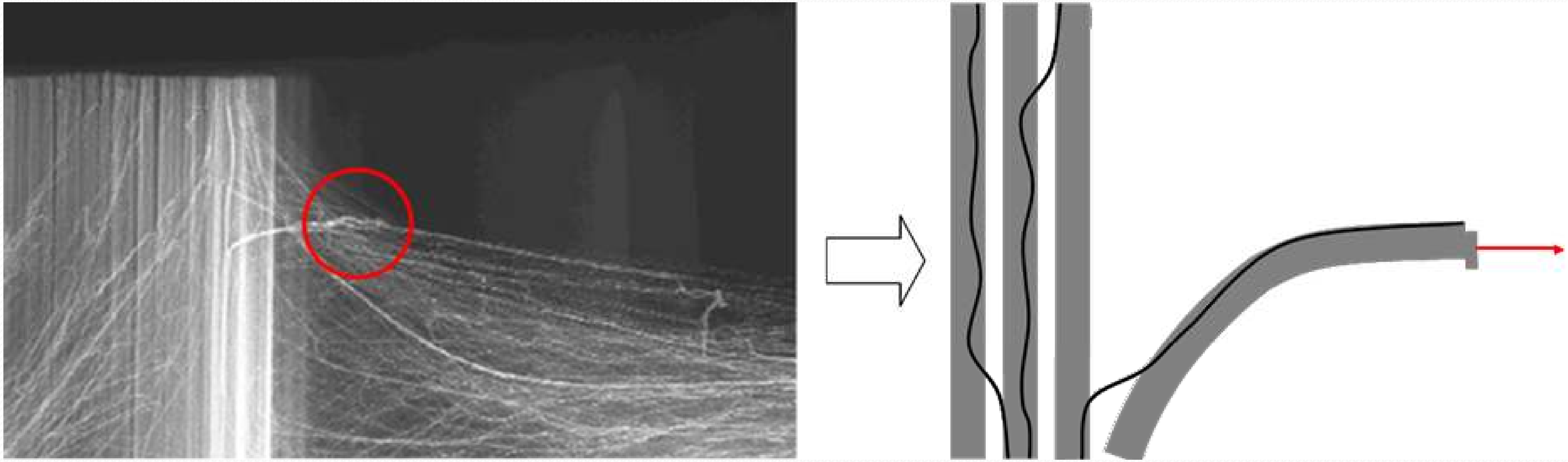
Instituto de Física "Gleb Wataghin"

Curso de verão 2014

Minicurso: Modelagem de materiais nanoestruturados com *Física Básica*



GSONM

Prof. Dr. Alexandre Fontes da Fonseca – DFA – IFGW

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Resumo da apresentação:

1. Introdução

2. Florestas de Nanotubos Helicoidais

3. Formação de Fios de Nanotubos de Carbono

4. Comentários

5. Idéias e projetos futuros ...

Introdução

David J. Srolovitz, University of Pennsylvania

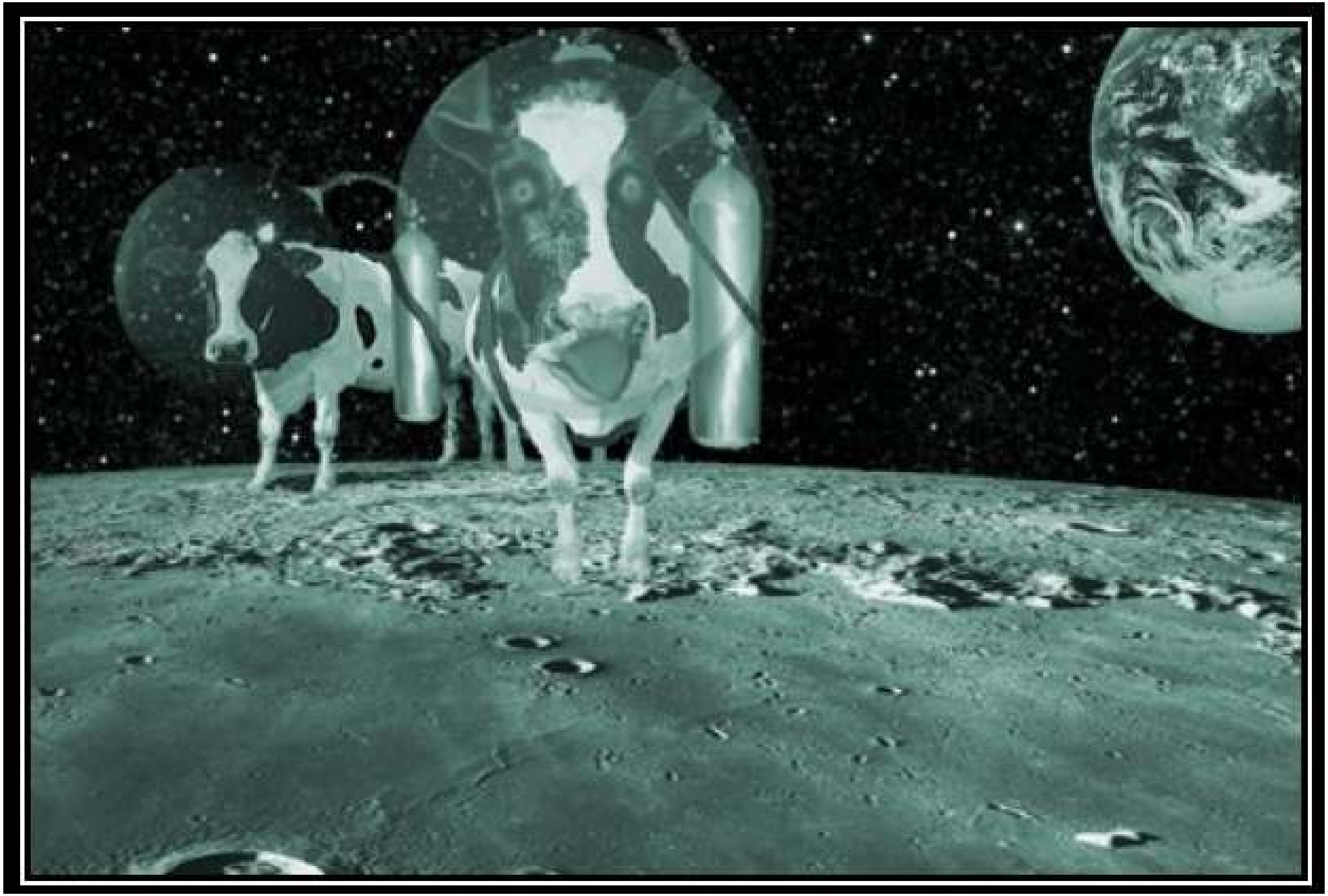
Materials Theory Award Talk 2013
"Polycrystal Microstructures At-Scale"

Como modelar uma vaca?

