Surface-dislocation interaction at the nanoscale

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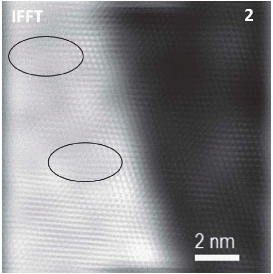
Outline

The paper is focused on collecting different surface elasticity models related to the Gurtin and Murdoch one (1975, 1978) and comparing the stress fields around the flat surface, which arise due to interaction of the periodic array of edge dislocations with the free surface. It is supposed that the semi-infinite elastic body is under the plane deformation and the dislocations can reach the distance to the surface up to several nanometers. For each model including the Gurtin and Murdoch one, the boundary equation is separately formulated in terms of complex variables. The solution of the problem for all models is presented in terms of the Fourier series for the stress field.

A dislocation array arising due to the lattice mismatch between the substrate and the deposited layer can deviate from the interface a few nanometers (Liu et al., 2011), as, for example, a result of emission from the surface/interface under loading (Lubarda, 2011, Wang et al., 2014,Zeng et al., 2012), and forms the dislocation wall parallel to the interface (Chu and Pan, 2014).



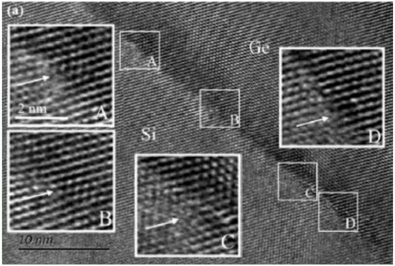


Figure: HRTEM images of Al/TiC (Maziarz et al., 2019, left) and Ge/Si (Zeng et al., 2012, right) heterostructures with the dislocation row near the interface.

Constitutive relations of surface elasticity

Gurtin and Murdoch (GM) (1975, 1978) – mathematical theory including surface stress and surface tension (residual surface stress)

Constitutive equation of the surface (GM linearized law)

$$\mathbf{\Sigma}^s = \tau_0 \mathbf{A} + (\lambda_s + \tau_0)\mathbf{A}\,\mathrm{tr}\,\mathbf{E}^s + 2(\mu_s - \tau_0)\mathbf{E}^s + \tau_0 \nabla_s \mathbf{u}, \qquad (1)$$

$\mathbf{\Sigma}^s$ – first Piola–Kirchhoff stress tensor, $\mathbf{E}^s$ – surface strain tensor, τ_0 – surface tension, $\mathbf{u}$ – displacement vector, $\mathbf{I}$ – unit 3D tensor, $\mathbf{A} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$, $\mathbf{n}$ – unit normal vector, $\nabla_s = \nabla - \mathbf{n}\,\partial/\partial n$ – 2-D nabla operator.

Simplified GM models used in the literature:

1. Only the first term in Eq. (1) is considered.
2. $\tau_0 = 0$ — widely used and more realistic.
3. $\lambda_s = 2\mu_s = 0$ — was compared with the complete GM model (1) by Mogilevskaya (JMPS, 2008).
4. $\mathbf{n} \cdot \nabla_\mathbf{s} \mathbf{u} = 0$ or $\nabla_s \mathbf{u} = 0$ — there is no one argument to use these assumptions.

? $\mathbf{\Sigma}^s = \tau_0 \mathbf{A} + \lambda_s \mathbf{A}\,\mathrm{tr}\,\mathbf{E}^s + 2\mu_s \mathbf{E}^s + \tau_0 \nabla_s \mathbf{u}$ ($\tau_0 \ll \lambda_s$ and $\tau_0 \ll \mu_s$)

Boundary value problem of elasticity with surface stress

Generalized Young–Laplace law – condition at the surface

$$\mathbf{\Sigma} \cdot \mathbf{n} = -\nabla_{\mathbf{s}} \cdot \mathbf{\Sigma}^{\mathbf{s}} \tag{2}$$

$\mathbf{\Sigma}$ – the volume stress tensor.

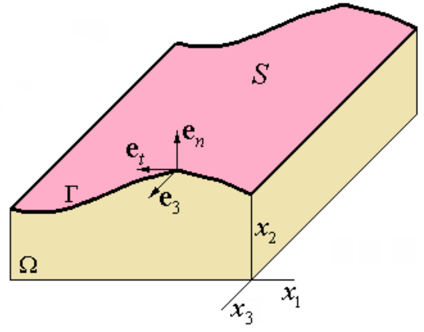
Constitutive equation of the bulk material (Hooke law)

$$\mathbf{\Sigma} = 2\mu\mathbf{E} + \lambda\mathbf{I}\,\mathrm{tr}\,\mathbf{E}, \quad \mathbf{E} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) \tag{3}$$

Inseparability condition of the surface and bulk material

$$\mathbf{u}^s = \mathbf{u}^b \equiv \mathbf{u} \tag{4}$$

Cylindrical surface S of the bulk material



Basic relations of plane strain problem ($\varepsilon_{33} = \varepsilon_{13} = \varepsilon_{23} = 0$)

