ON THE MODELING OF NANOCONTACTS

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This paper deals with the derivation of the nonlocal field equations for nanocontact mechanics. The nonlocal theory is very appropriate to describe long-range interactions among the particles in the material. To exemplify this approach, the problem of the nonlocal elastic contact for an elastic layer loaded by a rigid indenter is studied here. Classical and nonlocal solutions are compared. The nonlocal stress field is finite for all points of the contact domain, and has a maximum that does not occur at the boundary of the contact domain.

1. INTRODUCTION

The classical mechanics does not cover all the physical situations. For example, the systems whose dimensions are comparable with a characteristic inner length of the material imply long-range interactions of particles (Johnson [1], Cimmeli and Starita [2], Keer and Miller [3], Sabin [4]). The nonlocal theory is the best theory grounded for describing long-range interactions among the particles in materials. In such theory the stress has an energetic and an entropic components, both of them being intrinsically nonlocal. The stress at a location (atom, molecule, grain) is determined by the interatomic interactions in the neighbours around that location (Eringen [5-8], Artan [9]).

We are interested in the response of the body to external forces within an experimentally possible length and time scale. The domain of applicability of a continuum theory depends on the ratio $(\lambda/l, \tau/\tau_0)$ or $(\lambda/l, \omega_0/\omega)$, where λ is a characteristic length of the body (atomic distance, granular distance etc.), l is the external characteristic length associated with the external forces (waves, distances over which load distribution change sharply, geometrical and surface discontinuities), τ the time scale (or frequency ω) which is the minimum transmission time of a signal (or a frequency), and τ_0 is the external characteristic time or frequency) associated with the external forces (Eringen [8]). All classical theories assume $\lambda/l << 1$ and $\tau/\tau_0 << 1$, i.e. the external forces excite large numbers of subbodies simultaneously, so that subbodies interact and the result is a statistical average of the individual responses. For $\lambda/l = 1$ and $\tau/\tau_0 = 1$, the individual fields of subbodies (intermolecular and atomic forces) are important.

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Rev. Roum. Sci. Techn. – Méc. Appl., TOME 53, N° 3, P. 239–246, Bucarest, 2008

The balance laws of nonlocal continuum mechanics are identical to those of classical continuum mechanics. So, the balance laws for a body of volume V enclosed by a surface ∂V, state that the time rate of change of the field ϕ (mass, momentum, moment of momentum, energy) in the body, excluding the points on the discontinuity surface σ, which moves into the body with a velocity $\tilde{\mathbf{v}}$ in the direction of its unit normal $\mathbf{n}$, is balanced by the surface flux $\boldsymbol{\tau}$ and the body source g, namely (Eringen [5–8])

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{V-\sigma}\phi\mathrm{d}v-\int_{\partial V-\sigma}\boldsymbol{\tau}\cdot\mathrm{d}\mathbf{a}-\int_{\partial V-\sigma}g\mathrm{d}v=0\,. \tag{1.1}$$

By using the Green-Gauss theorem, (1.1) becomes

$$\int_{V-\sigma}\left[\phi_{,t}+\mathrm{div}(\phi\tilde{\mathbf{v}}-\boldsymbol{\tau})-g\right]\mathrm{d}v+\int_{\sigma}\left[\phi(\tilde{\mathbf{v}}-\mathbf{v})-\boldsymbol{\tau}\right]\cdot\mathbf{n}\mathrm{d}a=0\,, \tag{1.2}$$

where comma means the differentiation with the respective variable, $\tilde{\mathbf{v}}$ is the velocity vector, and the bracket is the jump of the mentioned quantity at σ. In the classical theory, (1.2) is valid for every part of the body, no matter how small it may be, and the localization condition yields to the vanishing of integrants in the integrals. In the nonlocal theory, this assumption is abandoned, but the localization is still possible by using certain localization residuals, which must integrate to zero.

These residuals are the effects of all other points of the body on one point of the body, that means the residuals are the long-range effects of all point $\mathbf{x}$ at which the balance laws are localised.

