ON THE MODELING OF NANOCONTACTS MADE OF THIN FILMS

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Abstract. The paper is using the nonlocal field equations for modelling a nanocontact made of thin films. The theory describes long-range interactions among the particles. An elastic layer loaded by a rigid indenter is considered. We show that the stress field is finite for all points and have a maximum value that does not occur at the boundary of the contact domain.

Key words: chalcogenide material, nanocontact, intermolecular.

1. INTRODUCTION

The classical mechanics is not working to all physical situations where the systems have dimensions comparable with the characteristic inner length of the material. The long-range interactions between the particles [1–4] are described by a nonlocal theory because the stress components at a location (atom, molecule, grain) need a description based on the interatomic interaction potentials [5–9].

The response of the body to external forces depends of the length and the time scale. That means, the response depends on the ratio $(\lambda / l, \tau / \tau_0)$ or $(\lambda / l, \omega_0 / \omega)$ where λ is the characteristic length of the body (can be an atomic distance, a granular distance etc.). Here, l is the external length associated with the external forces, τ the time scale or the frequency ω (the minimum transmission time of a signal or a frequency) and τ_0 is the external time or frequency associated with the external forces [8]. In general, the theories assume that $\lambda / l << 1$ and $\tau / \tau_0 << 1$. That means the external forces excite the all regions simultaneously, so that the regions interact each other and the result is a statistical average of the individual responses.

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For $\lambda / l = 1$ and $\tau / \tau_0 = 1$, the balance laws of the nonlocal theory are written by using the intermolecular and atomic forces. The balance laws for a body of a volume V and a surface ∂V, state that the time rate of a field ϕ (mass, momentum, moment of momentum, energy) is balanced by the surface flux $\boldsymbol{\tau}$ and the body source g [5–8]

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V-\sigma} \phi \mathrm{d}v - \int_{\partial V-\sigma} \boldsymbol{\tau}\cdot \mathrm{d}\mathbf{a} - \int_{\partial V-\sigma} g \mathrm{d}v = 0 . \tag{1}$$

In (1) we have excluded the points from the discontinuity surface which move into the body with a velocity in the direction of its unit normal.

The relation (1) can be rewritten by using the Green-Gauss theorem

$$\int_{V-\sigma} \left[\phi_{,t} + \mathrm{div}(\phi\tilde{\mathbf{v}} - \boldsymbol{\tau}) - g\right]\mathrm{d}v + \int_{\sigma} \left[\phi(\tilde{\mathbf{v}} - \mathbf{v}) - \boldsymbol{\tau}\right]\cdot \mathbf{n}\mathrm{d}a = 0 , \tag{2}$$

where $\tilde{\mathbf{v}}$ is the velocity vector, and the bracket is the jump of the quantity at σ.

The relation (2) is valid for every part of the body and the localization condition yields to the vanishing of integrants into the integrals.

In the following this assumption is abandoned, but the localization is yet possible by using the localization residuals which must integrate to zero.

The residuals describe the effects of all points of the body to one point inside the body. This means the residuals are the long-range terms of all point $\mathbf{x}$ at which the balance laws are localised.

The nonlocal continuum field theory is concerned with the physics of material bodies whose behavior at a material point is influenced by the state of all points of the body. The material points of a body have assigned some physically independent variables (*e.g.*, mass, charge, electric field, magnetic field).

The balance laws of the nonlocal theory are written as

$$\phi_{,t} + \mathrm{div}(\phi\tilde{\mathbf{v}} - \boldsymbol{\tau}) - g = \hat{g} \text{ in } V-\sigma,\ \left[\phi(\tilde{\mathbf{v}} - \mathbf{v}) - \boldsymbol{\tau}\right]\cdot \mathbf{n} = \hat{G} \text{ on } \sigma, \tag{3}$$

subject to

$$\int_{V-\sigma} \hat{g}\mathrm{d}v + \int_{\sigma} \hat{G}\mathrm{da} = 0 . \tag{4}$$