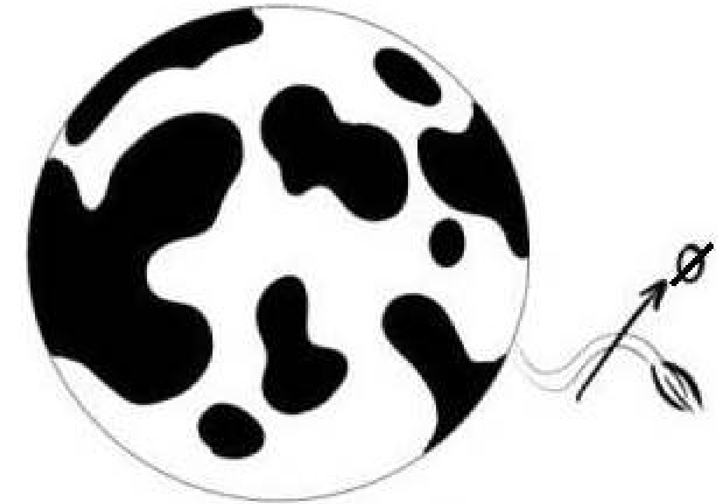
Por onde começar?

Como um bom físico(a) ...

Se vc quer estudar:



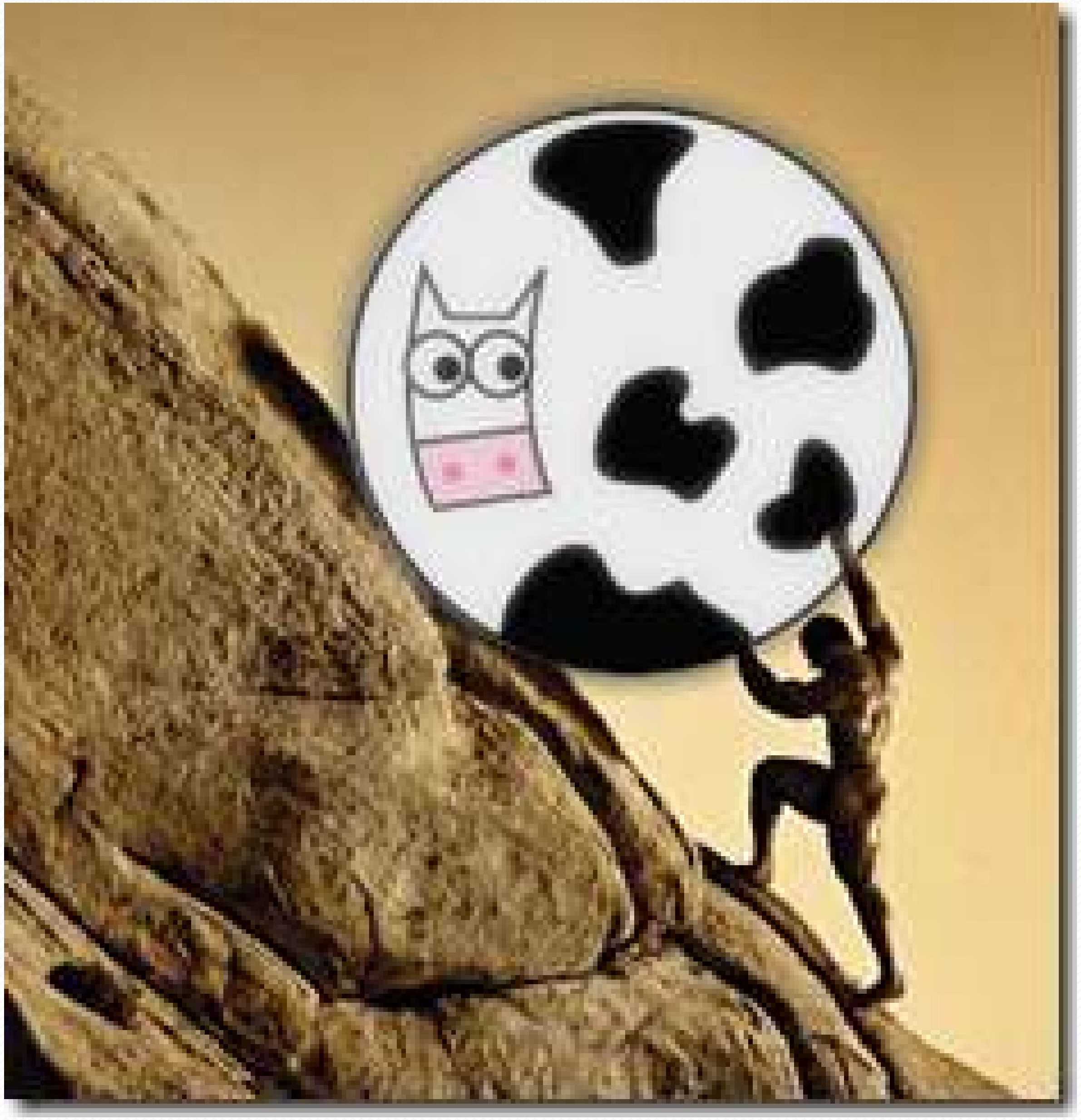
Daí, como um bom físico(a) ...



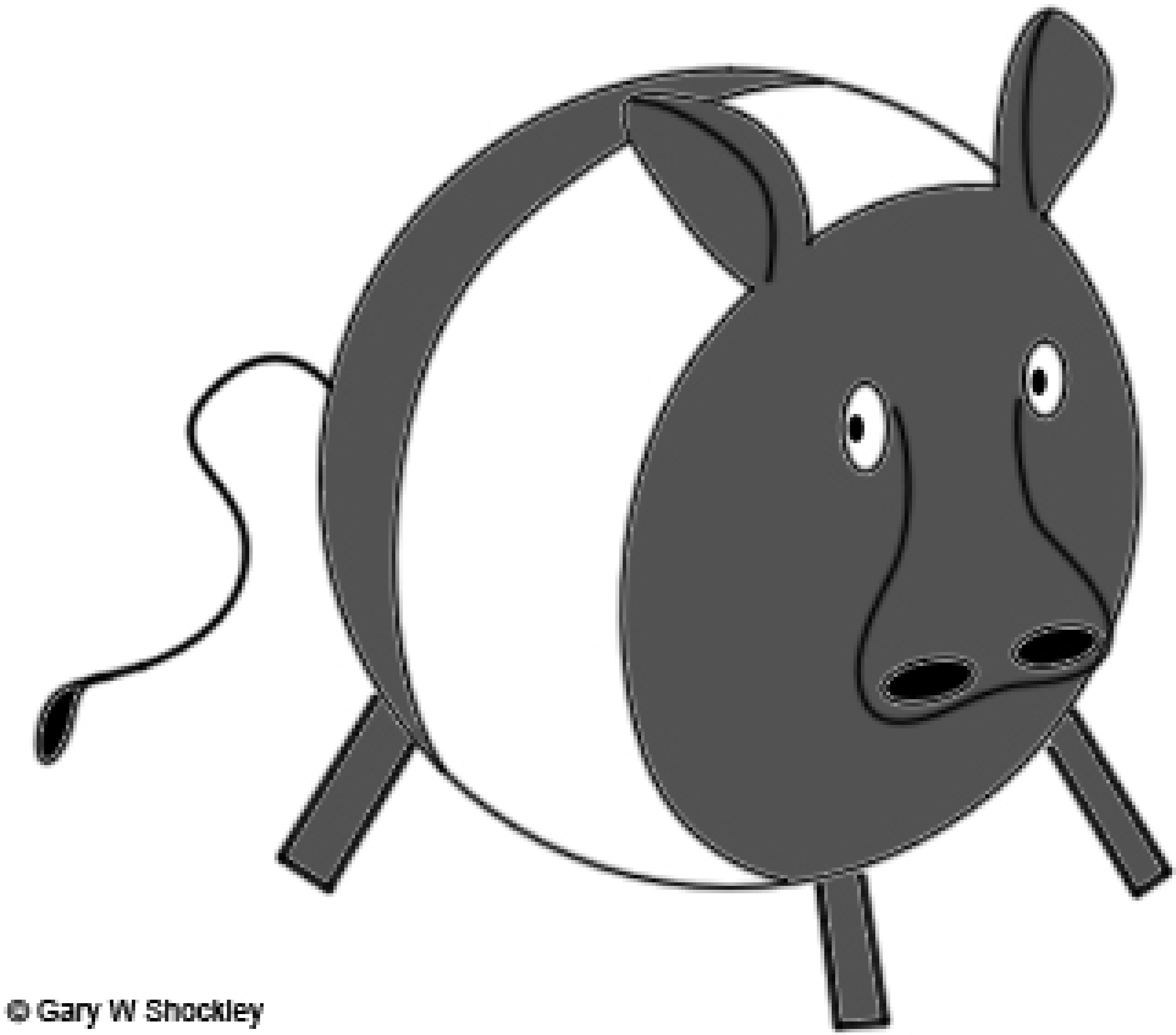
Considere uma vaca esférica de raio R ...

