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Dynamic analysis of nano-heterogeneities in a finite-sized solid by boundary and finite element methods

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ABSTRACT

This work addresses the elastodynamic problem for a finite-sized, elastic solid matrix containing multiple nano-heterogeneities of arbitrary shape, number and geometric configuration. The problem is formulated under plane strain conditions, and time-harmonic motions are assumed to hold. The aim is to evaluate the non-uniform stress and strain fields that develop in the solid matrix and to identify zones of dynamic stress concentration for the case of dynamic loads applied along the matrix boundary. The mechanical model used here is based on a combination of classical elastodynamic theory for the bulk solid under non-classical boundary conditions, supplemented with a localized constitutive equation for the solid-inclusion interface in the framework of the Gurtin–Murdoch theory of surface elasticity. As computational tools we use (a) the 2D boundary element method (BEM) with frequency-dependent fundamental solutions for the bulk solid and (b) the finite element method (FEM) software package ANSYS augmented by a macro-finite element for representing surface effects on the contour of the nano-inclusions. At first, accuracy of the numerical solutions obtained for the dynamic stress concentration factor (DSCF) and for the diffracted displacement wave field is satisfactorily established. Next, comparison studies are conducted to gauge the BEM and FEM separately. These are followed by extensive numerical simulations that show that both BEM and FEM are able to capture the dependence of the diffracted wave field and of the DSCF on the type of the inclusions, their overall configuration and the nature of applied dynamic loads. It is concluded that the interaction effect between the nano-heterogeneities and the external perimeter of the bounded solid matrix is of paramount importance.

1. Introduction

Wave propagation in homogeneous elastic continua is a well-known phenomenon and the numerical modeling effort involves solution of hyperbolic partial differential equations. The situation becomes far more complicated if the medium is heterogeneous, see Berezovski (2010). Elastic wave propagation through naturally occurring or man-made heterogeneous materials has attracted the attention of researchers from branches of science as diverse as seismology, material science, fracture mechanics, computational mechanics, etc. Another difficulty is that discontinuities such as cracks, cavities and inclusions complicate the overall picture by acting as scatterers and stress concentrators, thus causing reflection, refraction, diffraction and scattering phenomena that are not easy to quantify. In elastodynamics, the motion of waves in bounded solids is governed by the conservation law for linear momentum, the constitutive and kinematic relations, all complemented by initial as well as boundary continuity conditions along the solid boundaries, see Achenbach (1973). Computational tools available for solution of these problems within the frame of classical elastodynamics are as follows: (a) analytical and semi-analytical techniques dealing with regular geometries and employing wave function expansion methods (Kratochvil and Becker (2012), Li (2004), Pao and Mow (1971)), ray techniques (Babich (1956), Pao and Gajewski (1977)), complex function methods (Liu et al. (1982), Yang et al. (2015)), integral equation methods (Boström (2003), Lu and Hanyga (2004), Ayatollahi et al. (2009)), matrix methods including reflectivity methods and generalized coefficient techniques (Kennett (1983)), and finally mode matching techniques (Fah (1992), Panza et al. (2009)); (b) numerical techniques based on direct time and space discretization of the elastodynamic equations which lead to finite difference methods (Boore (1972), Kristek and Moczo (2003)) and finite element methods (Komatitsch et al. (2010), Nakasone et al. (2000), Santare et al. (2003), Wolf and Song (1996), Wolf (2003), Zhang and Katsube (1995)). The alternative use of integral representations based on reciprocity

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theorems and the concurrent introduction of fundamental solutions of the governing differential equations leads to mesh reducing boundary element methods (Dominguez (1993), Dravinski and Yu (2011), Kausel (2006), Kobayashi (1983), Manolis and Beskos (1988), Manolis and Dineva (2015), Parvanova et al. (2013, 2014), Valeva and Ivanova (1998)); (c) hybrid techniques that combine the previously mentioned techniques in various ways (Dineva et al. (2012), Gatmiri and Arson (2008), Gatmiri et al. (2008), Manolis et al. (2015), Manolis and Dineva (2015), Mogilevskaya and Crouch (2001, 2002)).

During the last few years it has been recognized that the properties of a given material might not be primarily controlled by its chemical composition, but rather by its microstructure and more so by size ranging from nanometers to micrometers. The widely discussed in the literature size effect cannot be described by models in the framework of continuum mechanics and this demands the development of alternative models and of high-performance computational tools. When the characteristic cross-sectional dimension of a solid is in microns, the ratio of surface area to volume becomes an important parameter and the solid is strongly influenced by surface characteristics. These lead to distinct mechanical properties as compared with their bulk solid counterparts. With the rapid development of nanomechanical systems, size-dependent phenomena in the wave fields that develop in nanostructures with defects such as holes and inclusions are insufficiently understood and need further study. More specifically, variations in the surface energy in nanostructures are caused by relaxation of bonds between the surface atoms and this lead to formation of surface residual stress, which is something that does not happen inside the solid core. This behavior is a surface stress effect and is described in the surface elasticity model introduced by Gurtin and Murdoch (1975). It has been determined that surface stress is a summation of surface residual stress and surface elasticity. In Gurtin and Murdoch (1975), the interfaces between the nanoinhomogeneity and the matrix are regarded as 'thin' material surfaces that possess their own mechanical properties and surface tension. Furthermore, non-classical boundary conditions are derived for the tractions along an interface expressing a stress jump as we move from matrix to inclusion, due to the presence of surface stress related to the deformation-dependent surface energy. We note in passing that if the defects present in a material at the nanoscale are cracks, even more advanced mechanical theories must be used as surface effects will surely change the crack tip singularity values, see Sendova and Walton (2010).

