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Technical Notes

Interface Debonding Between a Platelike Nanomaterial and the Substrate

Z.-H. Jin*
University of Maine, Orono, Maine 04469
and
L. Tan†
University of Nebraska, Lincoln, Nebraska 68588

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I. Introduction

PLATELIKE nanomaterials are found in many emerging advanced materials such as ultrathin films and nanolaminates [1], nanocomposites [2], and supramolecular materials [3]. Knowledge of mechanical properties and deformation responses of platelike nanomaterials and debonding characteristics between nanoplates and the substrate/matrix is critical to the successful application of those advanced materials. Moreover, the principle of mechanical detachment of platelike nanomaterials strongly adhering to a substrate plays an important role in a number of advanced technologies, such as optical surface cleaning and high-density integrated-circuit manufacturing [4].

A platelike nanomaterial usually has a thickness of a few nanometers and its in-plane dimensions are at least one order of magnitude larger. A continuum mechanics approach may be adopted to describe the field variations in the in-plane directions. The discrete characteristics in the thickness direction, however, have to be taken into account by considering the interatomic bonding between the atom layers. Sun and Zhang [5] and Zhang and Sun [6] proposed a semicontinuum methodology to describe the mechanical behavior of platelike nanomaterials. They developed a nanoplate model and found that the deflection of a nanoplate was underestimated using the continuum Mindlin plate theory. Hence, nanoplate theories, instead of classical continuum plate equations, should be used in the study of mechanical behavior of platelike nanomaterials.

In this Note, we employ the nanoplate theory in [5,6] and a cohesive zone model to investigate the interface debonding between a platelike nanomaterial and the substrate. Nondimensional forms of the nanoplate equations [6] are reformulated. A cohesive zone model characteristic of the van der Waals bond is used to describe the progressive nanoplate-substrate debonding. Analytical solutions of deflection of the nanoplate and interfacial crack extension due to the debonding are obtained. The energy dissipated during interface debonding is determined from the analytical solution.

II. Theoretical Formulations

A. Nanoplate Model

We employ the nanoplate theory in [5,6] to study cylindrical bending of a platelike nanomaterial with a simple cubic crystal structure. The basic equations governing the deflection w and the rotation of the cross section ψ are given by

$$
\begin{aligned}
&-2N\alpha_2 \frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + Na\alpha_2 \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + 2N\alpha_2 \frac{\mathrm{d}\psi}{\mathrm{d}x} + q = 0 \\
&A\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + Na\alpha_2 \frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + 2N\alpha_2\left(\psi - \frac{\mathrm{d}w}{\mathrm{d}x}\right) = 0
\end{aligned}
\tag{1}
$$

where a is the lattice parameter, $2N+1$ is the number of atomic layers, q is the transverse load, and A is a constant given by

$$
A = -\sum_{i=0}^{N-1}[2\alpha_1(1+i)^2 + 3\alpha_2(1+i)^2 + \alpha_2 i^2]a^2 \tag{2}
$$

in which α_1 and α_2 are the constants of atomic bonding force between the nearest atoms and between the next nearest atoms in a unit cell, respectively. The transverse shear force Q_x and bending moment M_x are related to w and ψ by

$$
\begin{aligned}
Q_x &= 2N\alpha_2 \frac{\mathrm{d}w}{\mathrm{d}x} - Na\alpha_2 \frac{\mathrm{d}\psi}{\mathrm{d}x} - 2N\alpha_2\psi \\
M_x &= -A\frac{\mathrm{d}\psi}{\mathrm{d}x} + 2N\alpha_2\left(\psi - \frac{\mathrm{d}w}{\mathrm{d}x}\right)
\end{aligned}
\tag{3}
$$

It is noted that the nanoplate model in [5,6] is a linear theory and thus may not be applied to a crack tip region. However, the theory may be employed to study fracture of interfaces with relatively weak bonding as the bulk may not undergo large deformation. Moreover, the theory may be used to study general crack extension with reasonable accuracy as long as the crack length is much larger than the size of the crack tip nonlinear deformation zone.