Supor que vc deseja estudar a interação entre vacas

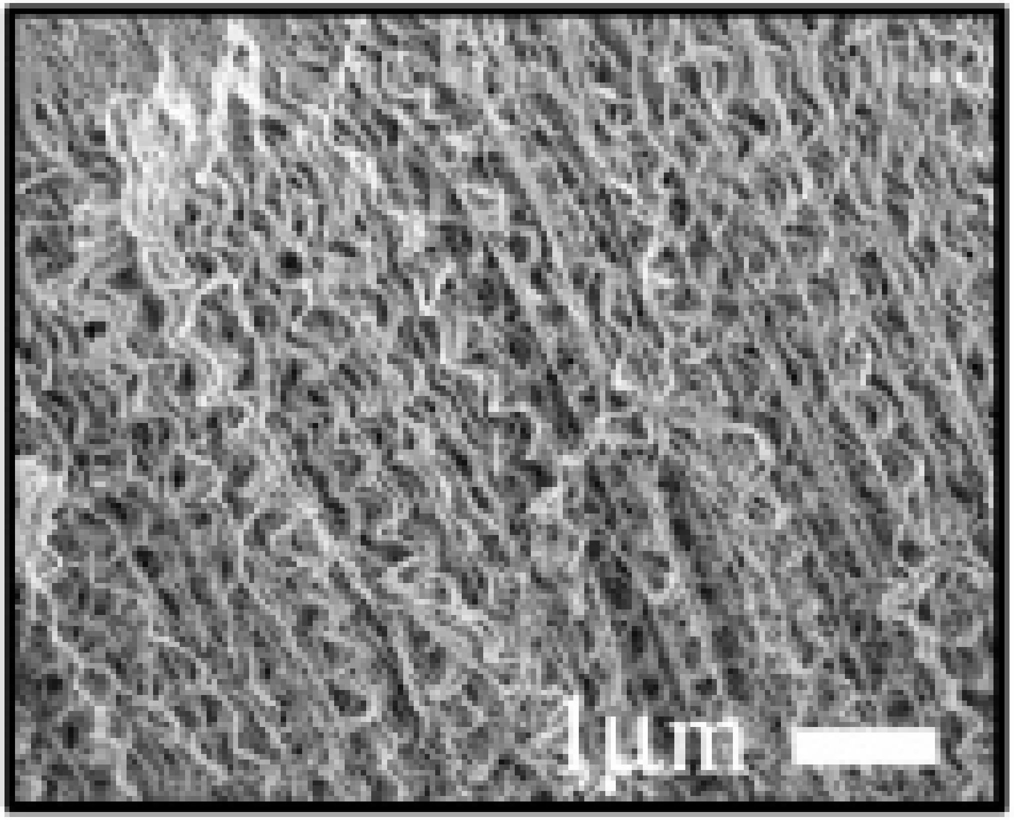
Vc pode querer estudar a descida ou Rolagem de uma vaca morro abaixo…

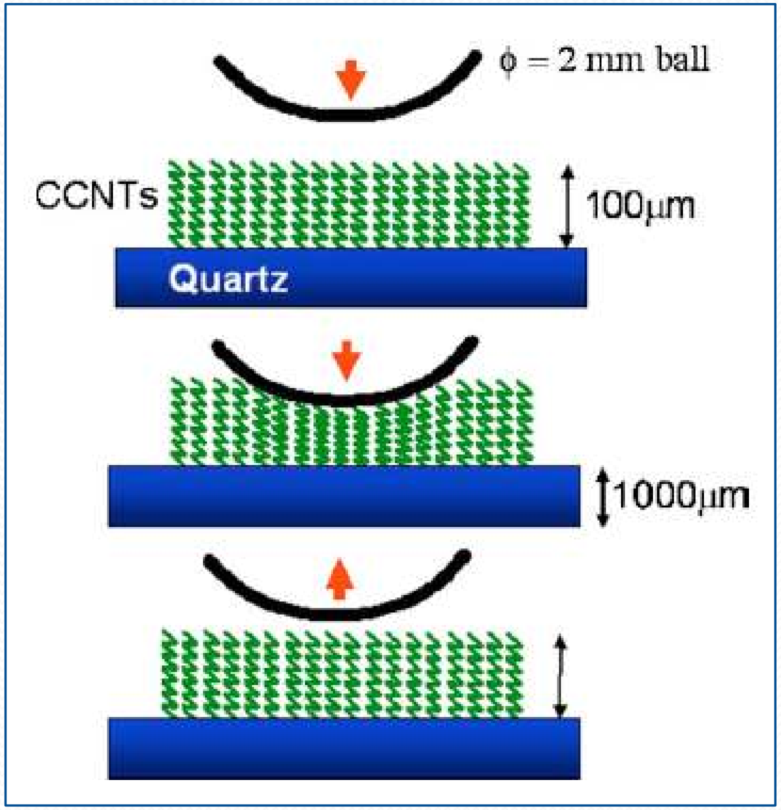


Aí, como um bom físico(a) ... vc descobre que precisa melhorar o modelo...