Surface stress tensor

$$\Sigma^{s} = \sigma^{s}_{tt}\mathbf{t} \otimes \mathbf{t} + \boldsymbol{\sigma}^{\mathbf{s}}_{\mathbf{tn}}\mathbf{n} \otimes \mathbf{t} + \boldsymbol{\sigma}^{\mathbf{s}}_{\mathbf{33}}\mathbf{k} \otimes \mathbf{k}. \tag{5}$$

Constitutive equations of the surface

$$\boldsymbol{\sigma}^{\mathbf{s}}_{\mathbf{tt}} = \boldsymbol{\tau_0} + (\boldsymbol{\lambda}_{\mathbf{s}} + 2\boldsymbol{\mu}_{\mathbf{s}})\varepsilon_{\mathbf{tt}}, \quad \boldsymbol{\sigma}^{\mathbf{s}}_{\mathbf{tn}} = \boldsymbol{\tau_0}(-\boldsymbol{u}_{\mathbf{t}}/\boldsymbol{R} + \partial \boldsymbol{u}_{\mathbf{n}}/\partial \boldsymbol{l}),$$

$$\boldsymbol{\sigma}^{\mathbf{s}}_{\mathbf{33}} = \boldsymbol{\tau_0} + (\boldsymbol{\lambda}_{\mathbf{s}} + \boldsymbol{\tau_0})\varepsilon_{\mathbf{tt}}. \tag{6}$$

Boundary equation of the original GM model in complex variables

$$\sigma_{nn} + i\sigma_{nt} = \left[\frac{\tau_0}{R} + \frac{M_s}{R}\mathrm{Re}\,\frac{\partial u}{\partial \zeta} + \tau_0 \mathrm{Im}\left(\frac{\partial^2 u}{\partial \zeta^2}e^{i\alpha_0}\right)\right] -$$

$$-i\left[M_s \mathrm{Re}\left(\frac{\partial^2 u}{\partial \zeta^2}e^{i\alpha_0}\right) - \frac{\tau_0}{R}\mathrm{Im}\frac{\partial u}{\partial \zeta}\right] \equiv -iq^s(\zeta), \tag{7}$$

$p = M_s + \tau_0$, $m = M_s - \tau_0$, $M_s = \lambda_s + 2\mu_s$, $u = u_1 + iu_2$, $\overline{u} = u_1 - iu_2$,
R – coverture radius of Γ, α_0 – angle between t and x_1 axes at the point $\zeta \in \Gamma$.

Boundary problem for half-plane with surface stress

Boundary condition in the case of the origin GM model

$$\sigma_{22} - i\sigma_{12} = -\frac{ip}{2}\frac{\partial^2 u}{\partial x_1^2} - \frac{im}{2}\overline{\frac{\partial^2 u}{\partial x_1^2}} \equiv -iq^s(x_1),\ x_2 = 0. \tag{8}$$

$q^s = q_1^s + iq_2^s$.

$\tau_0 = 0$ or $\mathbf{n} \cdot \nabla_{\mathbf{s}} \mathbf{u} = 0 \Rightarrow p = m = M_s$,
$\nabla_s \mathbf{u} = 0 \Rightarrow p = m = M_s - \tau_0$,
$\tau_0 \ll |\lambda_s|$ and $\tau_0 \ll |\mu_s| \Rightarrow p = m = M_s$,
$M_s = 0 \Rightarrow p = -m = \tau_0$.

Solution of the problem is reduced to solving the following integral equation

$$8\mu u'(x_1) - i(1-\varkappa)\left(pu''(x_1) + m\bar{u}''(x_1)\right) - \frac{1+\varkappa}{2\pi}\int_{-\infty}^{+\infty} \frac{pu''(t) + m\bar{u}''(t)}{t - x_1}dt = Q(x_1)), \tag{9}$$

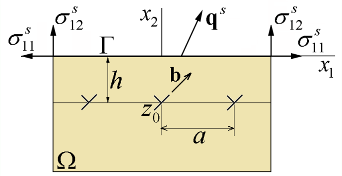
Function Q can depend on the traction at the surface, loading at infinity and internal sources of perturbations in the half-plane.

Dislocation array in a half-plane

$$Q(x_1) = 4(\varkappa+1)\left[H\operatorname{ctg}(\xi-\overline{\zeta}_0) + \overline{H}(\zeta_0-\overline{\zeta}_0)\operatorname{cosec}^2(\xi-\overline{\zeta}_0\right] +$$

$$4(1-\varkappa)H\operatorname{ctg}(\xi-\zeta_0) + 8iH. \qquad (10)$$

$$H = \frac{i\mu(b_1+ib_2)}{a(\varkappa+1)}, \quad \varkappa = \frac{\lambda+3\mu}{\lambda+\mu}, \quad \xi = \pi x_1/a, \quad \zeta_0 = -i\pi h/a.$$



$$\mathbf{b} = (b_1, b_2), \quad \mathbf{q}^s = (q_1^s, q_2^s)$$

Solution of the integral equation

Periodic function $Q(x_1)$ can be expanded into the complex Fourier series

$$Q(x_1) = A_0 + \sum_{k=1}^{\infty} \left(A_k e^{i l_k x_1} + B_k e^{-i l_k x_1} \right), \quad l_k = 2\pi k/a, \tag{11}$$

$$A_0 = \frac{1}{a} \int_{-a/2}^{a/2} Q(t)dt, \quad A_k = \frac{1}{a} \int_{-a/2}^{a/2} Q(t) e^{-i l_k x_1} dt, \quad B_k = \frac{1}{a} \int_{-a/2}^{a/2} Q(t) e^{i l_k x_1} dt.$$