B. Cohesive Zone Model

We assume that the platelike nanomaterial and the substrate are bonded by the van der Waals force, which is generally represented by the Lennard–Jones (L-J) potential. The nonlinearity of the L-J bonding force versus the atomic separation, however, excludes analytical treatment of the problem. We thus use the following cohesive zone model with constant cohesive traction to describe bonding/debonding between the nanoplate and the substrate:

$$
\sigma = \begin{cases} \sigma_0, & 0 \le \delta \le \delta_0 \\ 0, & \delta > \delta_0 \end{cases} \tag{4}
$$

where σ and σ_0 are the cohesive traction, δ the separation between the nanoplate and the substrate, and δ_0 a critical separation at which the cohesion is lost. This cohesive zone model has been frequently used to investigate progressive fracture in thin sheet metals experiencing localized plastic yielding [7] and in polymers undergoing crazing [8]. Unlike the cohesive force derived from the L-J potential, which exhibits a continuous softening behavior, the cohesive force in Eq. (4) softens suddenly at $\delta = \delta_0$. It is expected that the fundamental progressive failure characteristics such as the energy dissipation during crack extension may still be captured by the constant cohesive traction model if the cohesive energy density is chosen as that of an L-J potential model for two atomic planes [9] and the cohesive traction as the peak traction in the L-J model.

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*Department of Mechanical Engineering.

†Department of Engineering Mechanics, Nebraska Center for Materials and Nanoscience.

C. Debonding Between a Nanoplate and the Substrate

We consider interfacial debonding between a nanoplate and the substrate under the applied transverse load Q_0 (force per unit width) at edge $x = L$ as shown in Fig. 1, where L is the plate length. The nanoplate is fixed along the edge $x = 0$. We initially assume that the nanoplate and the substrate are perfectly bonded along the entire interface by a cohesive traction described by Eq. (4). The cohesion is lost at the loading edge $x = L$ when the deflection of the plate reaches the critical separation δ_0. The debonding then progressively proceeds with a bonding length of L_c. L_c decreases with increasing load during the progressive failure, with the deflection at the debonding front always being δ_0. The boundary conditions of the bending-debonding problem of the nanoplate can thus be formulated as follows:

$$w = 0, \qquad \psi = 0, \qquad x = 0 \tag{5}$$

$$\begin{aligned} Q_x &= 2N\alpha_2 \frac{\mathrm{d}w}{\mathrm{d}x} - Na\alpha_2 \frac{\mathrm{d}\psi}{\mathrm{d}x} - 2N\alpha_2\psi = Q_0, \qquad x = L \\ M_x &= -A \frac{\mathrm{d}\psi}{\mathrm{d}x} + Na\alpha_2\psi - Na\alpha_2 \frac{\mathrm{d}w}{\mathrm{d}x} = 0, \qquad x = L \end{aligned} \tag{6}$$

Introduce the following nondimensional quantities:

$$\begin{aligned} &\bar{x} = x/L, \qquad \bar{w} = w/a, \qquad \bar{\psi} = \psi(a/L) \\ &\bar{\sigma}_0 = \sigma_0(a/\alpha_2), \qquad \bar{Q}_0 = Q_0/\alpha_2 \end{aligned} \tag{7}$$

$$\begin{aligned} &\varepsilon = a/L, \qquad \bar{L}_c = L_c/L \\ &\bar{A} = -\sum_{i=0}^{N-1}\left[2\frac{\alpha_1}{\alpha_2}(1+i)^2 + 3(1+i)^2 + i^2\right] \end{aligned} \tag{8}$$

The basic governing equations of the nanoplate cohesively bonded to the substrate become

$$\begin{aligned} &-2N\varepsilon^2 \frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + N\varepsilon^3 \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + 2N\varepsilon^2 \frac{\mathrm{d}\psi}{\mathrm{d}x} - \bar{\sigma}_0 H(L_c - x) = 0, \\ &A\varepsilon^3 \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + N\varepsilon^2 \frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + 2N\varepsilon\left(\psi - \frac{\mathrm{d}w}{\mathrm{d}x}\right) = 0 \end{aligned} \tag{9}$$