Modelagem de nanoestruturas com *Física Básica*
Florestas de Nanotubos Helicoidais

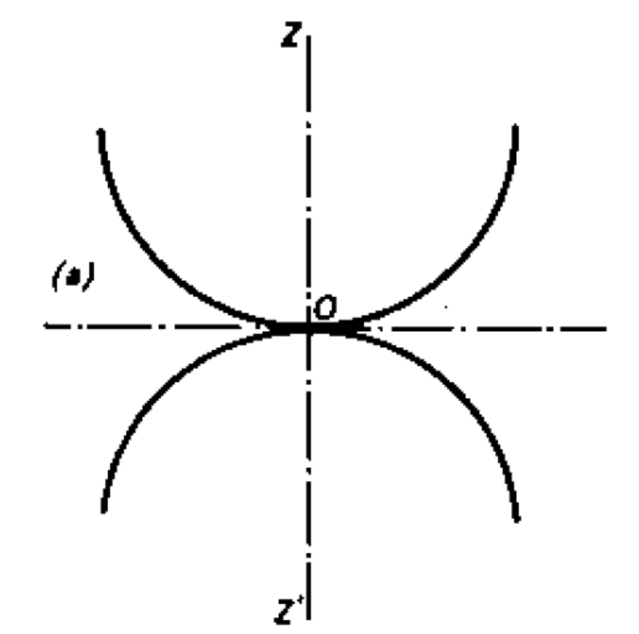


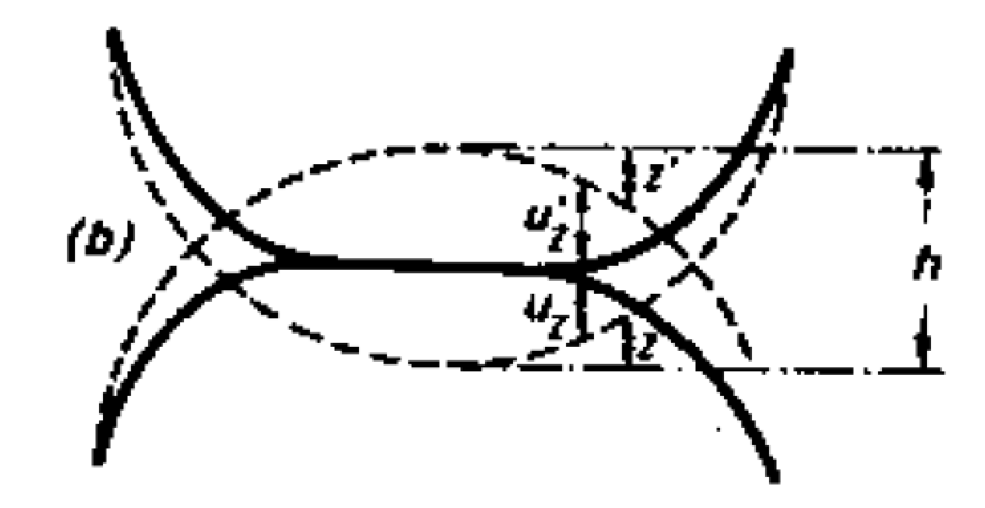


Daraio's result: $F \propto \delta^{2.2}$

Hertz theory of contact: $F \propto \delta^{\frac{3}{2}}$

Teoria de Hertz (1882):



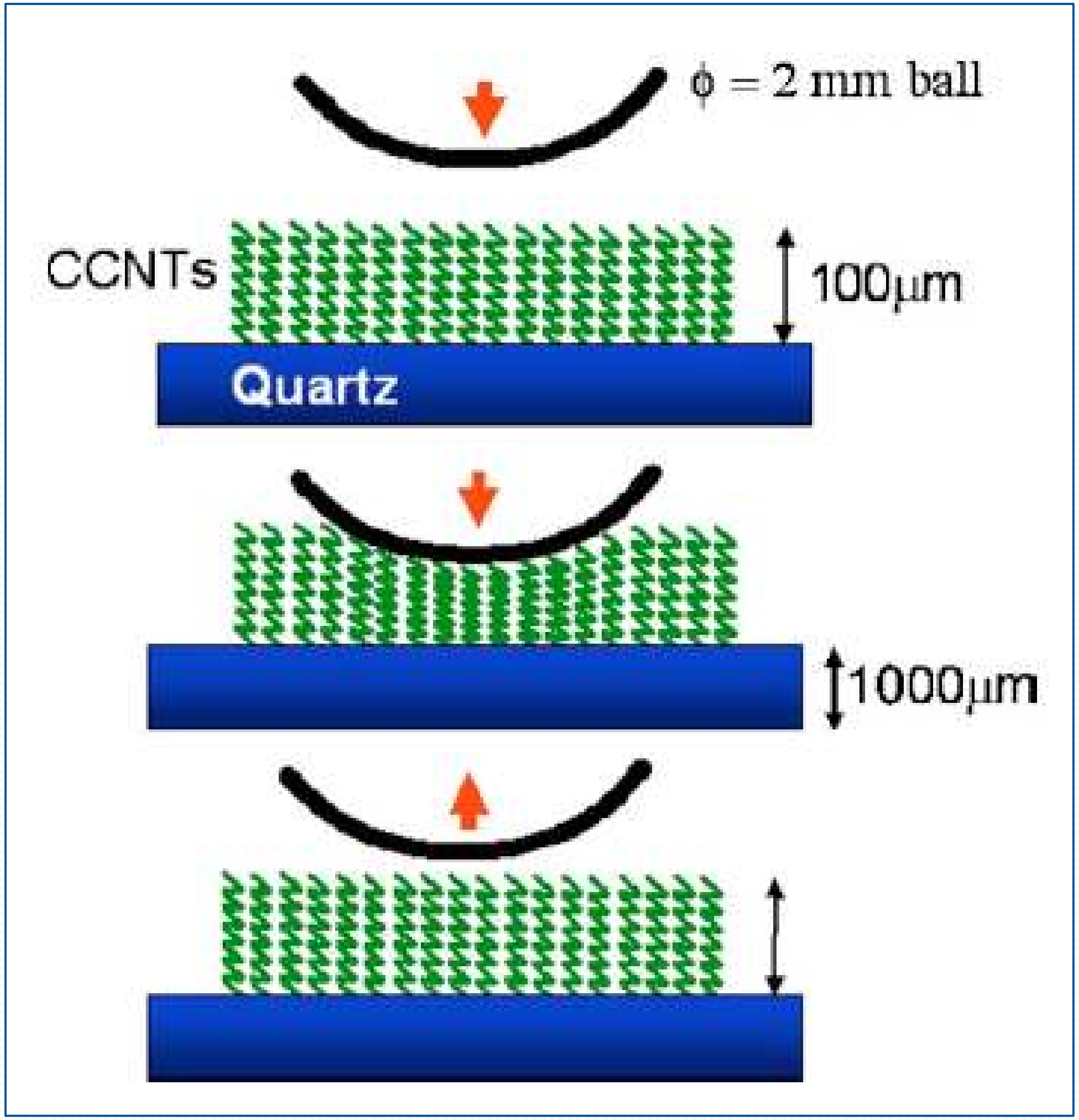


Hertz theory of contact:

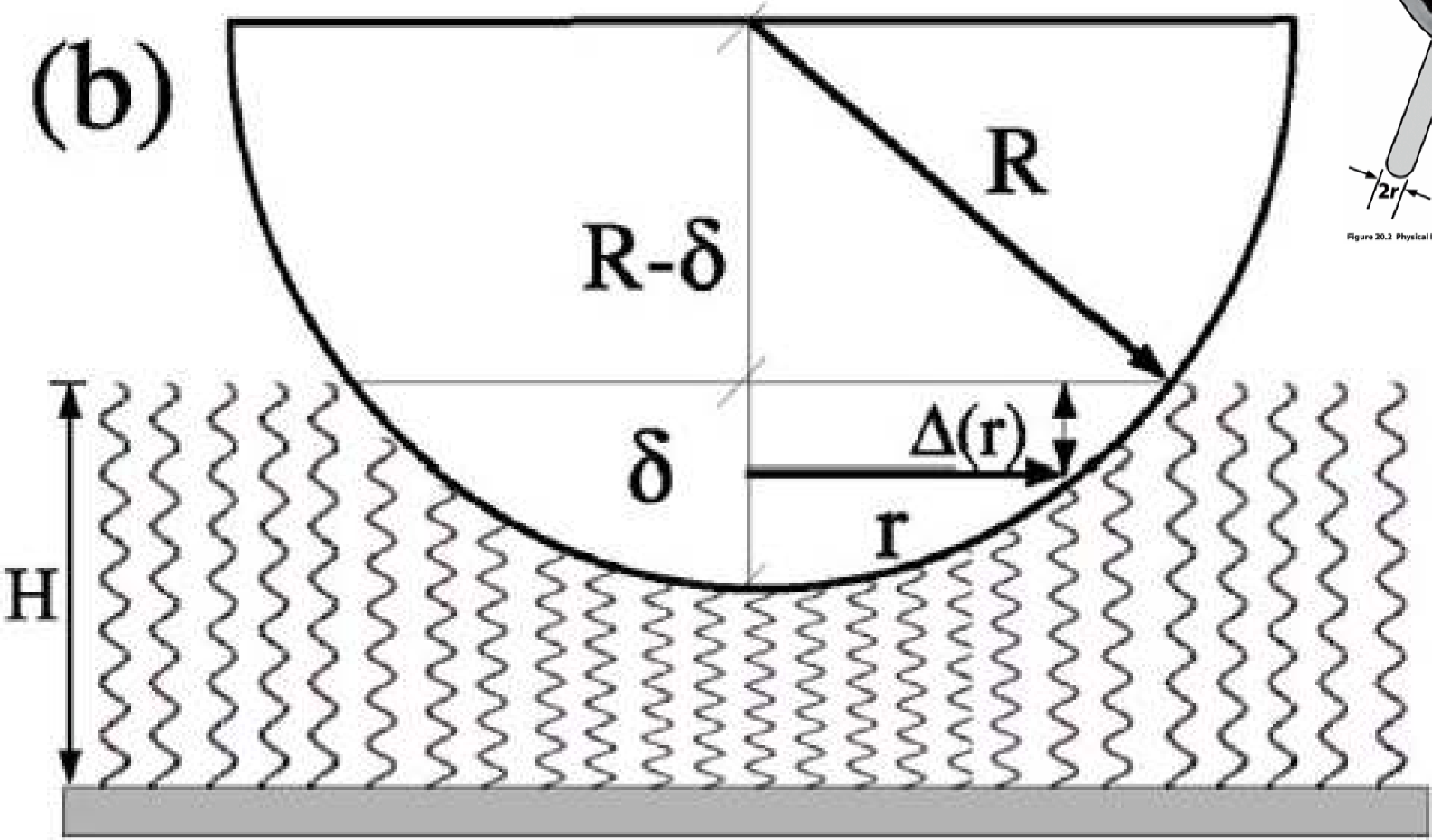
$$F \propto \delta^{\frac{3}{2}}$$

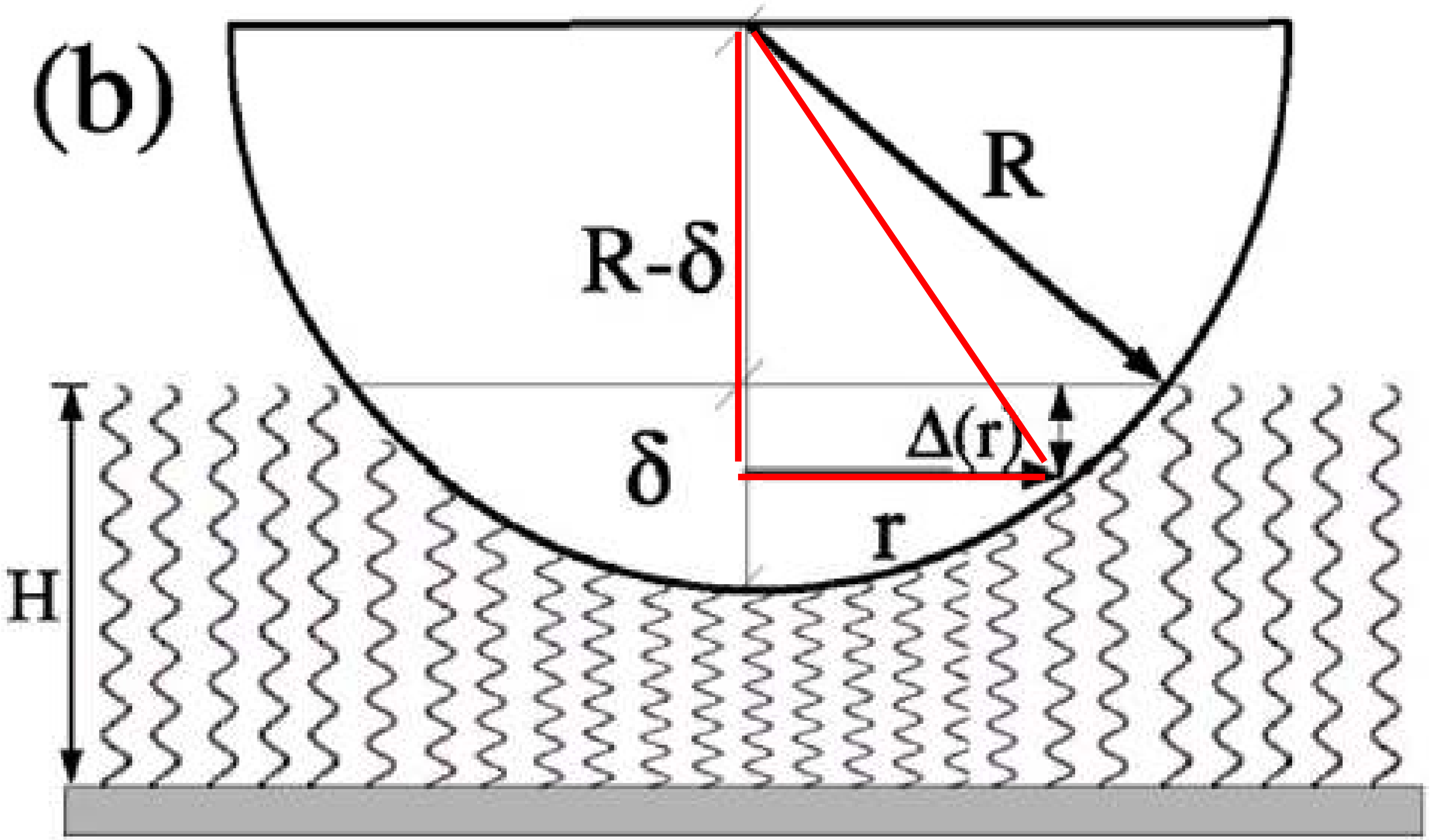
Modelagem de nanoestruturas com *Física Básica*

Florestas de Nanotubos Helicoidais



Daí, como um bom físico(a) ...

