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**COLLABORATIVE RESEARCH AND DEVELOPMENT  
(CR&D)**

**Delivery Order 0060: Gradient Materials Morphology Modeling  
Support**

**Ernie Pan**

**University of Akron**

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**Final Report**

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<b>14. ABSTRACT</b> This research in support of the Air Force Research Laboratory Materials and Manufacturing Directorate was conducted at Wright-Patterson AFB, Ohio from 7 August 2006 through 8 August 2007. Dislocation mobility and stability in nanocrystals and electronic materials are influenced by the material composition and interface conditions. Its mobility and stability then affect the mechanical behaviors of the composites. In the JMPS paper, we first address, in detail, the problem of a screw dislocation located in an annular coating layer which is imperfectly bonded to the inner circular inhomogeneity and to the outer unbounded matrix. Both the inhomogeneity-coating interface and coating-matrix interface are modeled by a linear spring with vanishing thickness to account for the possible damage occurring on the interface. An analytic solution in series form is derived by means of complex variable method, with all the unknown constants being determined explicitly. The solution is then applied to the study of the dislocation mobility and stability due to its interaction with the two imperfect interfaces.					
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# **Final Report for Task Order 0060 On Gradient Materials Morphology Modeling Support**

by

Ernie Pan

Computer Modeling & Simulation Group  
Department of Civil Engineering and Department of Applied Mathematics,  
University of Akron, OH 44325-3905  
Email: pan2@uakron.edu  
Tel: 330-972-6739

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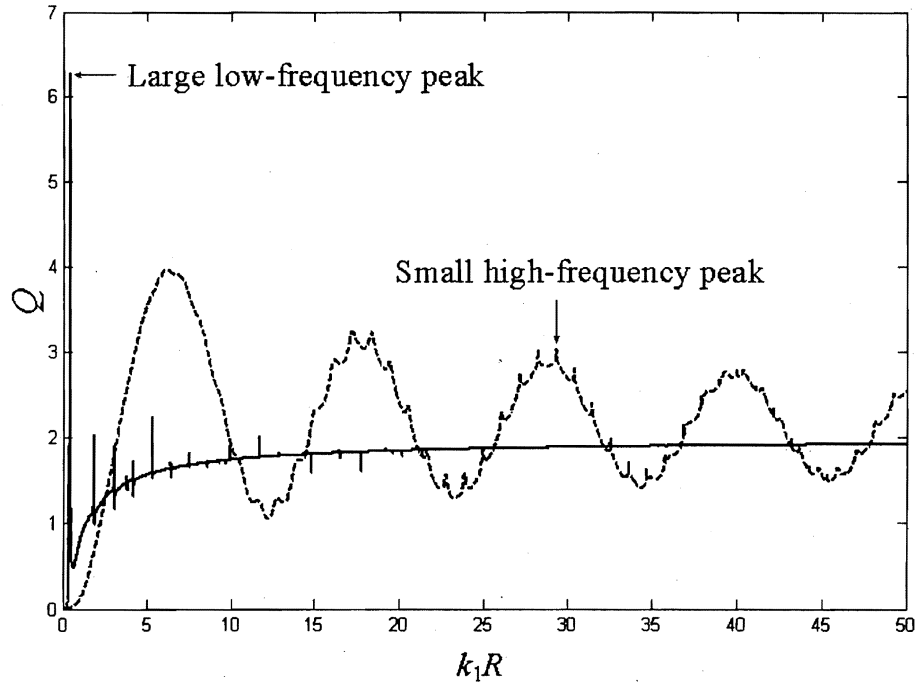
Thanks to the sponsorship by AFRL 06-S531-060-C1 and the supervision of Dr. Ajit Roy at AFRL, we have accomplished a couple of important subtasks under the four main tasks outlined in the proposal. These accomplishments have been published or accepted for publication in five peer reviewed journal papers.