where $H()$ is the Heaviside step function. The overbar for the nondimensional quantities is omitted for simplicity. The nondimensional boundary conditions at $x = 0$ are still given in Eq. (5), and the conditions at the loading edge become

$$\begin{aligned} &2N\varepsilon \frac{\mathrm{d}w}{\mathrm{d}x} - N\varepsilon^2 \frac{\mathrm{d}\psi}{\mathrm{d}x} - 2N\varepsilon\psi = \bar{Q}_0, \qquad x = 1 \\ &-\bar{A}\varepsilon^2 \frac{\mathrm{d}\psi}{\mathrm{d}x} + N\varepsilon\psi - N\varepsilon \frac{\mathrm{d}w}{\mathrm{d}x} = 0, \qquad x = 1 \end{aligned} \tag{10}$$

In addition to the above boundary conditions, we also need the following continuity conditions at the debonding front:

$$\begin{aligned} &w|_{x=L_c^-} = w|_{x=L_c^+}, \qquad \psi|_{x=L_c^-} = \psi|_{x=L_c^+} \\ &Q_x|_{x=L_c^-} = Q_x|_{x=L_c^+}, \qquad M_x|_{x=L_c^-} = M_x|_{x=L_c^+} \end{aligned} \tag{11}$$

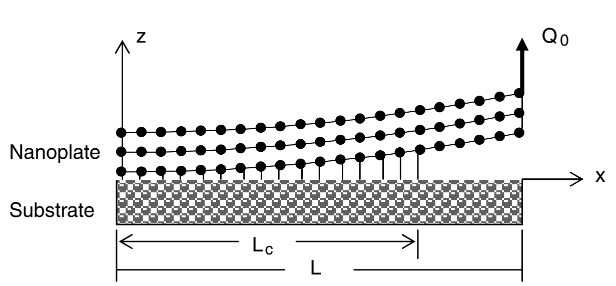

Fig. 1 Interface debonding between a nanoplate and the substrate.

D. Solution

By solving the debonding-bending problem of the nanoplate described in the above subsection, we obtain the solution for the nondimensional deflection as follows:

$$\begin{aligned} w = &-\frac{\bar{\sigma}_0}{2\varepsilon^2(2\bar{A}+N)}\left[-\frac{(\varepsilon+L_c)L_c}{\varepsilon}x + \left(\frac{1}{2} - \frac{L_c^2}{\varepsilon^2}\right)x^2 \right.\\ &\left.+ \frac{2L_c}{3\varepsilon^2}x^3 - \frac{L_c^2}{\varepsilon^2}x^4\right] - \frac{\bar{\sigma}_0}{2N\varepsilon}\left(L_c x - \frac{1}{2}x^2\right) \\ &+ \frac{\bar{Q}_0}{2\varepsilon^2(2\bar{A}+N)}\left[-(2+\varepsilon)x - \frac{2}{\varepsilon}x^2 + \frac{2}{3\varepsilon}x^3\right] \\ &+ \frac{\bar{Q}_0}{2N\varepsilon}x, \qquad 0 \le x \le L_c \end{aligned} \tag{12}$$

$$\begin{aligned} w = &-\frac{\bar{\sigma}_0}{2\varepsilon^2(2\bar{A}+N)}\left[\frac{\bar{A}}{N}L_c^2 + \frac{L_c^4}{6\varepsilon^2} - \left(\frac{L_c^2}{\varepsilon} + \frac{2L_c^3}{3\varepsilon^2}\right)x\right] \\ &+ \frac{\bar{Q}_0}{2\varepsilon^2(2\bar{A}+N)}\left[-(2+\varepsilon)x - \frac{2}{\varepsilon}x^2 + \frac{2}{3\varepsilon}x^3\right] \\ &+ \frac{\bar{Q}_0}{2N\varepsilon}x, \qquad L_c \le x \le 1 \end{aligned} \tag{13}$$