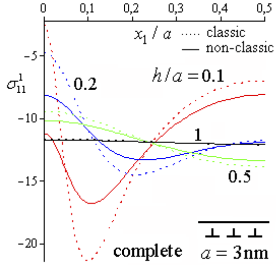
It allows obtaining the solution of integral equation (9) in the form:

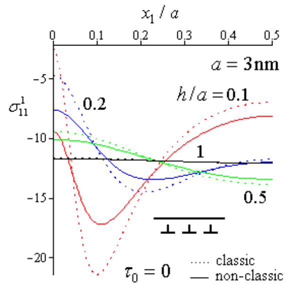
$$u'(x_1) = a_0 + \sum_{k=1}^{\infty} \left(a_k e^{i l_k x_1} + b_k e^{-i l_k x_1} \right). \tag{12}$$

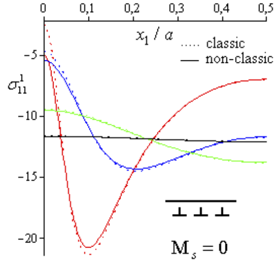
As a result, the stress field is evaluated in the explicit form.

The elastic parameters of surface and bulk materials taken in the numerical investigations are $\lambda_s = 6.8511$ N/m, $\mu_s = -0.3755$ N/m, $\tau_0 = 1$ N/m, $\lambda = 58.17$ GPa, $\mu = 26.13$ GPa.

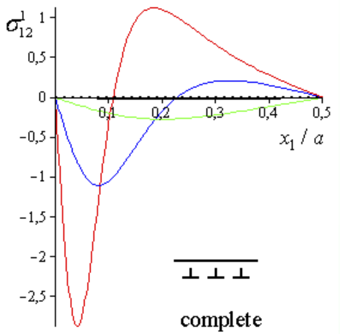
Hoop stress at the free planar surface

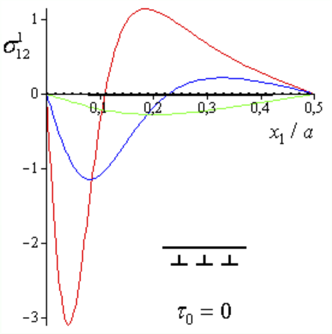




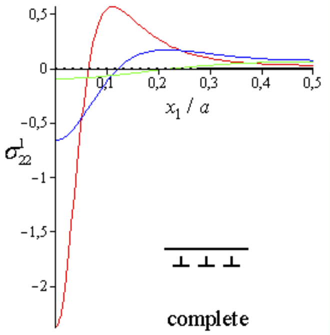


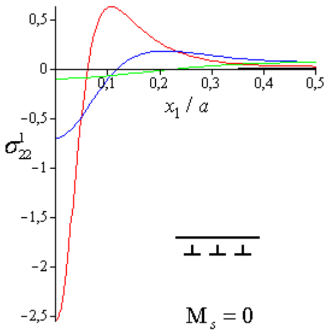
Tangential traction at the free planar surface





Normal traction at the free planar surface





Conclusions

- The closer dislocations to the surface the greater effect of both the surface elasticity and surface tension.
- The first term of constitutive GM equation (1) alone can be considered only in the case of a curvilinear surface.
- Most different simplified versions of the GM model ($\tau_0 = 0$, $\mathbf{n} \cdot \nabla_{\mathbf{s}} \mathbf{u} = 0, \tau_0 \ll \{|\lambda_s|, |\mu_s|\}$) yield the same boundary equation in the case of a planar surface and so lead to the same elastic fields.
- Except for the exotic version $M_s = 0$, all simplified versions of the GM model lead to the zero normal traction at the surface while this traction by the complete GM model has the same order as the tangential one.

Recent publications

1.Grekov M.A., Sergeva T.S. Interaction of edge dislocation array with bimaterial interface incorporating interface elasticity. Int. J. Eng. Sci. 2020. V. 149. 103233.

2. Grekov M.A., Sergeva T.S. Periodic Green functions for two-component medium with interface stresses at the planar interface. AIP Conference Proceedings. 2018. V. 1959. P. 070014.

3. Grekov M.A., Sergeeva T.S., Pronina Y.G., Sedova O.S. A periodic set of edge dislocations in an elastic solid with a planar boundary incorporating surface effects. Eng. Fract. Mech. 2017. V. 186. P. 423-435.

Thank you for your attention!