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### SUMMARY

• d (XFEM) a d • • We fee  $a = a_i f_i ac_i ba_i d_i c_i f_i e_i e_i d_i d_i$ . . . . . • Id Içfac• ad • fac• •ff•c • •c a ca b• a c f a cicic•. T• ci •d XFEM• • • a c a ca b• a c ii a •c a ca b i da; ai• c b• c d c ii • b ca a d d ac• • d• • icfac• ad • fac• a; •a a d•d, • i a•i acci i f c c ca a ca • icfac• •ff•c , cid i icfac• • •; , ; •, • a c a d • fac• d•c • . . W• a da • • , ; • d a ; a c b i d i • • i fac•- ;• - $\begin{aligned} \mathbf{d}_{\mathbf{c}} &= \mathbf{c} \cdot \mathbf{a} \cdot \mathbf{a} &= \mathbf{f} \quad \mathbf{i} \cdot \mathbf{v} \cdot \mathbf{i} \quad \mathbf{a} \cdot \mathbf{d} \cdot \mathbf{b} \cdot \mathbf{a} \cdot \mathbf{c} \quad \mathbf{a} \quad \mathbf{c} \quad \mathbf{c} \quad \mathbf{b} \quad \mathbf{f}_{\mathbf{c}} \quad \mathbf{v} \cdot \mathbf{c} \quad \mathbf{c} \\ & \cdot \mathbf{a} \quad \mathbf{c} \quad \mathbf{v} \cdot \mathbf{f} \mathbf{f} \cdot \mathbf{v} \quad \mathbf{f} \quad \mathbf{a} \quad \mathbf{b} \cdot \mathbf{a} \quad \mathbf{c} \quad \mathbf{c} \quad \mathbf{a} \cdot \mathbf{v} \quad \mathbf{c} \quad \mathbf{c} \quad \mathbf{c} \quad \mathbf{c} \quad \mathbf{c} \\ & \cdot \mathbf{a} \quad \mathbf{a} \quad \mathbf{c} \quad \mathbf{c}$  $1 \in fac - c - dc - c - a = fa$  1 - 1 = a = a - c - fc = c - a = da - c - c - da = c - a = c - da = c - a = c - da = c - a =• Isfac • Carc Bs de. T • • I • case I cao a ba •dı a •...•d • d ca b• 1 • d a d c • • f rac; ca\_r \_ r; fac• •ff•c \_ ac • •c a ca b• a ; r••r a d c \_ • a b•a r d•; r••; a •d •c a ca d•f; a . iface offect ac e e a cabe a f C \_ f \_ © 2010 J W. • & S , L d.

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KEY WORDS:  $i \notin fac \bullet \bullet a = c = ; i \notin fac \bullet \notin \bullet ; a = \# c i \notin \bullet ; XFEM; \bullet \bullet \bullet$ 

### **INTRODUCTION**

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<sup>\*</sup>C c;  $\bullet_{i}$  d  $\bullet_{i}$  c : F; a c J. V  $\bullet_{i}$   $\bullet_{i}$  , D  $\bullet_{i}$   $\bullet_{i}$  f C  $\cdot_{i}$  E  $\cdot_{i}$   $\bullet_{i}$  a d A; c  $\bullet_{i}$  c  $\cdot_{i}$  a E  $\cdot_{i}$   $\bullet_{i}$   $\cdot_{i}$   $\cdot_{i}$  J  $\bullet_{i}$  f C  $\cdot_{i}$  a d a B  $\cdot_{i}$  d  $\bullet_{i}$  , Ca  $\cdot_{i}$  B 428, B  $\cdot_{i}$  d  $\bullet_{i}$  , CO 80309-0428, U.S.A. E- a : f; a c  $\bullet_{i}$   $\bullet_{i}$   $\bullet_{i}$  c  $\bullet_{i}$  a d  $\bullet_{i}$ 