- [1] Wang, X., Pan, E., Roy, A. K., 2007. New phenomena concerning a screw dislocation interacting with two imperfect interfaces. **Journal of the Mechanics and Physics of Solids** (In press, published online).
- [2] Wang, X., Pan E., Roy, A. K., 2007. Scattering of antiplane shear wave by a piezoelectric circular cylinder with an imperfect interface. **Acta Mechanica** (In press, published online).
- [3] Wang, X., Pan, E., Roy, A. K., 2007. A functionally graded plane with a circular inclusion under uniform antiplane eigenstrain. **ASME Journal of Applied Mechanics** (In press, to appear in the September issue).
- [4] Wang, X., Pan, E., Roy, A. K., 2007. Three-dimensional Green's functions for a steady point heat source in a functionally graded half-space and some related problems. **International Journal of Engineering Science** (In press, published online).
- [5] Wang, X., Pan, E., Roy, A. K., 2007. A circular inhomogeneity with viscoelastic interface under antiplane shear. **AIAA Journal** (Accepted).

**Listed below is a more detailed description on our achievements.**

- Dislocation mobility and stability in nanocrystals and electronic materials are influenced by the material composition and interface conditions. Its mobility and stability then affect the mechanical behaviors of the composites. In the **JMPS paper [1]**, we first address, in detail, the problem of a screw dislocation located in an annular coating layer which is imperfectly bonded to the inner circular inhomogeneity and to the outer unbounded matrix. Both the inhomogeneity-coating interface and coating-matrix interface are modeled by a linear spring with vanishing thickness to account for the possible damage occurring on the interface. An analytic solution in series form is derived by means of complex variable method, with all the unknown constants being determined explicitly. The solution is then applied to the study of the dislocation mobility and stability due to its interaction with the two imperfect interfaces. The most interesting finding is that when the middle coating layer is more compliant than both the inner inhomogeneity and the outer unbounded matrix and when the interface rigidity parameters for the two imperfect interfaces are greater than certain values, one stable and two unstable equilibrium positions can exist for the dislocation. Furthermore, under certain conditions an equilibrium position, which can be either stable or unstable (i.e., a saddle point), can exist, which has never been observed in previous studies. Results for a screw dislocation interacting with two parallel straight imperfect interfaces are also presented as the limiting case where the radius of the inner inhomogeneity approaches infinity while the thickness of the coating layer is fixed.
- In the **Acta Mechanica paper [2]**, we present analytical solutions for the scattering of antiplane shear wave by a piezoelectric circular cylinder with an imperfect interface. We first consider the simple case in which the imperfection is homogeneous along the interface. Two typical imperfect interfaces are addressed: 1) mechanically compliant and dielectrically weakly conducting interface; 2) mechanically compliant and dielectrically highly conducting interface. The expressions for the directivity pattern and scattering cross-section of the scattered antiplane shears wave are derived.

We then investigate the more difficult problem in which the imperfection is circumferentially inhomogeneous along the interface. A concise expression for an inhomogeneously compliant and weakly conducting interface is derived by means of matrix notation. Numerical examples are presented to demonstrate the effect of the imperfection and the circumferential inhomogeneity of the interface on the directivity patterns and scattering cross-sections of the scattered antiplane shear wave. The circumferentially inhomogeneous interface is also utilized to model the interface where an arbitrary number of cracks exist. Results show that when every part of the interface is rather compliant, large low-frequency peaks of the scattered cross-sections as shown in Fig. 1, which correspond to the resonance scattering, can be observed no matter whether the interface is homogeneous or inhomogeneous. The appearance of large low-frequency peaks can be well explained by estimating the natural frequency of the corresponding reduced mass-spring system where the cylinder is assumed as a rigid body. Peaks of the scattered cross-sections spanning from low frequencies to high frequencies can be observed for a partially debonded



**Fig. 1** Scattering cross-sections of the scattered shear wave for a perfect interface (dashed lines) and for a rather compliant and insulating interface  $\alpha=0.1\mu_1/R$ ,  $\beta=0$  (solid lines).

cylinder.

- In the JAM paper [3], the problem of a functionally graded plane with a circular inclusion under a uniform antiplane eigenstrain is investigated, where the shear modulus varies exponentially along the  $x$ -direction. By introducing a new function which satisfies the Helmholtz equation, the general solution to the original problem is derived in terms of series expansion. Numerical results are then presented which demonstrate clearly that for a functionally graded plane, the strain and stress fields inside the circular inclusion under uniform antiplane eigenstrains are intrinsically nonuniform. This phenomenon differs to the corresponding homogeneous material case where both the strain and stress fields are uniform inside the circular inclusion.