So, the master balance laws of the nonlocal theory are

$$\phi_{,t}+\mathrm{div}(\phi\tilde{\mathbf{v}}-\boldsymbol{\tau})-g=\hat{g}\ \text{ in }\ V-\sigma\,,\quad \left[\phi(\tilde{\mathbf{v}}-\mathbf{v})-\boldsymbol{\tau}\right]\cdot\mathbf{n}=\hat{G}\ \text{ on }\ \sigma\,, \tag{1.3}$$

subject to

$$\int_{V-\sigma}\hat{g}\mathrm{d}v+\int_{\sigma}\hat{G}\mathrm{da}=0\,. \tag{1.4}$$

From (1.3) and (1.4), the nonlocal balance laws for mass, momentum, moment of momentum and energy are

$$\rho_{,t}+\mathrm{div}(\rho\tilde{\mathbf{v}})=\hat{\rho}\,, \tag{1.5}$$

$$\mathrm{div}\,\mathbf{t}_k+\rho(\mathbf{f}-\dot{\tilde{\mathbf{v}}})=\hat{\rho}\tilde{\mathbf{v}}-\rho\hat{\mathbf{f}}\,, \tag{1.6}$$

$$\mathbf{i}_k\times\mathbf{t}_k-\rho(\mathbf{x}\times\hat{\mathbf{f}}-\hat{\mathbf{l}})=0\,, \tag{1.7}$$

$$-\rho\dot{\varepsilon}+\mathbf{t}_k\cdot\tilde{\mathbf{v}}_{,k}+\nabla\cdot\mathbf{q}+\rho h-\hat{\rho}(\varepsilon-\frac{1}{2}\tilde{v}\cdot\tilde{v})-\rho\hat{\mathbf{f}}\cdot\tilde{\mathbf{v}}+\rho\hat{h}=0, \tag{1.8}$$

$$\int_V \hat{\rho}\mathrm{d}v = 0\,,\quad \int_V \rho\hat{\mathbf{f}}\,\mathrm{d}v = 0\,,\ \int_V \rho\hat{\mathbf{l}}\,\mathrm{d}v = 0\,,\ \int_V \rho\hat{h}\,\mathrm{d}v = 0\,, \tag{1.9}$$

where a superposed dot a material time derivative. Here, ρ is the mass density, $\mathbf{t}_k = \mathbf{t}_{kl} i_l$ 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 second law of thermodynamics is obtained from (1.3)

$$\rho\dot{\eta} - \nabla\cdot\mathbf{q} - \frac{\rho h}{\theta} - \rho\hat{b} + \hat{\rho}\eta \geq 0 \quad \text{in } V-\sigma\,, \tag{1.10}$$

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

$$\int_V \rho\hat{b}\,\mathrm{d}v = 0\,. \tag{1.11}$$

2. THE NONLOCAL ELASTIC SOLIDS

THEOREM 2.1 (Eringen 1972). *For the linear theory of nonlocal elastic materials, whose natural state is free of nonlocal effects, the nonlocal body force vanishes, i.e.* $\hat{f}_k = 0$.

THEOREM 2.2 (Eringen 1972). *The constitutive equations of the nonlocal linear homogeneous and isotropic elastic solids and residuals do not violate the global entropy inequality (1.10) and (1.11) if and only if they are of the form*

$$t_{kl} = \lambda e_{rr}\delta_{kl} + 2\mu e_{kl} + \int_{V-\sigma} (\lambda_1' e_{rr}' \delta_{kl} + 2\mu_1' e_{kl}')\mathrm{d}v'\,, \tag{2.1}$$

$$\Sigma = \Sigma_0 + \frac{1}{2}\lambda(e_{kk})^2 + \mu e_{kl} d_{kl} + \int_{V-\sigma} (\frac{1}{2}\lambda_1' e_{kk} e_{ll}' + \mu_1' e_{kl} e_{kl}')\mathrm{d}v'\,,\quad \hat{\rho} = 0\,,\ \hat{f}_k = 0\,, \tag{2.2}$$

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*

$$e_{kl}=\frac{1}{2}(u_{k,l}+u_{l,k})\,, \tag{2.3}$$

and u_k *the components of the displacement vector*.