The bonding length L_c is determined by the condition that deflection at the debonding front equals δ_0, i.e.,

$$\begin{aligned} &-\frac{\bar{\sigma}_0}{2\varepsilon^2(2\bar{A}+N)}\left[\frac{\bar{A}}{N}L_c^2 - \frac{L_c^3}{\varepsilon} - \frac{L_c^4}{2\varepsilon^2}\right] \\ &+ \frac{\bar{Q}_0}{2\varepsilon^2(2\bar{A}+N)}\left[-(2+\varepsilon)L_c - \frac{2}{\varepsilon}L_c^2 + \frac{2}{3\varepsilon}L_c^3\right] + \frac{\bar{Q}_0}{2N\varepsilon}L_c = \frac{\delta_0}{a} \end{aligned} \tag{14}$$

The maximum deflection at the loading edge ($x = 1$) is given by

$$\begin{aligned} w_{\max} = w(1) = &-\frac{\bar{\sigma}_0}{2\varepsilon^2(2\bar{A}+N)}\left[\frac{\bar{A}}{N}L_c^2 + \frac{L_c^4}{6\varepsilon^2} - \frac{L_c^2}{\varepsilon} - \frac{2L_c^3}{3\varepsilon^2}\right] \\ &+ \frac{\bar{Q}_0}{2\varepsilon^2(2\bar{A}+N)}\left[-2 + \varepsilon - \frac{4}{3\varepsilon}\right] + \frac{\bar{Q}_0}{2N\varepsilon} \end{aligned} \tag{15}$$

The energy stored in the deformed nanoplate and dissipated during interfacial debonding may be calculated as the work done by the applied load, i.e., the area under the curve of Q_0 versus $w_{\max}$ given by

$$E_{\mathrm{debond}} = \int_0^{w_{\max}} Q_0 \, \mathrm{d}w_{\max} \tag{16}$$

We note that Eq. (15) implies a nonlinear relationship between Q_0 and $w_{\max}$ because the debonding length $L - L_c$ also depends on Q_0.

III. Numerical Results

This section presents numerical examples of interfacial debonding between a NaCl nanoplate and a glass substrate. The properties for the NaCl nanoplate are given as follows [6]: $\alpha_1 = 2.02$ nN/nm, $\alpha_2 = 1.10$ nN/nm, and $a = 0.174$ nm. The plate length is assumed as $L = 100a$. A nanoplate with 11 layers of atoms ($N = 5$ corresponding to a plate thickness of 1.74 nm) is used in the calculation. We also assume the following cohesive properties for the interface between the nanoplate and the substrate: $\sigma_0 = 15$ MPa and $\delta_0 = 0.348$ nm. The cohesive energy density is $\Gamma_0 = \sigma_0\delta_0 = 5.22$ mJ/m^2 which, in terms of order of magnitude, is consistent with the estimate of work of adhesion due to the van der Waals force between NaCl nanoparticles and a soda lime glass substrate [4], especially in the presence of high relative humidity. We note that the assumed interface cohesive traction is much lower than the

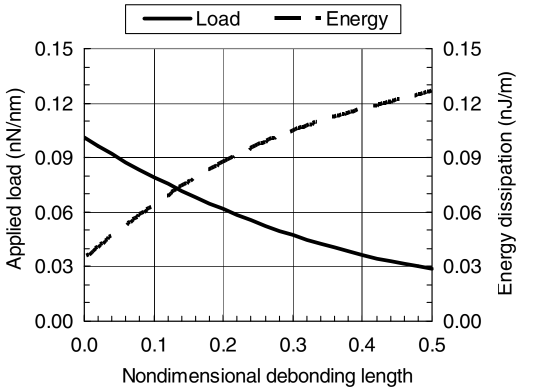

Fig. 2 Load and energy required to debond the nanoplate of unit width versus the debonding length.

theoretical strength of NaCl, which justifies the use of the linear nanoplate theory [5,6].