The nonlocal balance laws for mass, momentum, moment of momentum and energy become by using (3) and (4)

$$\rho_{,t} + \mathrm{div}(\rho\tilde{\mathbf{v}}) = \hat{\rho} , \tag{5}$$

$$\mathrm{div}\,\mathbf{t}_k + \rho(\mathbf{f} - \dot{\tilde{\mathbf{v}}}) = \hat{\rho}\tilde{\mathbf{v}} - \rho\hat{\mathbf{f}} , \tag{6}$$

$$\mathbf{i}_k \times \mathbf{t}_k - \rho(\mathbf{x} \times \hat{\mathbf{f}} - \hat{\mathbf{l}}) = 0\,, \tag{7}$$

$$-\rho\dot{\varepsilon} + \mathbf{t}_k \cdot \tilde{\mathbf{v}}_{,k} + \nabla \cdot \mathbf{q} + \rho h - \hat{\rho}(\varepsilon - \frac{1}{2}\tilde{v} \cdot \tilde{v}) - \rho\hat{\mathbf{f}} \cdot \tilde{\mathbf{v}} + \rho\hat{h} = 0, \tag{8}$$

$$\int_V \hat{\rho}\mathrm{d}v = 0, \quad \int_V \rho\hat{\mathbf{f}}\,\mathrm{d}v = 0, \quad \int_V \rho\hat{\mathbf{l}}\,\mathrm{d}v = 0, \quad \int_V \rho\hat{h}\,\mathrm{d}v = 0\,, \tag{9}$$

where a superposed dot a material time derivative. Here, ρ is the mass density, $\mathbf{t}_k = \mathbf{t}_{kl}\iota_l$ the stress tensor, $\mathbf{i}_k$ the Cartesian unit vectors, ε the internal energy density, $\mathbf{q}$ the heat flow vector, h heat source per unit mass, $\hat{\rho}$ the mass residual, $\hat{\mathbf{f}}$ the body force residual, $\hat{\mathbf{l}}$ the body couple residual, $\hat{h}$ the energy residual, all residuals being the nonlocal production of these quantities per unit mass due to the rest of the body.

The residuals describe the effects of all points of the body to one point inside the body. The second law of thermodynamics gives

$$\rho\dot{\eta} - \nabla \cdot \mathbf{q} - \frac{\rho h}{\theta} - \rho\hat{b} + \hat{\rho}\eta \geq 0 \,\mathrm{in}\, V - \sigma\,, \tag{10}$$

where η is the entropy density, θ is the absolute temperature and $\hat{b}$ is entropy residual subject to

$$\int_V \rho\hat{b}\,\mathrm{d}v = 0\,. \tag{11}$$

2. THE NONLOCAL THEORY

We start with some results demonstrated by Eringen in 1972 [5] .

The first result is related to the linear theory of the nonlocal elastic materials, whose natural state is free of the nonlocal effects. Eringen states that that the nonlocal body force vanishes, i.e. $\hat{f}_k = 0$.

The second results states that the constitutive equations of the nonlocal linear homogeneous and isotropic elastic solids and residuals do not violate the global entropy inequality (10) and (11) if and only if they are of the form

$$t_{kl} = \lambda e_{rr}\delta_{kl} + 2\mu e_{kl} + \int_{V-\sigma} (\lambda_1' e_{rr}' \delta_{kl} + 2\mu_1' e_{kl}')\mathrm{d}v' \tag{12}$$

$$\Sigma = \Sigma_0 + \frac{1}{2}\lambda(e_{kk})^2 + \mu e_{kl} d_{kl} + \int\limits_{V-\sigma} (\frac{1}{2}\lambda'_1 e_{kk} e'_{ll} + \mu'_1 e_{kl} e'_{kl})\mathrm{d}v' ,$$
$$\hat{\rho} = 0 ,\ \hat{f}_k = 0 , \tag{13}$$

where λ, μ are the classical Lamé elastic constants, and λ' and μ' are the nonlocal Lamé elastic functions which depend on $|\mathbf{x}' - \mathbf{x}|$, Σ is a functional over all argument functions of $\mathbf{x}'$ covering the entire body, defined by $\rho_0\psi = \Sigma(\mathbf{x}', \mathbf{x}'_{,k})$, with $\psi = \varepsilon - \theta\eta$ the free energy functional, Σ_0 refers to the value in the natural state, and ρ_0 the density in the natural state, δ_{kl} is the Kronecher delta, e_{kl} is the strain tensor of the linear theory

$$e_{kl} = \frac{1}{2}(u_{k,l} + u_{l,k}) , \tag{14}$$

and u_k the components of the displacement vector.

The prime index indicates that they depend on $\mathbf{x}'$ and $t' \le t$, where $\mathbf{x}'$ is any other point in the body and t' any time at or prior to present time t. The conditions $\hat{\rho} = 0$, $\hat{f}_k = 0$ means that we don't have the mass and body force nonlocal production in the body.

The nonlocal Lamé elastic functions $\lambda'(|\mathbf{x}' - \mathbf{x}|)$ and $\mu'(|\mathbf{x}' - \mathbf{x}|)$ are positive decreasing functions of $|\mathbf{x}' - \mathbf{x}|$.