A prime placed on quantities 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 influence functions, which are positive decreasing functions of $|\mathbf{x}'-\mathbf{x}|$. Another form of (2.1) and (2.2) is obtained by incorporating λ and μ into λ' and μ'

$$t_{kl}=\int_{V-\sigma}[\lambda'(|\mathbf{x}'-\mathbf{x}|)e'_{rr}(\mathbf{x}')\delta_{kl}+2\mu'(|\mathbf{x}'-\mathbf{x}|)e'_{kl}(\mathbf{x}')]\mathrm{d}v'(\mathbf{x}')\,, \tag{2.4}$$

$$\Sigma=\Sigma_0+\int_{V-\sigma}[\frac{1}{2}\lambda'(|\mathbf{x}'-\mathbf{x}|)e_{kk}(\mathbf{x})e'_{ll}(\mathbf{x}')+\mu'(|\mathbf{x}'-\mathbf{x}|)e_{kl}(\mathbf{x})e'_{kl}(\mathbf{x}')]\mathrm{d}v'(\mathbf{x}')\,. \tag{2.5}$$

3. THE NONLOCAL CONTACT PROBLEM

Nanoindentation is a technique for determining the mechanical properties of materials at very small scales (thin films, thin surface layers, and very small volumes of material). One of the great advantages of nanoindentation is that properties such as the hardness and elastic modulus can be measured by simple analyses of indentation load-displacement data (Kelchner, Plimpton and Hamilton [10], Bhushan [11]). In this paper 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. 3.1).

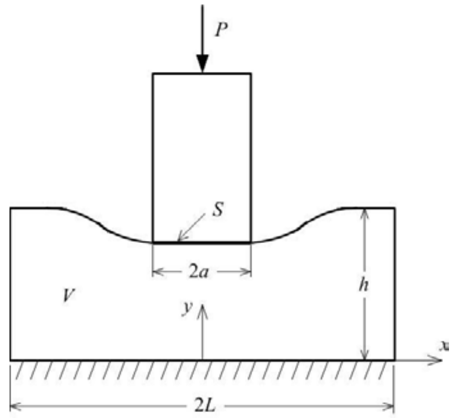

Fig. 3.1 – The scheme for the indentation problem.

The contact along the interface is frictionless, no tensile tractions can be transmitted across the interface. The layer is subjected to vertical body forces due to gravity. Let us note by V the volume of the layer and by S the surface between the indenter and the layer. The physical response of any point in V depends on the state of whole volume. This dependence can be described by the constitutive laws (2.4) written for the layer

$$t_{kl} = \int_{V_1} [\lambda'(|\mathbf{x}'-\mathbf{x}|) e'^{1}_{rr}(\mathbf{x}')\delta_{kl} + 2\mu'(|\mathbf{x}'-\mathbf{x}|) e'^{1}_{kl}(\mathbf{x}')] \mathrm{d}v'(\mathbf{x}') . \tag{3.1}$$

The Lamé constants for a nonlocal medium can be taken as

$$\lambda'(|\mathbf{x}'-\mathbf{x}|) = \alpha(|\mathbf{x}'-\mathbf{x}|)\lambda \ , \ \ \mu \ (|\mathbf{x}'-\mathbf{x}|) = \alpha(|\mathbf{x}'-\mathbf{x}|)\mu \ , \tag{3.2}$$

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 $\mathbf{x}$.

Eringen [8] has showed that

$$t_{kl} = \int_{V} \alpha(|\mathbf{x}'-\mathbf{x}|)\sigma_{kl}(\mathbf{x}')\mathrm{d}v'(\mathbf{x}') , \tag{3.3}$$

where $\sigma_{kl}(\mathbf{x}')$ are the local stress fields.

For the kernel function we consider the Artan representation [9]

$$\alpha(|\mathbf{x}'-\mathbf{x}|) = \begin{cases} B\left\{1-\dfrac{|\mathbf{x}'-\mathbf{x}|}{d}\right\}, & |\mathbf{x}'-\mathbf{x}|< d, \\ 0, & |\mathbf{x}'-\mathbf{x}|> d, \end{cases} \tag{3.4}$$

where $B = 1/d$, with d a atomic distance. For the indentation problems it is usually to take $d = 4\times 10^{7}\,\mathrm{cm}$ (Artan [9]).

The local stress field under the frictionless punch is (Civelek, Erdogan and Cakiroglu [12], Solomon [13])

$$\sigma(x) = -\rho g h + \\ + \frac{1}{\pi h}\int_{-a}^{a}\int_{-L}^{L} \sigma(t)\frac{\exp(u)[(1+u)\exp(2u)+u-1]}{\exp(4u)+4u\exp(2u)-1}\cos[(t-x)\frac{u}{h}]\mathrm{d}u\mathrm{d}t, \tag{3.5}$$

$$\int_{-a}^{a} \sigma(t)\mathrm{d}t = P . \tag{3.6}$$

The nonlocal stress field under the punch is calculated by using (3.3)

$$t(x) = \int_{x-d}^{x+d} \left(1-\frac{|x-x'|}{d}\right)\sigma(x)\mathrm{d}x' , \tag{3.7}$$

where $\sigma(x)$ is given by (3.5) and (3.6).

