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SUMMARY

We present a new approach based on coupling the extended finite element method (XFEM) and level \bullet to determining to study surface effects on the mechanical behavior of nanostructures. The coupled surface effects on the mechanical behavior of nanostructures. The coupled $XFEM$ -v-lease acontinuum solution to nanomechanical boundary value problems in the nanomechanical boundary value problems in the α cdc \ldots b ζ and diace in both strain and interface and interface are easily and interfaces are easily handled, which simultaneously account $f \in \mathbb{C}$ and f accounting surface energy, including surface energy, stress, including surface energy, stress, including surface energy, stress, including surface energy, stress, including elasticiately and interface decohesion. We validate the proposed approach by studying the proposed approximately study of the surface-stress-
decohesion. In the surface-stress-stress-stress-stress-stress-stress-stress-str drove and $f \longrightarrow \text{with } a \neq 1$ as the surface $a \rightarrow a \rightarrow c$ as the surface surface f vasticity to the effective stiffness of nanobeams. For each case, we compare the numerical results with $\frac{1}{2}$ new analytical solutions that we have defined for the problems; for the problems; for the problem involving the ι sface-setress-driven relaxation of a homogeneous nanoplate, we further validate the proposed approach of approach ι b comparing the results with the results with the results with the results with the results of the re \bullet is face Cauchy–Born model. These numerical results show that the proposed vertical be used to gain critical into the method into how surface effects in according to mechanical behavior ad ρ , we nade properties of the composite nanobeams under generalized mechanical deformation. C_{c} ϵ *y* \odot 2010 J W \bullet & S \bullet , L d.

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KEY WORDS: ι sface earsticity; surface set; nano-structure; XFEM; ee

INTRODUCTION

 $T \rightarrow \infty$ is not allow that materials in the understanding that materials whose units whose α features de at the nanometer length scales exhibit scales exhibit mechanical behavior and properties that \mathbf{r}

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C $rac{ac}{c}$ is a contraction sponsors: NSF; contraction in b is cmMI-0900607, CMMI-0750395

First 1. General outline of the nano-structure under study.

SURFACE EFFECTS ON NANO MATERIALS 1471

F_J $i \in S$. (a) E_{nr}iched downtown is cut by the interface ($x \rightarrow y$; (b) enriched do and completely entitled enriched exactles for a close interface; and cutting plane to define the set of f and cutting plane to define to define to define to define to define the set of f and cutting plane to define the se $c_4 \circ a_2 \circ c_1$ in a square damin

 \mathbf{w}_p^* , we

$$
I_{I}(x) = \begin{cases} N_{I}(x) & 0 \\ 0 & N_{I}(x) \end{cases} \tag{17}
$$

where \mathbf{r} is *N_I* () are finite extended shape \mathbf{r} , *N_J* () are \bullet associated with the nodes of an element that \bullet and \bullet face $(F_{.115} \bullet 3(b))$ and $H()$ and $\chi()$ are equired the required discontinuities with the requirement functions with the requirement functions with the requirement of $F_{.115}$ $(\epsilon \cdot d \cdot f \cdot c)$ and Heaviside function, $\epsilon \cdot \epsilon$, $\epsilon \cdot \epsilon$, $\epsilon \cdot \epsilon$ is the total (16), *n* is the total total total (16), *n* is the total and number of d_{\bullet} , whereas m_{\bullet} is the number of enriched d_{\bullet} (*m* $\leq n$). By definition, and $e \cdot c$ oder do below to an element that is cut by the interface as depicted in Figure 3. To de e ere es functions are gara fashion, esclusion a level set function () such that a vertace deed by \neq intervalent and intervaled intersection of the intervale. With the sign of ϕ is opposite in the sign of all ϕ at two sign of ϕ $f(x) = x - y$ and the unit of a set of the sets is the interface interface interface is determined by the gradient f \bullet fic. $\phi(x)$ a f:

$$
\left(\begin{array}{c}\n\end{array}\right) = \frac{\nabla \phi(x)}{\|\nabla \phi(x)\|}\n\tag{18}
$$