We consider an infinite FGM in the  $x$ - $y$  plane, and assume that the shear modulus  $\mu$  of the FGM varies exponentially in  $x$ -direction as

$$\mu = e^{2\beta x} \mu_0, \quad (1)$$

where  $\mu_0$  is the homogeneous shear modulus and  $\beta$  the gradient factor of the FGM.

We also assume that, within the FGM, there is a circular inclusion  $r = \sqrt{x^2 + y^2} \leq R$  which undergoes uniform antiplane eigenstrains  $\varepsilon_{xx}^*$  and  $\varepsilon_{yy}^*$ . The boundary condition along the inclusion-matrix interface  $r = R$  is assumed to be fully bonded, and can be expressed in terms of the out-of-plane elastic displacements  $w^{(1)}$  inside the inclusion and  $w^{(2)}$  outside, as

$$\begin{aligned} w^{(1)} + w^* &= w^{(2)}, \\ \frac{\partial w^{(1)}}{\partial r} &= \frac{\partial w^{(2)}}{\partial r}, \end{aligned} \quad (r = R) \quad (2)$$

where  $w^* = r(\varepsilon_{xx}^* - i\varepsilon_{yy}^*)e^{i\theta} + r(\varepsilon_{xx}^* + i\varepsilon_{yy}^*)e^{-i\theta}$  is the additional displacement corresponding to the uniform eigenstrains  $\varepsilon_{xx}^*, \varepsilon_{yy}^*$ .

We now introduce a new function  $\varphi$  which is related to  $w$  through the following relation

$$w = e^{-\beta x} \varphi \quad (3)$$

It is easy to show that, in terms of the new function  $\varphi$ , the boundary condition (2) can be equivalently expressed as

$$\begin{aligned}\varphi^{(2)} - \varphi^{(1)} &= e^{\beta x} w^*, \\ \frac{\partial \varphi^{(2)}}{\partial r} - \frac{\partial \varphi^{(1)}}{\partial r} &= \beta e^{\beta x} \cos \theta w^*,\end{aligned}\quad (r = R) \quad (4)$$

where  $\varphi^{(1)}$  and  $\varphi^{(2)}$  are within and outside the inclusion, respectively. They satisfy the following Helmholtz equations

$$\begin{aligned}\frac{\partial^2 \varphi^{(1)}}{\partial x^2} + \frac{\partial^2 \varphi^{(1)}}{\partial y^2} - \beta^2 \varphi^{(1)} &= 0, \quad \sqrt{x^2 + y^2} \leq R \\ \frac{\partial^2 \varphi^{(2)}}{\partial x^2} + \frac{\partial^2 \varphi^{(2)}}{\partial y^2} - \beta^2 \varphi^{(2)} &= 0, \quad \sqrt{x^2 + y^2} \geq R\end{aligned} \quad (5)$$

In view of Eq. (5),  $\varphi^{(1)}$  and  $\varphi^{(2)}$  can be expressed in terms of series expansion as

$$\varphi^{(1)} = \sum_{n=-\infty}^{+\infty} A_n^{(1)} I_n(|\beta|r) e^{in\theta}, \quad 0 \leq r \leq R \quad (6)$$

$$\varphi^{(2)} = \sum_{n=-\infty}^{+\infty} A_n^{(2)} K_n(|\beta|r) e^{in\theta}, \quad r \geq R \quad (7)$$

where  $I_n$  and  $K_n$  are the modified  $n$ th-order Bessel functions of the first and second kinds, respectively;  $A_n^{(1)}$  and  $A_n^{(2)}$  are unknown coefficients to be determined.