Relations (12) and (13) are rewritten by incorporating λ and μ into λ' and μ'

$$t_{kl} = \int\limits_{V-\sigma} [\lambda'(|\mathbf{x}' - \mathbf{x}|)e'_{rr}(\mathbf{x}')\delta_{kl} + 2\mu'(|\mathbf{x}' - \mathbf{x}|)e'_{kl}(\mathbf{x}')]\mathrm{d}v'(\mathbf{x}') , \tag{15}$$

$$\Sigma = \Sigma_0 + \int\limits_{V-\sigma} \Big[\frac{1}{2}\lambda'(|\mathbf{x}' - \mathbf{x}|)e_{kk}(\mathbf{x})e'_{ll}(\mathbf{x}') + \mu'(|\mathbf{x}' - \mathbf{x}|)e_{kl}(\mathbf{x})e'_{kl}(\mathbf{x}')\Big]\mathrm{d}v'(\mathbf{x}'). \tag{16}$$

3. THE NONLOCAL CONTACT PROBLEM

One of the great advantages of nanoindentation is that the properties such as the hardness and elastic modulus can be measured by simple analyses of indentation load-displacement data [10, 11]. This technique is used for determining the mechanical properties of thin films, thin surface layers and very small volumes of material at very small scales. The plane problem of a layer of thickness h and length $2L$ on a rigid horizontal plane, loaded by a rectangular rigid indenter with a flat horizontal base of width $2a$ is considered, Fig. 1. The contact along the interface is frictionless and we suppose that no tensile stress or tractions can be transmitted across the interface.

The layer is subjected to vertical gravity body forces. Here, V is the volume of the layer and S is the surface between the indenter and the layer.

The response of any point in V depends on the state of whole volume described by the constitutive laws (15) written for the layer

$$t_{kl} = \int_{V_1} [\lambda' (|\mathbf{x}' - \mathbf{x}|) e'^{1}_{rr}(\mathbf{x}')\delta_{kl} + 2\mu' (|\mathbf{x}' - \mathbf{x}|) e'^{1}_{kl}(\mathbf{x}')] \mathrm{d}v'(\mathbf{x}') . \quad (17)$$

The Lamé constants for a nonlocal medium are

$$\lambda' (|\mathbf{x}' - \mathbf{x}|) = \alpha(|\mathbf{x}' - \mathbf{x}|)\lambda,\ \mu (|\mathbf{x}' - \mathbf{x}|) = \alpha(|\mathbf{x}' - \mathbf{x}|)\mu , \quad (18)$$

where λ and μ are the Lamé constants for the nonlocal case, and $\alpha(|\mathbf{x}' - \mathbf{x}|)$ is the nonlocal kernel function which measures the effect of the strain at $\mathbf{x}'$ on the stress at $\mathbf{x}$.

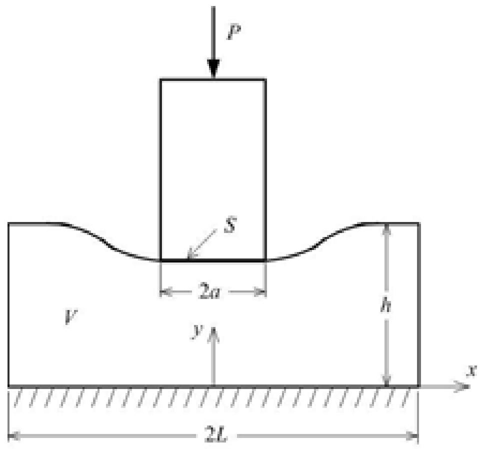

Fig. 1 – The indentation scheme.

Eringen [8] state that

$$t_{kl} = \int_{V} \alpha(|\mathbf{x}' - \mathbf{x}|)\sigma_{kl}(\mathbf{x}')\mathrm{d}v'(\mathbf{x}') , \quad (19)$$

with the local stress field $\sigma_{kl}(\mathbf{x}')$.

The kernel function is given by the Artan representation [9]

$$\alpha(|\mathbf{x}'-\mathbf{x}|)=\begin{cases} B\left\{1-\dfrac{|\mathbf{x}'-\mathbf{x}|}{d}\right\}, & |\mathbf{x}'-\mathbf{x}|<d, \\ 0, & |\mathbf{x}'-\mathbf{x}|>d, \end{cases} \tag{20}$$

where $B=1/d$, with d the atomic distance, $d=4\times10^{7}\,\text{cm}$ [9].