Let us now focus on the Heaviside and ridge functions appearing in (16). Referring to Figure 4, \bullet H \bullet a d \bullet from \bullet a \bullet a \bullet a ridge displacement (strong displacement (strong displacement (strong displacement (strong displacement); in contrast, a strong displacement (strong displacement of \bullet); in co function causes a id in strain field id or interface that is related values of interface that is related values of interface that is related values of id or interface that is related values of id or interface that is derivative of displacement. With α into details, the Heaviside and ridge functions are responsible functions are r d **d** \bullet d**ime** \bullet d**ime**nsion):

$$
H(\phi) = \begin{array}{ccccc} 1 & \phi/ \ 0 \\ 0 & \phi & 0 \end{array} \quad \text{a d} \quad \chi_j(\) = |\phi(\)| - |\phi(\)| \tag{19}
$$

 T is finite extended by the deformation of nano-composites is not depend by s_1 **b** s_1 **d** s_2 **d** s_3 **d** s_4 **a e from** (16) **i b a f f f l g i i** (14) and (15). For this, strain, and early matrices are first rewritten in Voice notation [27].

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F₁ $s = 4$. A $t = \pm a$ f $s = f(a) - a$ denoted by define strong and define strong and valid continuity, $c \neq 0$, $c \neq 0$.

Bulk energy

Starting with the bulk energy,the finite element approximation -*W*˜ *^e ^b* of -*W^e ^b* gives rise to the a dad \bullet , \bullet \bullet :

$$
\delta \tilde{W}_b^e = \frac{\delta \epsilon^e : e^e \cdot \epsilon^e d\Omega}{\Omega} = \delta^{eT} \cdot \frac{e^T \{ e^e \} e^T d\Omega \cdot e}{\Omega} \tag{20}
$$

where *e* and { e } are bulk constitutive relation as for element *e* in tensorial and Voigt a ρ , ρ , ρ , ρ , ρ and in terms of the standard matrix is ρ the shape functions $\frac{1}{2}$

External energy

Fa, the finite element approximation of the external energy is only associated with standard and standard $a \cdot f(c)$, and $i \cdot g \cdot b$:

$$
\delta \tilde{W}^e_{\bullet} = \delta^{eT} \cdot \Omega^{eT} d\Omega + \frac{e^{T}}{\partial \Omega_F} d\Gamma
$$
 (30)

Final XFEM equation

U r E r a (20) , (22) , (28) , and (30) , and the weak form in (14) and (15), \bullet XFEM \bullet r and for one one element of $f \circ f$.

$$
\left(\begin{array}{cc} e & e \\ b & d \end{array}\right) \cdot e = e - e \tag{31}
$$

where the nodal displace e is contributions from the contributions from the contributions of contributions from the contributions of contributions of contributions of contributions of contributions of contributions of c die $1 + 1$, and $s + 1$ die $1 + 1 + 1$

$$
e = [\quad \left\{ \nabla \quad \right\} \quad \in
$$

d

F_{IS} = 5. T_i ca i a normal elements: (a) normal elements: (b) and (c) = ϵ c = d = = = ϵ .

continuous across across c_1 and c_2 and c_3 and c_4 require the existence of a strong discontinuity, but f if \star if \star is leads and indical study of an indical stiffness matrix \star indical study indical study in \star is an indical ζ vanishing stiffness). The second stategy, which is described in this paper, overcome this paper, overcome this paper, overcome this paper, overcome the strategy of the strategy of the strategy of the strategy of the by considering a stiffness in the external stiffness in the external region, together with the existence of f a displace entirely across the free boundary. The strong discontinuity and ensures that the free boundary discontinuity across that the format t diac vidivident fields in the theory in the dependent, and thus the material Ω_2 $d \bullet$ introduction. The same reference relief $d \circ f$ is due the introduction of both a strategy the intervals of both a strong strategy of both and wand discontinuity (to describe surface elasticity) on the effect.

In the paper, bilinear four and are used. Furthermore, for integrating are used. F_1 purposes, four Gaussian are considered in normal and partial and partially enriched elements. In addition, for $[34]$, $b-c.a \rightarrow a \rightarrow c$ of both sides and interface in an enriched element. The interface in an interface in an interface in an interface in method allows to define enough \mathbf{f} integration integration in the integration in the enriched region; in the enriched region; in the energy of \mathbf{f} is a set of \mathbf{f} is a set of \mathbf{f} is a set of \mathbf{f} i finally, the integration on surface is performed under the integration of $f(x)$ assumption that the integration of $f(x)$ a say \bullet costs in and \bullet . Figure 5 shows the gauss points and sub-sears \mathbf{u} different situations.