By enforcing the boundary condition (4), we determine the unknown expansion coefficients in Eqs. (6) and (7) as

$$\begin{aligned}\begin{bmatrix} A_n^{(1)} \\ A_n^{(2)} \end{bmatrix} &= \frac{R}{K_n(|\beta|R) I_n'(|\beta|R) - I_n(|\beta|R) K_n'(|\beta|R)} \begin{bmatrix} K_n'(|\beta|R) & -K_n(|\beta|R) \\ I_n'(|\beta|R) & -I_n(|\beta|R) \end{bmatrix} \\ &\times \begin{bmatrix} I_{n-1}(\beta R)(\varepsilon_{zx}^* - i\varepsilon_{zy}^*) + I_{n+1}(\beta R)(\varepsilon_{zx}^* + i\varepsilon_{zy}^*) \\ \frac{\beta}{2|\beta|} \{ [I_{n-2}(\beta R) + I_n(\beta R)](\varepsilon_{zx}^* - i\varepsilon_{zy}^*) + [I_n(\beta R) + I_{n+2}(\beta R)](\varepsilon_{zx}^* + i\varepsilon_{zy}^*) \} \end{bmatrix},\end{aligned} \quad (8)$$

where the prime (') denotes the derivative with respect to the variable in the parenthesis.

- In the **IJES paper [4]**, three-dimensional Green's functions are derived for a steady point heat source in a functionally graded half-space, in which the thermal conductivity varies exponentially along an arbitrary direction. We first introduce an



auxiliary function which satisfies an inhomogeneous Helmholtz equation. Then by virtue of the image method which was first proposed by Sommerfeld for the homogeneous half-space Green's function of a steady point heat source, we arrive at an explicit expression for this auxiliary function. With this auxiliary function, we finally derive the three-dimensional Green's functions due to a steady point heat source in a functionally graded half-space. Also investigated in this paper are the temperature field induced by a point heat source moving at a constant speed in a functionally graded infinite space; the electric potential due to a static point electric charge in a dielectric space with electric field gradient effects; and two-dimensional time-harmonic dynamic Green's functions for homogeneous and functionally graded materials with strain gradient effects.

The explicit expression of the three-dimensional Green's functions due to a steady point heat source in a functionally graded half-space can be finally derived as

$$T = \frac{H}{4\pi k_0} \exp\left[-\frac{\beta_1 x + \beta_2 y + \beta_3(z+h)}{2}\right] \left\{ \frac{\exp\left[-\alpha\sqrt{x^2 + y^2 + (z-h)^2}\right]}{\sqrt{x^2 + y^2 + (z-h)^2}} + \frac{\exp\left[-\alpha\sqrt{x^2 + y^2 + (z+h)^2}\right]}{\sqrt{x^2 + y^2 + (z+h)^2}} - 2\gamma \int_0^{+\infty} \frac{\exp\left[-\alpha\sqrt{x^2 + y^2 + (z+h+\eta)^2} - \gamma\eta\right]}{\sqrt{x^2 + y^2 + (z+h+\eta)^2}} d\eta \right\},$$

(z ≥ 0) (9)

where  $\alpha = \frac{\sqrt{\beta_1^2 + \beta_2^2 + \beta_3^2}}{2}$ ,  $\gamma = \lambda + \frac{\beta_3}{2}$  and  $k_0, \beta_1, \beta_2, \beta_3$  are material constants.

The temperature field induced by a point heat source moving at a constant speed in a functionally graded infinite space is

$$T = \frac{H}{4\pi k_0} \frac{1}{\sqrt{(x-Vt)^2 + y^2 + z^2}} \times \exp\left[-\frac{(V/k_d)(x-Vt) + \beta_2 y + \beta_3 z}{2} - \frac{\sqrt{(V/k_d)^2 + \beta_2^2 + \beta_3^2}}{2} \sqrt{(x-Vt)^2 + y^2 + z^2}\right]$$

(10)

The electric potential due to a static point electric charge in a dielectric space with electric field gradient effects is

$$\phi = \frac{Q}{4\pi\epsilon} \frac{1 - \exp\left(-l^{-1}\sqrt{x^2 + y^2 + z^2}\right)}{\sqrt{x^2 + y^2 + z^2}}. \quad (11)$$

It is of interest to observe that Eq. (11) for the expression of the electric potential due to a point charge in a dielectric ceramic with electric field gradient effects is still *finite* (or non-singular) when  $r = \sqrt{x^2 + y^2 + z^2} \rightarrow 0$  (i.e., when approaching the location of the electric charge). More specifically

$$\lim_{r \rightarrow 0} \phi = \frac{Q}{4\pi\epsilon l}, \quad (12)$$

which is inversely proportional to  $l$ . Furthermore it can be proved that

$$\lim_{r \rightarrow 0} \frac{d^n \phi}{dr^n} = (-1)^n \frac{Q}{4\pi\epsilon (n+1)l^{n+1}}, \quad (n = 0, 1, 2, 3, \dots), \quad (13)$$

where  $\frac{d^0 \phi}{dr^0} = \phi$ .