C ; ac, r; a ;: NSF; c ; ac, r; a r b; : CMMI-0900607, CMMI-0750395



 $F_{\mathcal{F}}(\mathfrak{g}\bullet 1,\,G\bullet\,\mathfrak{g}\mathfrak{a}\,\mathfrak{g})=\mathfrak{f}\,\,\bullet\,\mathfrak{g}\,\,\bullet\,\mathfrak{g}(\mathfrak{g}\bullet\mathfrak{g}\bullet\mathfrak{g})=\mathfrak{g}(\mathfrak{g}\circ\mathfrak{g}\bullet\mathfrak{g})$ 



## SURFACE EFFECTS ON NANO MATERIALS



 $F_{i'} = (-3, (a) = (-2, -d) + (-2, -d) +$ 

₩, ₩

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

$$() = \frac{\nabla\phi(x)}{\|\nabla\phi(x)\|} \tag{18}$$

Let  $\mathbf{f} \circ \mathbf{o}$  • Heal de a d c de  $\mathbf{f}_1 \circ \mathbf{c}$  a  $\mathbf{a}_1 \cdot \mathbf{a}_2 \cdot \mathbf{c}_1 \cdot \mathbf{c}_1$  (16). Referent  $\mathbf{F}_1 + \mathbf{c} \cdot \mathbf{d}_1$ • Heal de  $\mathbf{f}_1 \circ \mathbf{c}_1$  a  $\mathbf{a}_1 = \mathbf{d}_2$  ace  $\mathbf{e}_1 (\mathbf{c}_1 + \mathbf{d}_2 + \mathbf{c}_1)$ ;  $\mathbf{c}_1 \circ \mathbf{c}_2$  a  $\mathbf{a}_2 \cdot \mathbf{d}_1 \cdot \mathbf{c}_1$  $\mathbf{f}_1 \circ \mathbf{c}_2 \circ \mathbf{a}_1 = \mathbf{c}_2 \circ \mathbf{a}_1 \cdot \mathbf{c}_2$  a  $\mathbf{d}_1 \circ \mathbf{d}_2 \circ \mathbf{c}_1 \cdot \mathbf{c}_1$  ) ace  $\mathbf{e}_1 \circ \mathbf{c}_2 \circ \mathbf{c}_2$  a  $\mathbf{c}_1 \circ \mathbf{c}_2 \circ \mathbf{c}_2$   $\mathbf{d}_1 \circ \mathbf{c}_2 \cdot \mathbf{c}_2$   $\mathbf{d}_2 \circ \mathbf{c}_1 \cdot \mathbf{c}_2$   $\mathbf{d}_2 \circ \mathbf{c}_2 \cdot \mathbf{c}_2$   $\mathbf{d}_1 \circ \mathbf{c}_2 \cdot \mathbf{c}_2$   $\mathbf{d}_2 \circ \mathbf{c}_2 \circ \mathbf{c}_2$   $\mathbf{d}_2 \circ \mathbf{c}_2$   $\mathbf{d$ 

$$H(\phi) = \frac{1}{0} \frac{\phi/0}{\phi_{0}} \quad \text{a d} \quad \chi_{j}(\ ) = |\phi(\ )| - |\phi(\ _{j})| \tag{19}$$

 $T \bullet [\bullet \bullet \bullet \bullet \bullet] a = (\bullet \bullet] a = (\bullet] a =$ 

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 $F_{i'} \leftarrow 4. A_{i'} \bullet \Rightarrow a_{i'} f_{i'} = f_{i'} (a) \Rightarrow a_{i'} d \bullet a_{i'} d \bullet (b) = d_{i'} \bullet f_{i'} c_{i'} d \bullet \bullet = f_{i'} a_{i'} d \bullet = f$ 

### Bulk energy

$$\delta \tilde{W}_{b}^{e} = {}_{\Omega} \delta \epsilon^{e} : {}^{e} : \epsilon^{e} d\Omega = \delta {}^{eT} \cdot {}_{\Omega} {}^{eT} \{ {}^{e} \} {}^{e} d\Omega \cdot {}^{e}$$
(20)