NUMERICAL EXAMPLES

In order the aforementioned model and for validation purposes, we investigate we allowed properties of α final properties and compare the numerical results with a a canalytical solutions. In particular, we concentrate on the following point

- T \bullet strain relation of nanoplates subjected to subject the subject of the subjected to subject the subject of α $ca \rightarrow a$ \rightarrow \rightarrow \rightarrow $a \rightarrow a$ d a composite bilayered plate.
- T \mathbf{r} is face each value of in the axial stiffness of nanoplates (both in uniaxial deformation in unitative of nanoplates (both in unitative of nanoplates in unitative of nanoplates in the axial deformation of $\$ a adb $d \cdot$).
- T eff + C f + C b and f surface decohesion and surface elasticity on the overall contracts. \bullet c a case, \bullet f a a \bullet and an inclusion.

For each problem, $a \neq a$, $\neq fac$ interfaces (including the structure) are modeled using the structure of the structure b stad and c \mathbf{r} . The strong and weak discontinuity allows the strong discontinuity allows the structure under structure

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F_{rig} = 6. Sc = a c f a g d a g a =, a d = ζ = i g xFEM disc= a

Figure 7. A comparison of surface-stress-driven compressive axial strain and using E range (40) ad XFEM a \rightarrow \rightarrow d a \rightarrow a \rightarrow \rightarrow

from Equation (40) and the XFEM simulations are actively match exactly. Equations (40), va ve ve ved veffect $f P$, say, surface value constants and boundary conditions; becar of the Poisson ratio and surface elastic constants and subset of \mathbb{R} FEM ca can all α .

B.can $\bullet \gg t$, \bullet can $\bullet \bullet$ contributed t in \bullet \bullet + time in (41) and ϵ \bullet as:

$$
\frac{F}{\blacktriangleright} = \sigma t + 2\tau \tag{42}
$$

If *E* and S_{1111} a. the bulk Young's modulus and a surface earlier constant, respectively, ca_c \cdot a:

$$
1 = \frac{\sigma}{E} \quad \text{a d} \quad 2 = \frac{\tau}{S_{1111}} \tag{43}
$$

where 1 and 2 are the axial strains in the axial strains in the bulk and surface, respectively. Combining Equations in the bulk and surface, respectively. Combining Equations in the axial strains in the axial strains in t (42) a d (43) a d \cdot \cdot a \cdot \cdot = \cdot \cdot *L*, \cdot b a :

$$
\frac{E_P}{\delta L} = \frac{Et}{L} + \frac{2S_{1111}}{L} = K_b + K_s \tag{44}
$$

where *K_b* and *K_s* are the bulk and surface and if if it is respectively. From (44), we note that if it is a stiffness of the interval stiffness, respectively. $a \le a \le c \le f \le r$ gold as $p \le r$ in Table I are considered, because the $Y \cap r'$ dulus *E* is to ϵ or a section of the surface stiffness *K_s* with be negligible for ϵ arge $a \bullet$, which is good in contract of smaller smaller $a \bullet a$ in $a \bullet$. Furthermore, Equation (44) denotes the aspect ratio of the aspect ratio of the plate t as a significant effect on the bulk, ad the $f \cdot f \cdot a$ and F_{ℓ} stiffness of the nanoplate. $f \rightarrow a$ as $\bullet \bullet \bullet$, where a aspect $a \downarrow L$ as $\bullet \circ$ constant at 10. As can be \mathbf{v} Figure 9, and excellent agreement is found between the theoretical solution in Equation (44)

F_{igure} 9. Surface effects on the size-dependent axial stiffness of a gold nanoplate and a gold nanoplate a gold nanoplate a gold nanoplate $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ a a constant f 10.

Figure 10. General outline of $f = \frac{1}{2}$ fixed bi-layered nano-beam including both surface and interface $f = 1$.

If \bullet d \bullet \bullet τ_1^0 , τ_2^0 , and τ_{12}^0 and \bullet is face \bullet expression of surface \bullet is \bullet if \bullet is \bullet \bullet interface f and and 2 , \bullet induced moment (*M*) in the induced moment (*M*) in $\bullet c$ and \bullet the material and surface $\bullet a$ and c , \bullet we difference between \bullet \bullet and \bullet 1 $a d 2 a:$

$$
M = (\tau_{1\blacktriangleright}^{0})(t - x) - (\tau_{2\blacktriangleright}^{0})x + (\tau_{12\blacktriangleright}^{0}) \frac{t}{2} - x
$$
\n(47)

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F_J $i \in \{11, (a) \mid A \mid a \in \{2, a\} \}$ be the XFEM and theory (Equations (49)–(51)) due both surface and interface stress for a bi-a wid $P_{\rm A}$ Ni a chavered \sim and \sim deflection comparison along a bi-layered P_t(N_i a abi-level XFEM and \bullet comparison (52)) due b ι sface and interface seeds.