By using the dimensionless quantities

$$s=\frac{t}{a},\; q=\frac{x}{L},\; f(s)=\frac{\sigma(as)}{\rho gh}, \tag{3.8}$$

the equations (3.5) and (3.6) become

$$\frac{\sigma(x)}{\rho gh}=-1+ \\ +\frac{aL}{\pi h}\int_{-1}^{1}\int_{-1}^{1} f(s)\frac{\exp(qL)[(1+qL)\exp(2qL)+qL-1]}{\exp(4qL)+4qL\exp(2qL)-1}\cos[(as-x)\frac{qL}{h}]\mathrm{d}q\mathrm{d}s, \tag{3.9}$$

$$\frac{a}{h}\int_{-1}^{1} f(s)\mathrm{d}s=\frac{P}{\rho gh^2}. \tag{3.10}$$

The contact stresses are calculated for $a/h=0.5$, $L/h=15$, by using a Gaussian integration formula. Figs. 3.2 and 3.3 show the difference between the local and the nonlocal fields of stresses near the boundary of the contact domain for $a/h=0.5$ and respectively $a/h=0.3$. Both figures show that, if the points are situated in the neighbourhood of the boundary $x/a>0.95$ for the first case, and $x/a>0.965$ for the second, 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.

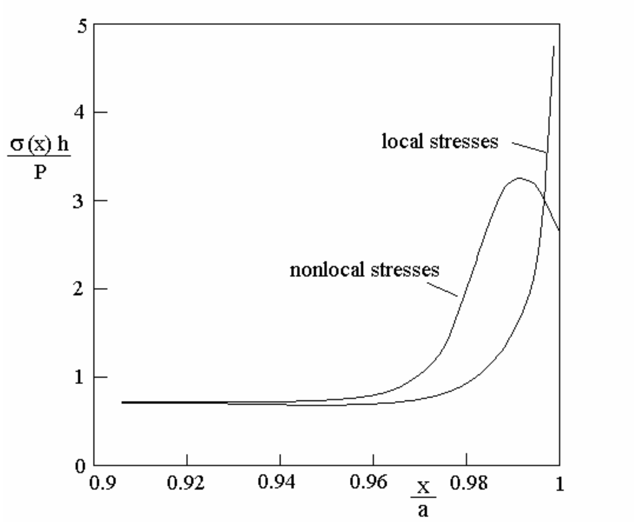

Fig. 3.2 – The local and nonlocal stresses
near the boundary of the contact domain for $a/h=0.5$.

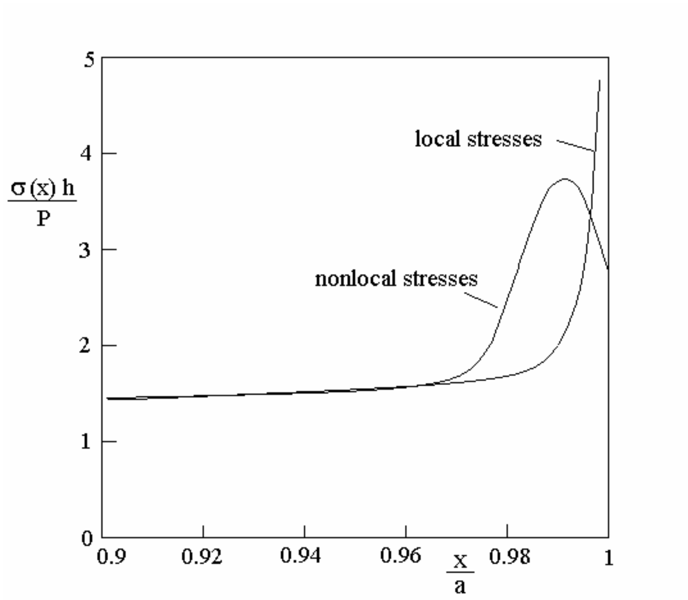

Fig. 3.3 – The local and nonlocal stresses
near the boundary of the contact domain for $a/h = 0.3$.