A brief literature review for in-plane wave motion in heterogeneous nano-solids described by the Gurtin–Murdoch model points to the following: (a) most computational techniques used are actually analytical methods, and use of the boundary element method (BEM), which is most efficient for problems with low surface to volume ratios, is mostly absent (see Parvanova et al. 2015) for unbounded solids), except for static solutions. Also, the finite element method (FEM) is used to evaluate the contribution of surface stress to the total potential energy (see Wang et al. 2010) and the Gurtin–Murdoch surface stress model is implemented in commercial program ANSYS (2009) through its user programmable features. (b) There are no results for solution of in-plane wave diffraction problems in bounded heterogeneous solids at nanoscale; (c) in-plane diffraction of time-harmonic P- and SV- waves by nano-holes and nano-inclusions in unbounded solids were studied analytically in Ru et al. (2009), Wang et al. (2006), Wang (2009), and Zhang et al. (2011). More specifically, the wave function expansion method was used to derive analytical expressions for diffracted wave fields in the infinite elastic, isotropic plane with two circular holes in Wang (2009). Next, Wang et al. (2006) considered the diffraction of planar P- waves by a nano-sized circular hole using wave function expansion method. The same method was applied in Zhang and Katsube (1995) to study the diffraction of elastic waves by an array of cylindrical holes, including the effects of surface elasticity. The diffractions of planar P- and SV- waves by a cylindrical nano-cavity and nano-inclusion were investigated in Ru et al. (2009). Finally, Fang et al. (2010) analytically evaluated the presence of surfaces/interfaces on the dynamic stress around single circular hole, a single circular inclusion and two interacting circular nano-inclusions in an infinite matrix under P-waves.

A systematic study of the dynamic response of a finite elastic, isotropic solid with multiple heterogeneities at the nano-scale, which act both as wave scatterers and stress concentrators, seems necessary. To the authors' knowledge, the majority of current results in the field are for unbounded solids under static loads. In this respect, we believe that new results that take into account the interaction effect between the multiple inclusions and the external perimeter of the solid matrix at the nano-scale is both interesting and important. The present work is an effort in this direction and can be viewed as a continuation of our previous work (Parvanova et al. 2015) on the BEM modeling of wave scattering phenomena in an infinite elastic plane. Thus, we present new results for the interaction effect between the multiple nano-inclusions and the external perimeter of the elastic matrix.

More specifically, we focus on the 2D, time-harmonic elastodynamic problem for a finite, isotropic elastic solid at the nano-scale containing multiple heterogeneities of arbitrary configuration. To this purpose, we develop, verify and use for numerical simulations the following computational tools: (i) A BEM with 2D frequency-dependent fundamental solutions for the bulk solid; (ii) an FEM implementing of the surface effect on the contour of the nano-inclusion as one macro-finite element in the ANSYS (2009) software package. The paper is organized as follows: (a) we start with the formulation of the 2D elastodynamic problem for a finite, elastic and isotropic solid matrix with heterogeneous structure at the nano-scale solid under time-harmonic waves in Section 2; (b) we continue with a BEM reformulation at all interfaces to include surface effects in Section 3; (c) the FEM formulation and solution is developed in Section 4; (d) verification studies follow in Section 5 for the proposed numerical scheme; (e) comparison studies between the BEM and FEM follow in Section 6; (f) extensive parametric studies are conducted in Section 7 to investigate the effect of size-dependent effects in the solid matrix and finally (g) Section 8 lists the conclusions of the present study.

2. Problem statement

Consider wave motion in the plane $x_3 = 0$ for a Cartesian coordinate system $O\text{-}x_1x_2x_3$, where a finite-sized, elastic and isotropic solid with boundary Γ is subjected to time-harmonic loads with frequency ω, see Fig. 1. The solid matrix contains multiple nano-inclusions with boundaries Γ_I^n or nano-cavities Γ_H^n, where $n = 1, 2,\ldots, N$, of arbitrary shape, number, size and configuration. We assume that heterogeneities do not intersect and we denote their total surfaces as $\Gamma_I = \bigcup_{n=1}^{N} \Gamma_I^n$ and $\Gamma_H = \bigcup_{n=1}^{N} \Gamma_H^n$. The total boundary is then $S = \Gamma \cup \Gamma_H$ in the case of cavities (or holes) and $S = \Gamma \cup \Gamma_I$ in the case of inclusions. The material properties (Lamè constants and density) are denoted as λ_M, μ_M, ρ_M for the solid matrix and $\lambda_{I,n}, \mu_{I,n}, \rho_{I,n}$ for the nth inclusion. Furthermore, the displacement vector $u_i(x_1, x_2, \omega)$, (where $i, j = 1, 2$), the stresses $\sigma_{ij}(x_1, x_2, \omega)$ and the corresponding traction vector $t_i(x_1, x_2, \omega) = \sigma_{ij}(x_1, x_2, \omega)n_j$, ($n_j$ is the outward pointing unit normal vector) all satisfy the equations of motion in the bulk solid. In the absence of body forces, these are:

$$\sigma_{ij,i} + \rho\omega^2 u_j = 0 \tag{1}$$

where

$$\sigma_{ij} = \begin{cases} C_{ijkl}^{M} u_{k,l}^{M} (matrix) \\ C_{ijkl}^{I,n} u_{k,l}^{I,n} (n-th\ inclusion) \end{cases},$$

$$C_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),\ \rho = \begin{cases} \rho_M \\ \rho_{I,n} \end{cases} \tag{2}$$