Figure 2 shows the response of applied load Q_0 versus nondimensional debonding length, and the energy required to debond the nanoplate of unit width (nm) versus the debonding length. Debonding first occurs at a load of 0.1013 nN/nm. The load then decreases with increasing debonding length. The load decreases to 0.0287 nN/nm when the debonding length reaches half the plate length ($L_c = 0.5$). The fixed support boundary condition at $x = 0$ together with the cohesive force would require significantly higher load to propagate the interface crack into the region near the fixed end. Hence, debonding beyond half the plate length is not considered in this study. It is also seen that the energy increases with increasing debonding length as expected. The energy per unit width increases to 0.1263 nN-nm (or nJ/m) at a debonding length of $L - L_c = 0.5L$. In other words, the energy density required to detach the single nanoplate of 1.74 nm thickness at a debonding length of 8.7 nm is about $0.015\ \mathrm{J/m^2}$. The result has significant implications in engineering nanomaterials for energy absorption such as supramolecular materials composed of molecularly intercalated nanoflakes since progressive delamination of large number of nanoflakes could lead to significant energy dissipation. However, this requires a molecular approach to engineer the interlayer bonding properties, which will be reported elsewhere [3].

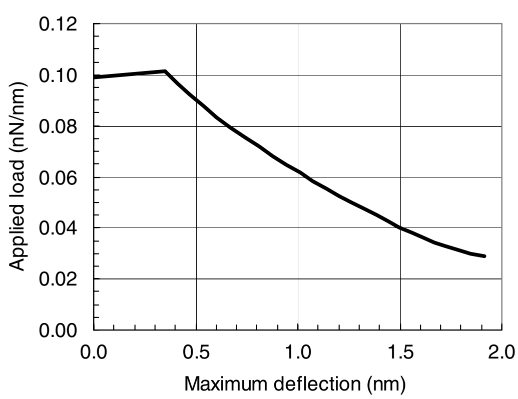

Fig. 3 Load versus maximum deflection response.

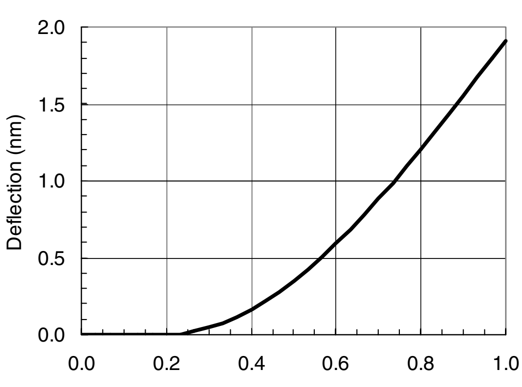

Fig. 4 Deflection curve for $L_c = 0.5$.

Figure 3 shows the response of applied load Q_0 versus maximum deflection at the edge of the nanoplate. An initial load of 0.09873 nN/nm is required to deflect the plate due to the action of interface cohesive traction σ_0. The load initially increases linearly with deflection until the interface starts to debond at the loading edge. The load then gradually decreases with increasing deflection because of the interfacial crack extension. The load reduces to 0.0287 nN/nm at a debonding length of $L - L_c = 0.5L$ at which the deflection of the loading edge reaches 1.91 nm.

Figure 4 shows deflection curve of the nanoplate at a nondimensional debonding length of 0.5. The corresponding applied load is 0.0287 nN/nm and the debonding length is $L - L_c = 0.5L$. The nanoplate and the substrate are perfectly bonded along $0 \leq x \leq 0.23$ due to the cohesive force. The plate and the substrate are still bonded along $0.23 < x \leq 0.5$ with a cohesive traction of σ_0, and are in the process of complete decohesion.

IV. Conclusions

This work investigates the interfacial debonding between a platelike nanomaterial and the substrate. The nanoplate is loaded by a transverse force at one edge and fixed at the other end. The analytical solution of the problem is obtained using a semicontinuum nanoplate theory [5,6] and a cohesive zone model characteristic of the van der Waals bond. The relationship between the applied load and debonding length, and the energy required to debond the nanoplate of unit width (nm) versus the debonding length are determined from the analytical solution. A linear relation between the deflection of the plate at the loading edge and the applied load prevails before the start of debonding. The load decreases monotonically with increasing debonding length once the debonding occurs and progressively propagates along the interface. It is important to use nanoplate models instead of classical continuum theories in evaluating the energy stored in the deformed nanoplate and dissipated during the progressive debonding between a platelike nanomaterial and the substrate/matrix because continuum theories underestimate the deformation.

Acknowledgments

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M. Hyer
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