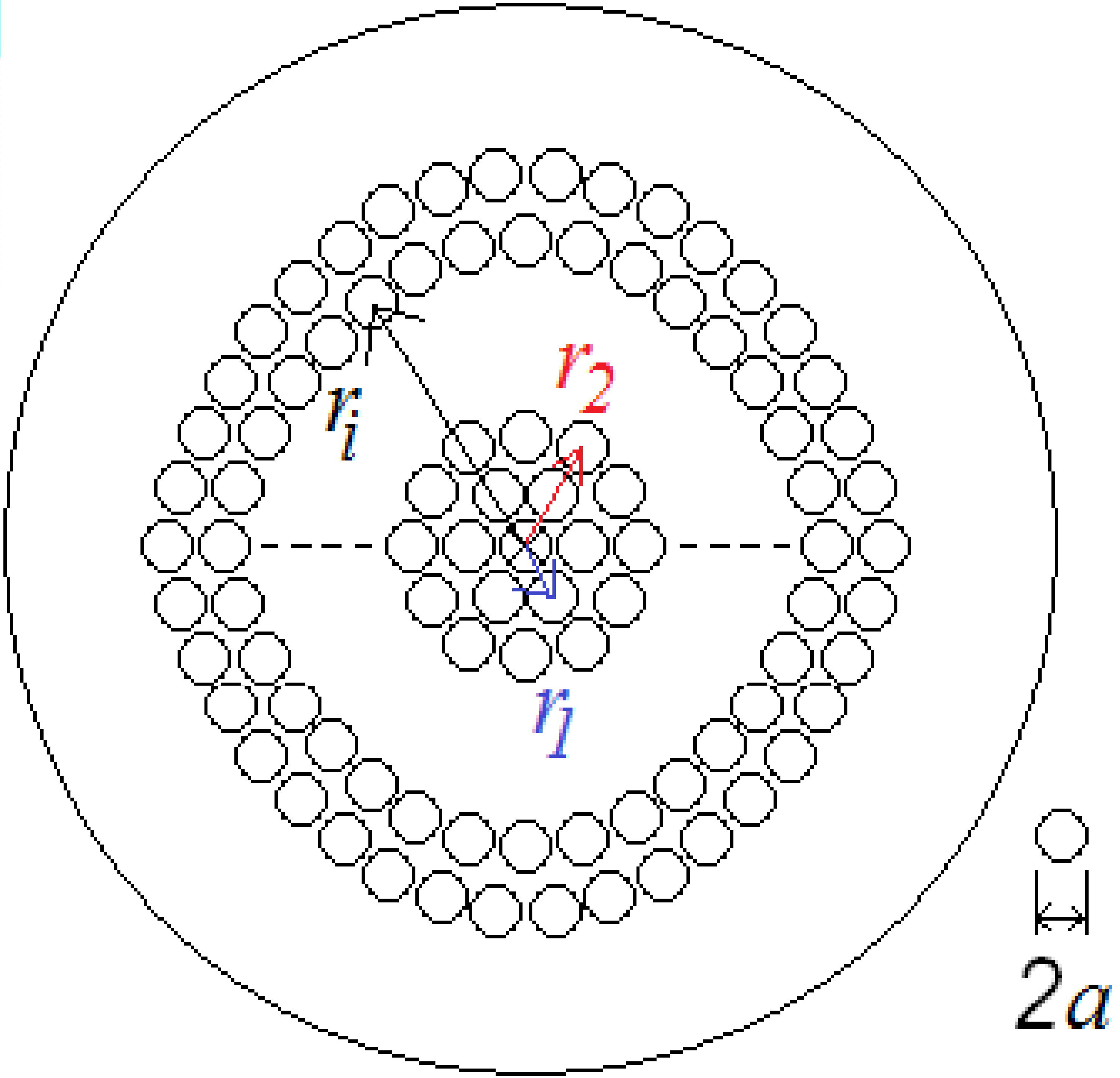




$$F = \sum k\,\Delta(r)$$

$$\Delta(r) = \sqrt{R^2 - r^2} - (R - \delta)$$

Florestas de Nanotubos Helicoidais



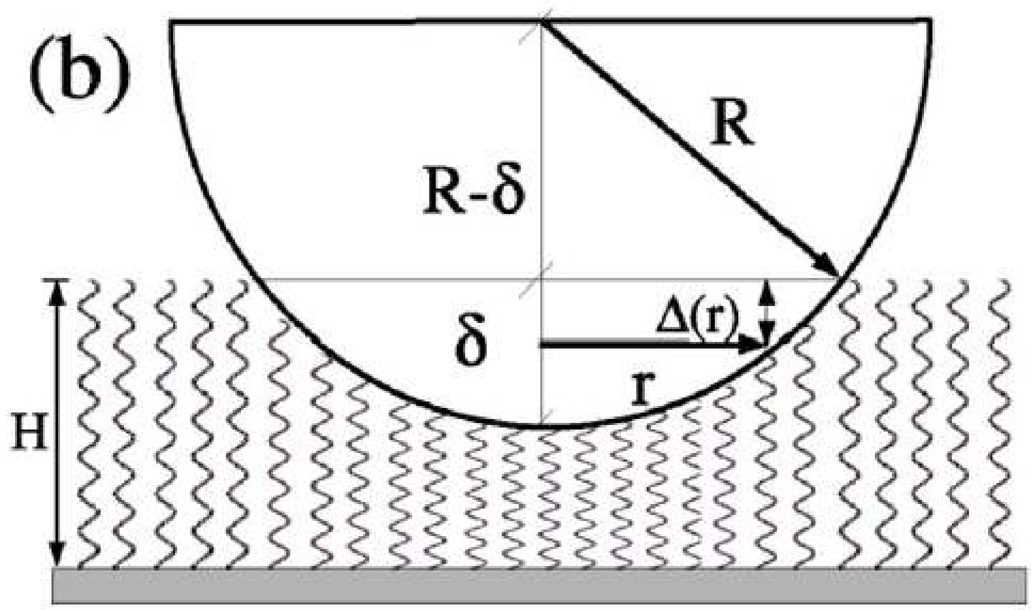
$$r_i = 2a * i$$

$$n_i \approx \frac{2\pi\, r_i}{2a}$$

$$n_i \approx 2\pi * i$$

$$n_0 = 1$$

Florestas de Nanotubos Helicoidais



$$F = k \sum_{i=0}^{M} n_i \Delta(r_i)$$

$$M = \frac{\sqrt{2R\delta - \delta^2}}{2a}$$

$$\Delta(r_M) = 0$$

$$\Delta(r) = \sqrt{R^2 - r^2} - (R - \delta)$$