External energy

F a , • • • • • a , c a f • • •; a • •; a a c a • d a da; d a • fi c , a d  $\cdot$  a b :

$$\delta \tilde{W}^{e}_{\bullet} = \delta \stackrel{e^{\mathrm{T}}}{\longrightarrow} \stackrel{e^{\mathrm{T}}}{\Omega} \mathrm{d}\Omega + \stackrel{e^{\mathrm{T}}}{\partial \Omega_{F}} \mathrm{d}\Gamma$$
(30)

Final XFEM equation

U \_ ' E ' a \_ (20), (22), (28), a d (30), a d · •a f ; (14) a d (15), • XFEM • ' a \_ f ; :  $f : a = a \cdot f : f$ 

$$\begin{pmatrix} e \\ b \end{pmatrix} + \begin{pmatrix} e \\ d \end{pmatrix} + \begin{pmatrix} e \\ s \end{pmatrix} \cdot \begin{pmatrix} e \\ \bullet \end{pmatrix} = \begin{pmatrix} e \\ \bullet \end{pmatrix} - \begin{pmatrix} e \\ s \end{pmatrix}$$
(31)

 $-\epsilon \cdot \cdot \cdot \cdot da d ac \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot df c \epsilon b f \epsilon \cdot c \cdot i \cdot i \cdot , \cdot a d c \cdot i \cdot , a d \epsilon \cdot \cdot dc \cdot i \cdot \cdot \cdot d$ 

$$\stackrel{e}{=} \begin{bmatrix} -\{ \nabla \} \\ d \end{bmatrix} \in \mathcal{A}$$



 $F_{I}$  : (a)  $\varsigma$  a · · · ; (b) a d (c) ·  $\varsigma_{-}$  c · d · · · .

I a  $\mathbf{x}$ , b  $\mathbf{x}$ , f  $\mathbf{y}$ , d  $\mathbf{y}$  a  $\mathbf{x}$ , f  $\mathbf{y}$ ,  $\mathbf{y}$ , f  $\mathbf{y}$ , a  $\mathbf{x}$ , a  $\mathbf{x$ 

### NUMERICAL EXAMPLES

- $T \cdot ca$ ,  $c \cdot aa$ ,  $f \cdot aa$ ,  $a \cdot b \cdot c \cdot d$ ,  $ca \cdot ca \cdot caa$ ,  $f \cdot aa$ ,  $a \cdot aa$ ,  $a \cdot aa$ ,  $a \cdot aa$ ,  $a \cdot ba$ ,  $a \cdot caa \cdot caa$ ,  $a \cdot ba$ ,  $a \cdot caa \cdot caa$ ,  $a \cdot ba$ ,  $a \cdot caa \cdot caa$ ,  $a \cdot ba$ ,  $a \cdot caa \cdot caa \cdot caa \cdot caa$ ,  $a \cdot caa \cdot caaa \cdot caa \cdot c$
- T •ff•c f c b a f 1; fac• d•c a d 1; fac• a c •; a • c a ca; • • f a a • a c · .

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File 6. Sc • a c f a d a , a d • e v i v XFEM d c • a .



 $F_{ris} \bullet 7. A c = a = f_{ris} fac \bullet - s \bullet - d = c = s \bullet - a = a = s = a = c = r \bullet d = r = E + a = (40)$ a d XFEM a r • r d a = a • • r .

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

If  $E = d S_{1111} a_{\bullet} \cdot b_{\bullet} Y_{1} r' d_{\bullet} a d a_{\bullet} a_{\bullet} c_{\bullet} c_{\bullet} a_{\bullet} c_{\bullet} a_{\bullet} c_{\bullet} \cdot a_{\bullet} c_{\bullet} c$ 

$$_{1} = \frac{\sigma}{E}$$
 a d  $_{2} = \frac{\tau}{S_{1111}}$  (43)

(42) ad (43) ad (43)

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





Fire 10. Go va 1 of de vob - a vod a -boa cid / b refaco a d vefaco offoc.