For the local case, the results are the same with those given by Civelek, Erdogan and Cakiroglu [12]. Near the boundary of the contact domain $x/a \to 1$, the stresses tend to infinity. For $d \to 0$ the nonlocal stresses are the same with the local stresses inside the contact domain. In other words, the nonlocal theory of elasticity will not provide new insight into the problem, for interior points of the contact domain. The nonlocal stress has a maximum, but this maximum stress does not occur at the boundary of the contact domain.

As a conclusion, the local and nonlocal solutions are practically constant under the punch for $x/a \le 0.95$ in the first case and $x/a \le 0.965$ in the second, but they differ near the boundary of the contact domain $x/a > 0.95$, and respectively $x/a > 0.965$, where severe stress gradient appears. For $x/a > 0.95$ and respectively $x/a > 0.965$ both solutions depend essentially on a/h. Superiority of the nonlocal theory consists in the perfect agreement with the experiments, where have been depicted finite stress fields under the punch and near/on the boundary of the contact domain (Johnson [1]). The nonlocal approaches in similar problems are discussed also in other papers (Picu [14], Artan [15-18]).

Acknowledgements. The authors gratefully acknowledge the financial support of the National Authority for Scientific Research Council (ANCS), Romania, through CEEX postdoctoral grant nr. 1531/2006.

Recived on Octomber 2, 2006

REFERENCES

1. Johnson, K. L., *Contact Mechanics,* Cambridge University Press, New York, 1985.
2. Cimmelli, V.A., Starita, G., *Nonlocal variational theories for systems with an interface*, Int. J. Engng. Sci., **28**, *7*, pp. 663–675, 1990.
3. Keer, L.M., Miller, G.R., *Contact between an elastically supported circular plate and a rigid indenter*, Int. J. Engng. Sci., **21**, *6*, pp. 681–690, 1983.
4. Sabin, G.C.W., *The impact of a rigid axisymmetric indentor on a viscoelastic half-space*, Int. J. Engng. Sci., **25**, *2*, pp. 235–251, 1987.
5. Eringen, A.C., *Linear theory of nonlocal elasticity and dispersion of plane waves*, Int. J. Engng. Sci., **10**, pp. 425–435, 1972.
6. Eringen, A.C., *On nonlocal continuum thermodynamics*, in: *Modern developments in thermo dynamics* (ed. B. Gal-Or), John Wiley and Sons, New York, pp. 121–142, 1974.
7. Eringen, A.C., *Continuum mechanics at the atomic scale*, Crystal Lattice defects, **7**, pp. 109–130, 1977.
8. Eringen, A.C., *Nonlocal continuum field theories*, Springer, 2002.
9. Artan, R., *Rigid parabolic stamp on a nonlocal elastic half plane*, Turk J. Engin Environ. Sci., **25**, pp. 611–616, 2001.
10. Kelchner, C.L., Plimpton, S.J., Hamilton, J.C., *Dislocation nucleation and defect structure during surface indentation*. Phys. Rev. B, **58,** p. 17, 1998.
11. Bhushan, B., *Nanomechanical properties of solid surfaces and this films*, in Handbook *of Micro/Nano Tribology*, (ed. Bhushan, B.) CRC Press, Inc.: Boca Raton, FL, pp. 321-396, 1995.
12. Civelek, M.B., Erdogan, F., Cakiroglu, A.O., *Interface separation for an elastic layer loaded by a rigid stamp*, Int. J. Engng. Sci., **16**, *9,* pp. 669–679, 1978.
13. Solomon, L., *Elasticitate liniară. Introducere matematică în statica solidului elastic*, Editura Academiei, Bucureşti, 1969.
14. Picu, R.C., *A nonlocal formulation of rubber elasticity*, International Journal for Multiscale Computational Engineering, **1**, *1*, pp. 23–32, 2003.
15. Artan, R., *Unsymmetrical rigid stamp on a nonlocal elastic half plane*, Int. J. Engng. Sci., **34**, pp. 933–941, 1996.
16. Artan, R., *Nonlocal elastic half plane loaded by a concentrated force*, Int. J. Engng. Sci., **34**, pp. 943–950, 1996.
17. Artan, R., *Rectangular rigid stamp on a nonlocal elastic half plane*, Int. J. Solids Structures, **33**, pp. 3577–3586, 1996.
18. Artan, R., *Unsymetrical elastic stamp on a nonlocal elastic half plane*, computers and structures, **63**, pp. 39–50, 1997.