$$r_M = 2a * M$$

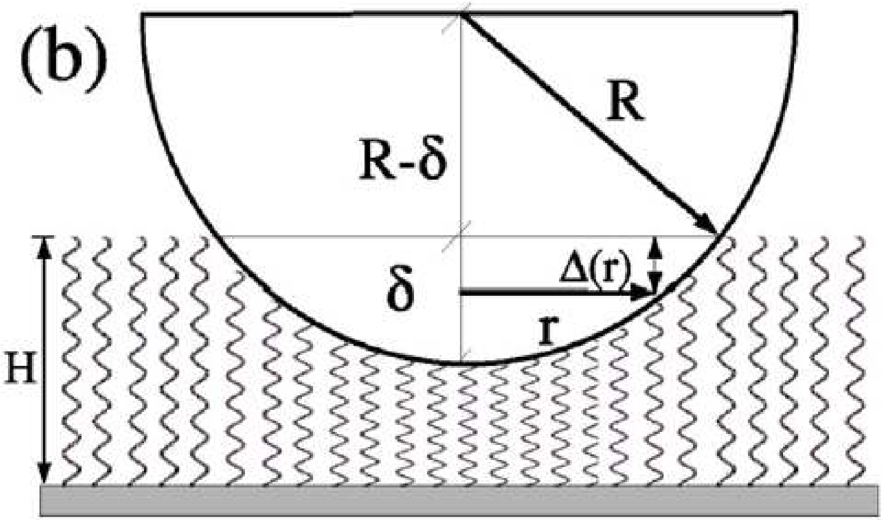
$$F = k \sum_{i=0}^{M} n_i \Delta(r_i) \qquad M = \frac{\sqrt{2R\delta - \delta^2}}{2a}$$

$$r_i = 2a * i$$

$$\Delta(r) = \sqrt{R^2 - r^2} - (R - \delta) \qquad n_i \approx 2\pi * i$$

$$\Rightarrow \quad F = F(\delta)$$

Daraio's result: $F \propto \delta^{2.2}$



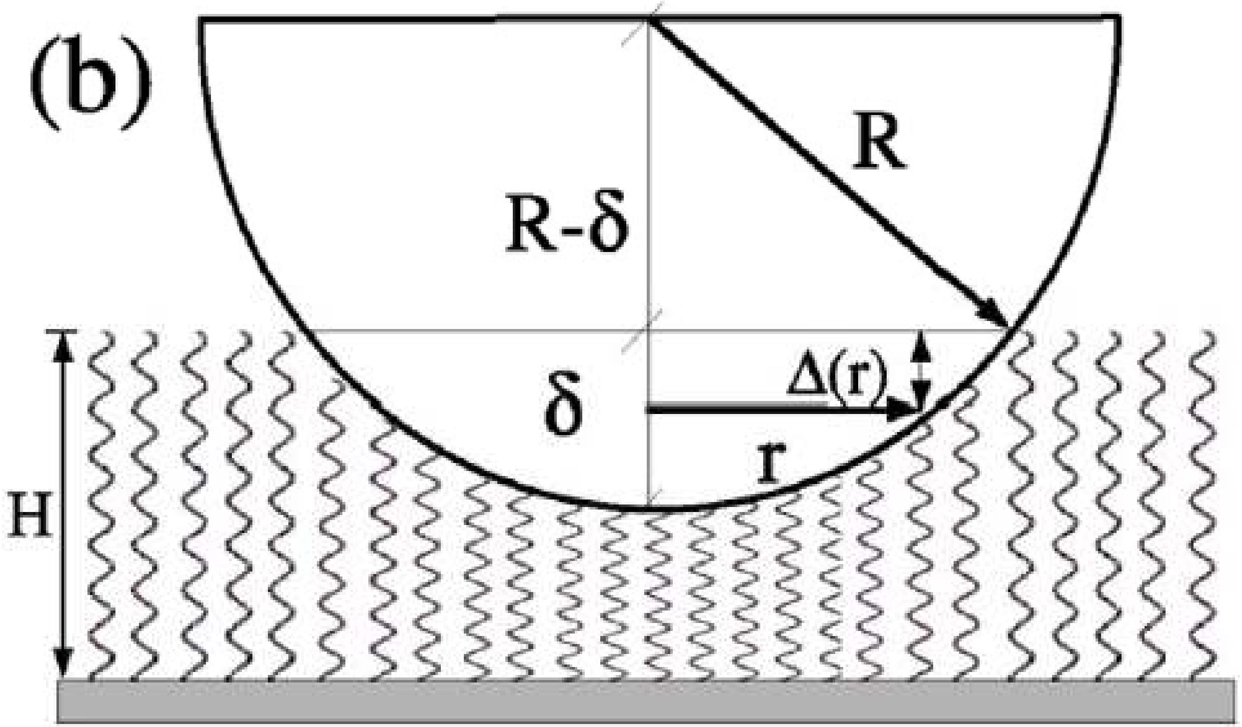
$$F = k \sum_{i=0}^{M} n_i \Delta(r_i) \qquad M = \frac{\sqrt{2R\delta - \delta^2}}{2a}$$