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

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 $F_{II} = 12$ . Sc • a c f a • d • d a b•a b• b a a • d f c• F.

$$\int_{A} \sigma_x y \, \mathrm{d}A + 2 \qquad f_s \frac{t}{2} \, \mathrm{d}z = -M \tag{53}$$

 $C \,\,, \,\, \varsigma_{-'} \quad @ \ 2010 \ J \qquad W_- \bullet \ \& \ S \quad , \ L \ d.$ 

$$=(\underbrace{y}_{a}, \underbrace{y}_{a})_{a} \text{ a d } \underbrace{b}_{1}, \underbrace{f}_{a}, \underbrace{(53)}_{A} \text{ b d a};$$

$$\frac{2E}{t}_{a} \underbrace{y^{2}}_{A} dA + S_{1111} t_{P} \text{ a} = -M$$
(54)

K  $I = y^2 dA$ ,  $\neg I = -c$   $\cdot f = -c$  a = -d = -z,  $\cdot c = -c$ 

$$_{a} = \frac{-M}{\frac{2EI}{t} + S_{1111}t}$$
(55)

F  $\epsilon$  •  $\epsilon$  • c a i a  $\epsilon$  • c =  $F_{II} \epsilon \bullet 12$ ,  $I = \frac{1}{12} \epsilon^3$ ; •  $\epsilon \bullet f \epsilon \bullet$ , • c =  $f E_{II} \epsilon \bullet 12$ ,  $I = \frac{1}{12} \epsilon^3$ ; •  $\epsilon \bullet f \epsilon \bullet$ , • c =  $f E_{II} \epsilon \bullet 12$ ,  $I = \frac{1}{12} \epsilon^3$ ; •  $\epsilon \bullet f \epsilon \bullet$ , • c =  $f E_{II} \epsilon \bullet 12$ ,  $f E_{II} \epsilon \bullet 12$ ,

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

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

If  $\bullet$  c d = F a d d





• T • • d ab • d •  $c_{1}$  b • c • a • a b • a  $c_{1}$  a - c • i c a a  $c_{2}$ c da ar • I i  $c_{2}$  • • a i • fi f  $c_{1}$  i d  $c_{1}$  i  $c_{1}$  fac • a d •  $c_{1}$  • fac •  $c_{1}$  • d • f  $c_{2}$  • d • f  $c_{2}$  a d  $f_{c}$  a c •  $c_{1}$  •  $c_{1}$  •  $c_{2}$  •

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#### REFERENCES

- 1. S a: a P, Ga S, B a · N. Eff-c f 1 s fac. Applied Physics Letters 2003; 2(4):535 537.
- 2. Da J, Ga K, Di ML. Si  $fac \cdot c \cdot d = c \cdot c \cdot a$  f i d a  $c \cdot Physical Review B 2004; 0. 075413.$
- 3. C T et al. S. •-d• d• a c  $\varsigma$  f i d $\varsigma$  c a a -c . • • fac•  $\varsigma$  • Acta Mechanica 2007; 1 :39 54.
- 4. Ca a; a a RC. Si cface a d e; face c effec . Progress in Surface Science 1994; 4 (1):1 38.
- 5. S VB. A c cao a f a c ; ; f a c FCC c; a <math>c cao a Physical Review B 2005; 1:094104.
- 6. M. C, Ji S, Ki; DA, K. SY. A ccao a f sface a c; see c see a c b a s. Physical Review B 2008; :075425.
- 7. Pa; HS, K PA. Sicfac · Carc B c a a ficfac c ff · c a c a c . Physical Review B 2007; :085408.

8. Pa; HS, Ca W, E, a HD, H a ' H. M • c a c f c; a • a c • . *MRS Bulletin* 2009; **34**(3):178–183. 90**7**54259999 0 .9968(d • c H1 ) 68(d • c H1 ) 0 Tc383.9(L • •;)9.8 L • 2(c a 103.2 • c •)( )0(• a 9.8) , a •, P ca R • c ; •fB