F_{14} \div 12. Sc \div a c f a \div d \div d a b \div a b \div b an applied force *F*.

a \bullet compare \bullet compare \bullet XFEM cost \bullet The bending equilibrium of the cross- \bullet ction shown in Figure 12 can be written as a shown in Figure 12 can be written as a section of \bullet

$$
\sigma_x y \, dA + 2 \qquad f_s \frac{t}{2} \, dz = -M \tag{53}
$$

 $\forall x \in \sigma_x$ is the axial stress of the cross-section and *f_s* is the force induced on the beam surface due to the surface elastic constant *S*₁₁₁₁; $f_s = S_{1111}$ may is the maximum aximum ax a co ς **.** and b is faces. By applying the standard ς on $\sigma_x = E$ and

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$$
= (\mathbf{y} \ \mathbf{y} \ \mathbf{a}) \quad \mathbf{a} \ \mathbf{a} \ \mathbf{d} + \mathbf{b} \quad \mathbf{y} \quad \mathbf{y} \quad \mathbf{y} \tag{53}
$$
\n
$$
= \frac{2E}{t} \quad \mathbf{a} \quad \mathbf{y}^2 \, \mathbf{d}A + S_{1111} t \quad \mathbf{a} = -M \tag{54}
$$

Known $I = y^2 dA$, where $I = \infty$ is section momentum axis *I* is section momentum axis *z*, one can write:

$$
a = \frac{-M}{\frac{2EI}{t} + S_{1111}t_{\blacktriangleright}}\tag{55}
$$

For the rectangular section shown in Figure 12, $I = \frac{1}{12} \times t^3$; we figure can simplify Equa- (55) :

$$
a = \frac{-M}{\blacktriangleright t(\frac{1}{6}Et + S_{1111})}
$$
\n(56)

 \bullet for \bullet can write:

$$
=\frac{-2My}{\blacktriangleright t^2(\frac{1}{6}Et + S_{1111})}
$$
(57)

If \bullet c $d \bullet F$ and *d*

Figure 14. General outline of the plate under study under study of the plate f and f and f interface interface interface f coehesion). Sub-elements close to interface are used for plotting purposes on α

 \bullet T \bullet defined is above to describe a splastic in nano-composite such as plasticity in nano-composite such as plasticity in α as α or damage. It is presented the study of studying state of surface $\frac{1}{\sqrt{2}}$ or the surface effects on t def ζ and and fraction of nano-composite structures.

 T odoby od methodology was verified against four numerical examples in the face $s = -d_1 - g = a$ a fa a a nad a n $-$ a multi-material a multi-material bi-layer nanoplate. \bullet a a ff \bullet f a a a \bullet , a d is face effec \bullet bending ffixed frace beam. In a cases, \bullet XFEM/level set in excellent set of a cases with the derived with the analytical solution. Furthermore, validation in the case of the surface-stress-driven relaxation of \bullet daga \bullet against \bullet daagb \bullet calculations. Atomistic and multiscale \bullet SCB calculations. Fa, in the last example, a combination of was addening to capture and strong discontinuities was used to capture \bullet interactions between surface decohesion and surface elasticity in a plate with a plate with an inclusion. The influence of surface properties and decohesion on the overall mechanical response of the composite of the composite \mathbf{r} plate could the assessed. Since surface early assessed with the inclusion on \mathbf{S}_1 associated with the inclusion, we call the inclusion of \mathbf{S}_2 associated with the inclusion, we call the inclusion of \mathbf{S}_1 as $b \leq -d$ a $-d \leq -d - d - c$ in the overall and $c \leq -d$ in the overall plate response when $c \in \mathbb{R}$ and as and devel. However, no singlet when the interface constant and interface constant of interface constant of interface constant and interface constant and interface constant and interface constant and interface const a $-d$.

Future will focus on incorporation in \mathbf{F}_t and interface decohesion in \bullet , \circ \bullet d framework \circ [38–40], as well as detailed investigations into how surface effects in actions in \bullet \bullet calcal properties of a nanomaterials.

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