The local stress field under the frictionless punch is [12, 13]

$$\sigma(x)=-\rho gh+ \\ +\frac{1}{\pi h}\int_{-a}^{a}\int_{-L}^{L}\sigma(t)\frac{\exp(u)[(1+u)\exp(2u)+u-1]}{\exp(4u)+4u\exp(2u)-1}\cos[(t-x)\frac{u}{h}]\mathrm{d}u\mathrm{d}t, \tag{21}$$

$$\int_{-a}^{a}\sigma(t)\mathrm{d}t=P\,. \tag{22}$$

The nonlocal stress under the punch is calculated from (19)

$$t(x)=\int_{x-d}^{x+d}\left(1-\frac{|x-x'|}{d}\right)\sigma(x)\mathrm{d}x', \tag{23}$$

where $\sigma(x)$ is given by (21) and (22).

By introducing the dimensionless quantities

$$s=\frac{t}{a},\quad q=\frac{x}{L},\quad f(s)=\frac{\sigma(as)}{\rho gh}, \tag{24}$$

the equations (21) and (22) become

$$\frac{\sigma(x)}{\rho gh}=-1+ \\ +\frac{aL}{\pi h}\int_{-1}^{1}\int_{-1}^{1}f(s)\frac{\exp(qL)[(1+qL)\exp(2qL)+qL-1]}{\exp(4qL)+4qL\exp(2qL)-1}\cdot \\ \cdot\cos[(as-x)\frac{qL}{h}]\mathrm{d}q\mathrm{d}s, \tag{25}$$

$$\frac{a}{h}\int_{-1}^{1}f(s)\mathrm{d}s=\frac{P}{\rho gh^{2}}\,. \tag{26}$$

Now, we calculate the contact stresses for $a/h=0.3$, $L/h=10$.The following results are observed.

For the local case, the results are identically to those given in [12].

Near the boundary of the contact domain $x/a \to 1$, the stress field tends to infinity.

For $d \to 0$ the stresses are the same with the local stresses inside the contact domain. This means that the nonlocal theory of elasticity will not provide new insight into the problem for the points into the contact domain.

Figures 2 and 3 show the difference between the local and nonlocal fields of stresses for $a/h = 0.5$ and respectively $a/h = 0.3$. The figures show that for the points of the neighbourhood of the boundary $x/a > 0.95$ for the first case, and for $x/a > 0.965$ for the second case, or on the boundary of the contact domain $x/a = 1$, then the difference between solutions obtained in both theories cannot be ignored. The nonlocal stresses are finite at all points of the boundary of the contact domain.

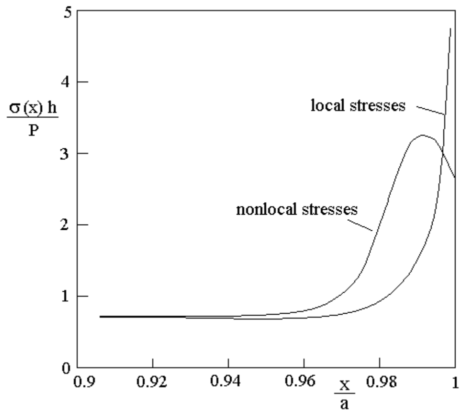

Fig. 2 – The local and nonlocal stresses near the boundary of the contact domain for $a/h = 0.5$.

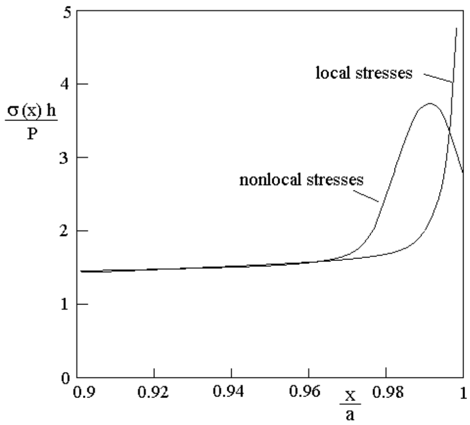

Fig. 3 – The local and nonlocal stresses near the boundary of the contact domain for $a/h = 0.3$.

The nonlocal stress has a maximum that does not occur at the boundary of the contact domain and appears before the contact domain boundary.

As a conclusion, the local and nonlocal solutions are constant under the punch for $x/a \le 0.93$ in the first case and $x/a \le 0.935$ in the second, but they differ near the boundary of the contact domain $x/a > 0.93$, and respectively $x/a > 0.935$, where severe stress gradient appears.

For $x/a > 0.93$ and respectively $x/a > 0.935$ the solutions depend on a/h. The conclusion is that the nonlocal theory in the perfect agreement with the experimental data, where have been depicted finite stress fields under the punch and near/on the boundary of the contact domain [1]. The nonlocal approaches in similar problems are discussed also in other papers [14, 15–18]). The chalcogenide materials characterisation and describing are found in [19–25].

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