The two-dimensional time-harmonic dynamic Green's functions for homogeneous and functionally graded materials with strain gradient effects are

$$w = \frac{p}{2\pi\sqrt{1+4k^2l^2}\mu} \left[ \frac{i\pi}{2} H_0^{(1)}(k_1 r) - K_0(k_2 r) \right], \quad (14)$$

for a homogeneous material, and

$$w = \frac{p\tilde{l}^2}{2\pi\sqrt{1+4\tilde{k}^2\tilde{l}^2}\mu_0} \exp\left(-\frac{\beta}{2}y\right) \left[ \frac{i\pi}{2} H_0^{(1)}(k_1 r) - K_0(k_2 r) \right], \quad (15)$$

or

$$w = \frac{p\tilde{l}^2}{2\pi\sqrt{1-4\tilde{k}^2\tilde{l}^2}\mu_0} \exp\left(-\frac{\beta}{2}y\right) [K_0(k_1 r) - K_0(k_2 r)], \quad (16)$$

for a functionally graded material.

- In the **AIAA paper** [5], we address in detail a circular inhomogeneity with viscoelastic interface subjected to remote uniform antiplane shear stresses. Both the inhomogeneity and the surrounding matrix are assumed to be elastic and quasi-static, while the interface is viscoelastic modeled by a linear spring and dashpot. Exact closed-form solutions for both the Kelvin-and Maxwell-type viscoelastic interfaces

are obtained by means of the complex variable method. It is observed that when the matrix is subjected to remote uniform shear stresses, the stress field inside the inhomogeneity, although time-dependent, is still uniform. The derived solutions are then used to predict the time-dependent effective shear modulus of the composite based on the Mori-Tanaka mean field approximation.

By using the Mori-Tanaka mean-field method, the time-dependent effective shear modulus of a composite containing randomly aligned fibers of the same radius with Kelvin-type interface on the  $xy$  plane can be derived to be

$$\mu^* = \mu_2 \frac{1 - c \left[ \frac{\mu_1 + \mu_2 + \chi(\mu_2 - \mu_1)}{(\chi + 1)(\mu_1 + \mu_2)} - \frac{2\mu_1}{(\chi + 1)(\mu_1 + \mu_2)} \exp\left(-\frac{\chi + 1}{\gamma} t\right) \right]}{1 + c \left[ \frac{\mu_1 + \mu_2 + \chi(\mu_2 - \mu_1)}{(\chi + 1)(\mu_1 + \mu_2)} - \frac{2\mu_1}{(\chi + 1)(\mu_1 + \mu_2)} \exp\left(-\frac{\chi + 1}{\gamma} t\right) \right]}, \quad (17)$$

where  $\mu^*$  is the time-dependent effective shear modulus,  $c$  is the volume fraction of the fiber. It is seen that the effect shear modulus is determined by the shear moduli of the fiber and the matrix, the volume fraction  $c$  of the fiber, the interface rigidity  $\chi$ , the characteristic time  $\gamma$ .

The time-dependent effective shear modulus of a composite containing randomly aligned fibers of the same radius with the Maxwell-type interface on the  $xy$  plane can be derived as

$$\mu^* = \mu_2 \frac{1 - c \left[ 1 - \frac{2\chi\mu_1}{(\chi + 1)(\mu_1 + \mu_2)} \exp\left(-\frac{\chi t}{\gamma(\chi + 1)}\right) \right]}{1 + c \left[ 1 - \frac{2\chi\mu_1}{(\chi + 1)(\mu_1 + \mu_2)} \exp\left(-\frac{\chi t}{\gamma(\chi + 1)}\right) \right]}. \quad (18)$$

It is added that the method presented here could be extended to address the interface described by a standard linear solid model, which combines the Maxwell-model and a linear spring in parallel.