.com/science/article/B6V2N-4N3P54F-1/2/1e75e57e78af7b959332c5a626d1a54b>)

Abstract: The paper presents a new numerical technique for solving axisymmetric problems with Laplace operator. It is similar to the method of fundamental solutions but it is based on the use of special basis functions which satisfy the majority of the boundary conditions of the problem considered. This reduces the number of unknowns and the size of the collocation matrix considerably. As it is shown in the paper, this technique can also be applied successfully in the cases when the solution domain has infinite boundaries in z or r directions. Numerical examples justifying the method are presented.

Keywords: Laplace equation; Axisymmetric problems; Fundamental solutions; Infinite domain

V. Kompis, M. Kompis and M. Kaukic, Method of continuous dipoles for modeling of materials reinforced by short micro-fibers, *Engineering Analysis with Boundary Elements*, Volume 31, Issue 5, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, May 2007, Pages 416-424.

(<http://www.sciencedirect.com/science/article/B6V2N-4N2D5Y9-1/2/dbc653c8289c942c537ecdef3a7a202a>)

Abstract: Method of continuous dipoles for modeling of the interaction of composites reinforced with fibers is presented in the paper. The dipoles are distributed along the fiber axis. All three components of dipoles are used to satisfy the boundary conditions along the fiber boundaries. The boundary conditions in strain components instead of displacements are used in the model, which simplifies the numerical solution. In resulting quasi-hyper-singular integral equations the integration is performed analytically. The dipole fields decay in infinity and they accurately simulate the near and far field interaction. The presented models are applicable to solution of problems of composites reinforced by straight fibers with large aspect ratio, which are most significant for practical purposes, as the fibers have large stiffness in tension, but not in bending. The fiber is considered to be rigid in the fiber axis direction.

Keywords: Composite material; Short and long fibers; Large aspect ratio; Quasi-hyper-singular integral equations; Method of continuous dipoles

Hamid R. Sadraie, Steven L. Crouch and Sofia G. Mogilevskaya, A boundary spectral method for elastostatic problems with multiple spherical cavities and inclusions, *Engineering Analysis with Boundary Elements*, Volume 31, Issue 5, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, May 2007, Pages 425-442.

(<http://www.sciencedirect.com/science/article/B6V2N-4N6NHF7-1/2/671845d4473e329a2e80c837936c4a57>)

Abstract: The problem of an infinite solid containing an arbitrary number of non-overlapping spherical cavities and inclusions with arbitrary sizes and locations is considered. The infinite solid and the spherical inclusions are made of different isotropic, linearly elastic materials. The spherical cavities are assumed to carry arbitrary tractions, and the spherical inclusions are assumed to be perfectly bonded to the infinite solid. The boundary and interfacial displacements and tractions are represented by truncated series of surface spherical harmonics. The problem involving multiple spherical features is replaced by a sequence of problems involving a single spherical feature via Schwarz's alternating method which accounts for the interactions in the course of an iterative process. Problems involving a single spherical feature are solved by employing the Papkovitch-Neuber functions, and the interactions are evaluated by applying a least squares method. A robust scheme is introduced to control the total errors on the spherical boundaries and interfaces and to choose the number of terms in the series expansions. Several numerical examples are given to address the efficiency and the accuracy of the proposed method. **Keywords:** Elasticity; Spherical cavities and inclusions; Spherical harmonics; Boundary spectral method; Alternating method; Least squares method

Chengzhi Li and Guanshui Xu, Geometrical effect on dislocation nucleation at crystal surface nanostructures, *Engineering Analysis with Boundary Elements*, Volume 31, Issue 5, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Pages 443-450.

(<http://www.sciencedirect.com/science/article/B6V2N-4N3GNRT-1/2/3ecd41273cbfb403bdd2ae0b17a87476>)

Abstract: Crystal surface nanostructures such as steps and trenches in microelectronic layer structures have been considered as stress concentrators that may facilitate dislocation nucleation. Quantitative characterization of the critical condition of this atomic scale process is of considerable interest for the development of high performance electronic devices. This paper addresses this issue using a multiscale approach based on the variational boundary integral formulation of the Peierls-Nabarro dislocation model. By representing the profiles of embryonic dislocations as the relative displacements between the two adjacent atomic layers along the slip planes, the critical conditions for dislocation nucleation are obtained by solving the stress dependent activation energies required to activate embryonic dislocations from their stable to unstable saddle point configurations. The geometrical effect of surface nanostructures such as steps and trenches on dislocation nucleation is ascertained quantitatively. Our results show that the atomic scale surface nanostructures can reduce the critical stress for dislocation nucleation by nearly an order of magnitude and the trench configurations are more prone to dislocation nucleation than the step configurations. Nucleation of versatile dislocations in multiple slip systems at crystal surfaces may be attributed surface nanostructures of a variety of geometries. **Keywords:** Dislocation nucleation; Surface nanostructure; Variational boundary integral method

C. Cercignani, A. Frangi, S. Lorenzani and B. Vigna, BEM approaches and simplified kinetic models for the analysis of damping in deformable MEMS, *Engineering Analysis with Boundary Elements*, Volume 31, Issue 5, *Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I*, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Pages 451-457.

(<http://www.sciencedirect.com/science/article/B6V2N-4N3GNRT-2/2/08d2993f9fe895870ff523e80e433161>)

Abstract: Microflows occurring in MEMS are addressed by applying a continuum BEM code for quasi-static Stokes flow accounting for slip boundary condition. Working conditions typical of transition and rarefied flows are treated in a simplified manner by employing a viscosity corrected

according to semi-analytical solutions for the linearized BGK model of Couette and Poiseuille flows. Numerical results are compared with experiments showing excellent agreement

Keywords: Multipole accelerators; Stokes flow; Damping forces; MEMS

Tomofumi Koyama and Lanru Jing, Effects of model scale and particle size on micro-mechanical properties and failure processes of rocks--A particle mechanics approach, Engineering Analysis with Boundary Elements, Volume 31, Issue 5, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, Innovative Numerical Methods for Micro and Nano Mechanics and Structures - Part I, May 2007, Pages 458-472.

(<http://www.sciencedirect.com/science/article/B6V2N-4N3GNRT-3/2/f3a43cded92d9209e57a1aa15f100da1>)

Abstract: A numerical procedure to determine the equivalent micro-mechanical properties of intact rocks is presented using a stochastic representative elementary volume (REV) concept and a particle mechanics approach. More than 200 models were generated in square regions with side lengths varying from 1 to 10 cm, using the Monte Carlo simulation technique. Generated particle models were then used for the calculation of equivalent micro-mechanical properties. Results with a core sample of diorite from Aspo, Sweden, show that the variance of the calculated values of mechanical properties decrease significantly as the side lengths of particle models increase, reaching a REV side length about 5 cm with an acceptable variation of 5%, which is equal to the minimum diameter of rock specimen for uniaxial compressive tests suggested by ISRM. The complete stress-strain curve of the diorite rock sample was predicted under uniaxial compression, as the basis for evaluating the damage and failure processes. The unique contribution of this paper is its study on impacts of sample size and particle size distributions on mechanical behaviour of rocks when particle mechanics approaches are used.

Keywords: Micro-mechanical properties; Failure process; Complete stress-strain curve; Particle mechanics approach; Representative elementary volume (REV); Stochastic simulation