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Dynamic strength around a coated nanowire with surfaces/interfaces in a half solid

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ABSTRACT

In this paper, the multiple scattering of anti-plane shear waves around a coated nanowire with surfaces/interfaces embedded in a half solid is studied, and the dynamic stress at the two surfaces/interfaces is presented. The boundary condition at the edge of the half solid is satisfied by the image method. The analytical solutions of displacements in the two half solids, in the coating layers, and inside the nanowire are expressed by wave function expansion method. The expanded mode coefficients are determined by satisfying the boundary conditions at the two surfaces/interfaces of the coated nanowire and the straight edge of the structure. The addition theorem for cylindrical wave function is employed to accomplish the superposition of displacement fields in the two half solids. Analyses show that the properties of the outer and inner interfaces show different effect on the dynamic stress around the nanowire. The dynamic stress distribution around the nanowire is also significantly related to the interfacial properties at the edge and the position of the nanowire.

1. Introduction

Composites embedded with nanowires are new and very promising materials for chemical and bio-chemical sensing since their geometrical properties can be tuned to match those of biological and chemical species. One of the most striking aspects of nanowires is the dramatically increase of surface-to-volume ratio due to the existence of coating layer [1].

Nanocomposites with nanowires may experience different working environments. Sensors from these materials will suffer from many kinds of loadings, and these loadings will degrade their function in serving life. Under these loadings, the stress concentration near the surface/interface can be a highly probable site of crack initiation and fracture because they often have weak bonding (low resistance to fracture) and stress concentration (high driving force for fracture) resulting from the deformation mismatch of dissimilar materials [2]. In past years, lots of theoretical and experimental works on the strength of nanocomposites resulting from surface/interface stress have been done. Fang et al. have studied a screw dislocation interacting with a coated nanowire with interface effects, and the interaction energy and force were calculated [3]. Using the molecular dynamics method, Tang et al. studied the mechanical properties of a silicon nanowire under uni-axial tension and compression [4].

The wave scattering around the inclusions, wires, multi-layers, and contacts in nanocomposite is a classical problem, which can be used to predict the dynamic response of structures [5–7]. In these papers, it is assumed that the elastic waves

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propagate in the infinite nanocomposites, which simplifies the wave propagation a great deal. Most recently, the propagation and multiple scattering of waves at the interfaces of two nanowires in an infinite solid have been investigated, and the surface/interface stress effect on the macroscopic dynamic stress was analyzed [8]. However, in practical engineering, the nanostructures are finite, and the reflection of elastic waves at the edges influences the wave fields and stability greatly. In many cases, it may play an important role. The nano-inclusions near the edge of finite structures present great difficulties and characteristics far beyond those present researches in which the body is in a boundless space.

In this paper, a half plane embedded with a coating nanowire under anti-plane shear waves is investigated, which is quite different from the infinite solids in Ref. [8], and the dynamic stresses at the two surfaces/interfaces are obtained. The boundary condition at the straight edge with interface effect is satisfied by the image method. The analytical solutions of displacements in the nanowires are expressed by wave function expansion method. The expanded mode coefficients are determined by satisfying the boundary conditions around the coated nanowire and the straight edge. The numerical solutions of dynamic stress concentration factor are graphically illustrated. The effects of the wave frequency, the material properties of wires, coating layers and interfaces, and the position of nanowire on the dynamic stress around the nanowires are analyzed.

2. Problem formulation

Consider a half solid embedded with a cylindrical nanowire with annular nanoscale coating layer, as depicted in Fig. 1. The outer and inner radii of the coating annulus are a_1 and a_2, respectively. The distance between the center of the cylindrical nanowire and the edge of the half solid is b .The interface stresses exist at the edge surface Γ, the outer interface Ω_1 and inner interface Ω_2 of the coating layer. It is assumed that an anti-plane shear wave with frequency ω impinges on the edge of the half solid. Let μ^m, ρ^m be the shear modulus and mass density of the matrix solid, μ^w, ρ^w those of the nanowire, and μ^c, ρ^c those of nanoscale coating layer. It should be noted that in the following, the superscripts m, w, and c represent the matrix solid, nanowire, and coating layer, respectively.

In nanocomposites with nanowires, interfaces around the nanowires play an important role in determining the dynamic strength of nanocomposites. To analyze the quantum confinement effect, the surface/interface theory is proposed. In the work of Gurtin and Murdoch [9], the surface/interface region is regarded as a layer of vanishing thickness adhering to the solid without slipping. The elastic field within the bulk solid is described by the differential equations of classical elasticity, while the interface has its own elastic constants and is characterized by an additional constitutive law. The shear modulus and mass density of the edge surface Γ, the outer interface Ω_1, and the inner interface Ω_2 are denoted as μ^{s0}, ρ^{s0}, μ^{s1}, ρ^{s1}, and μ^{s2}, ρ^{s2}, respectively. It should be noted that the mass density shows little effect on the dynamic stress in the solid, and is ignored in this paper.

The surface/interface properties can be determined by molecular dynamics simulations or experiments. Experimental methods to access the interfacial boundaries at an atomistic level are often complicated and the resolution is limited. Atomistic simulation is the theoretical and computational modelling of what happens at the atomic scale in solids and molecules, and it can provide important insight into the unexpected properties of surface/interface at the atomic and electronic level, which are very difficult to obtain from experiments. In addition, atomistic simulation can also be used to interpret existing experimental data and predict new phenomena.

The medium, coating layers, and wires are all assumed to be isotropic. When the anti-plane shear wave propagates in the medium, only the displacement component in the z direction exists. The governing equation in the medium can be expressed as

$$\frac{\partial^2 W}{\partial x^2}+\frac{\partial^2 W}{\partial y^2}=\frac{1}{c}\frac{\partial^2 W}{\partial t^2}, \tag{1}$$

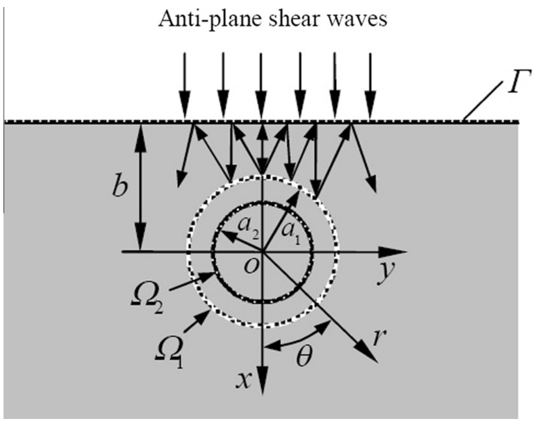

Fig. 1. A half solid with a cylindrical nanowire and the incident waves.