$$r_i = 2a * i$$

$$\Delta(r) = \sqrt{R^2 - r^2} - (R - \delta) \qquad n_i \approx 2\pi * i$$

$$F \cong k\delta + 2\pi k \sum_{i=1}^{M} i(\delta R - 2i^2 a^2)$$

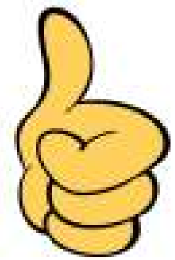
onde: $\delta / R \ll 1$



$$R = 1000\ \mu\text{m}$$

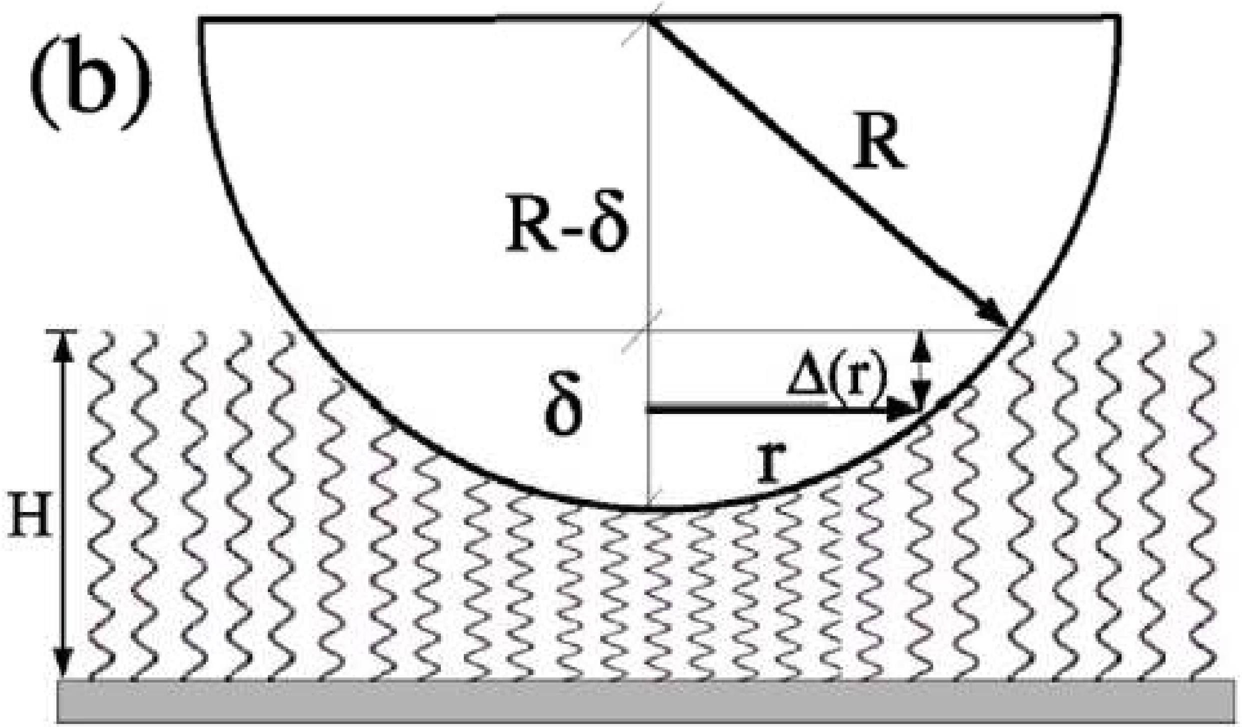
$$\delta = 3\ \mu\text{m}$$

$$2a = 0.45\ \mu\text{m}$$



$$F \cong k\delta + 2\pi k \sum_{i=1}^{M} i(\delta R - 2i^2 a^2)$$

onde: $\delta / R \ll 1$



Resultado:

$$F = k\frac{\pi R\delta^2}{4a^2}$$

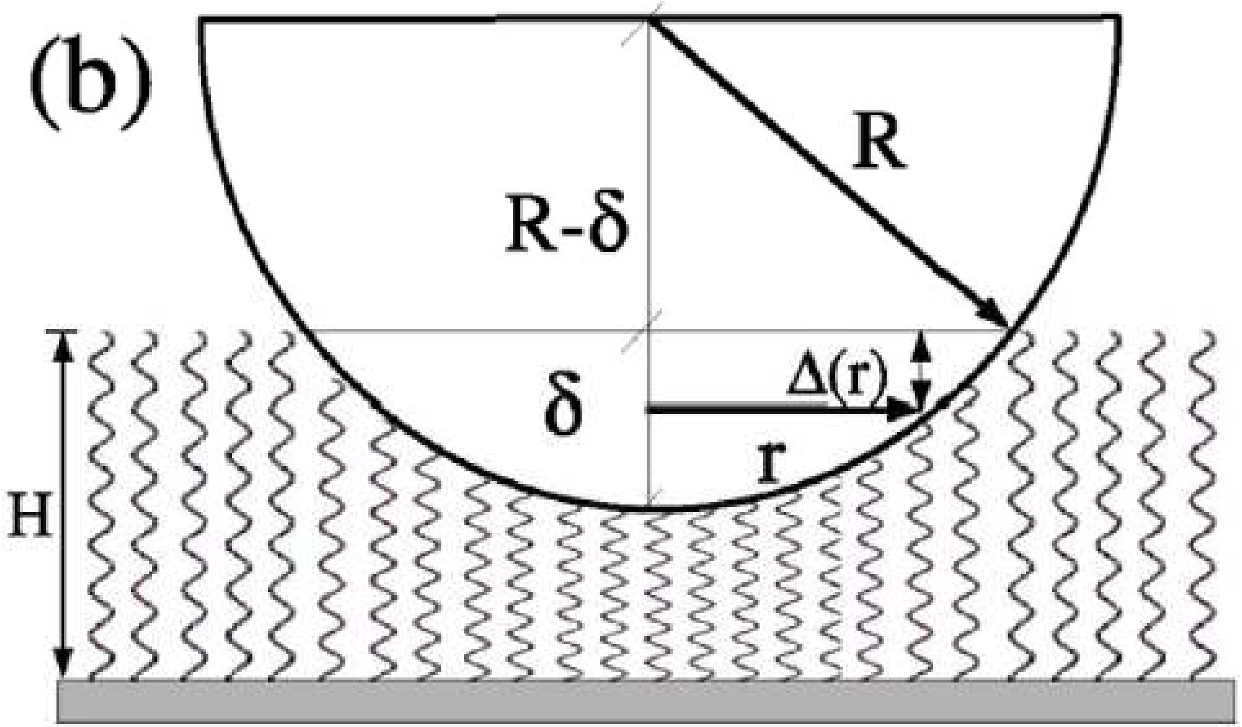
Meu modelo: $F \propto \delta^2$

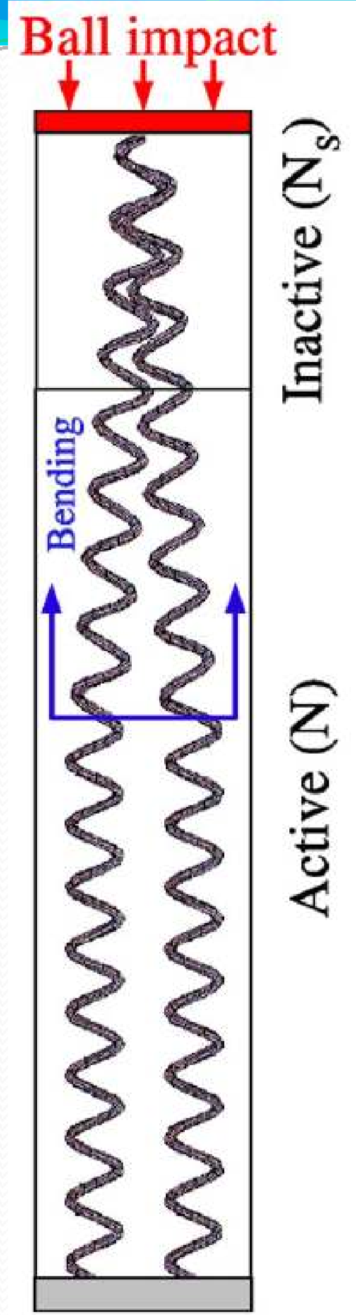
Daraio's result: $F \propto \delta^{2.2}$

Hertz theory of contact: $F \propto \delta^{\frac{3}{2}}$

Modelagem de nanoestruturas com *Física Básica*

Florestas de Nanotubos Helicoidais





O que faltava?

Incluir

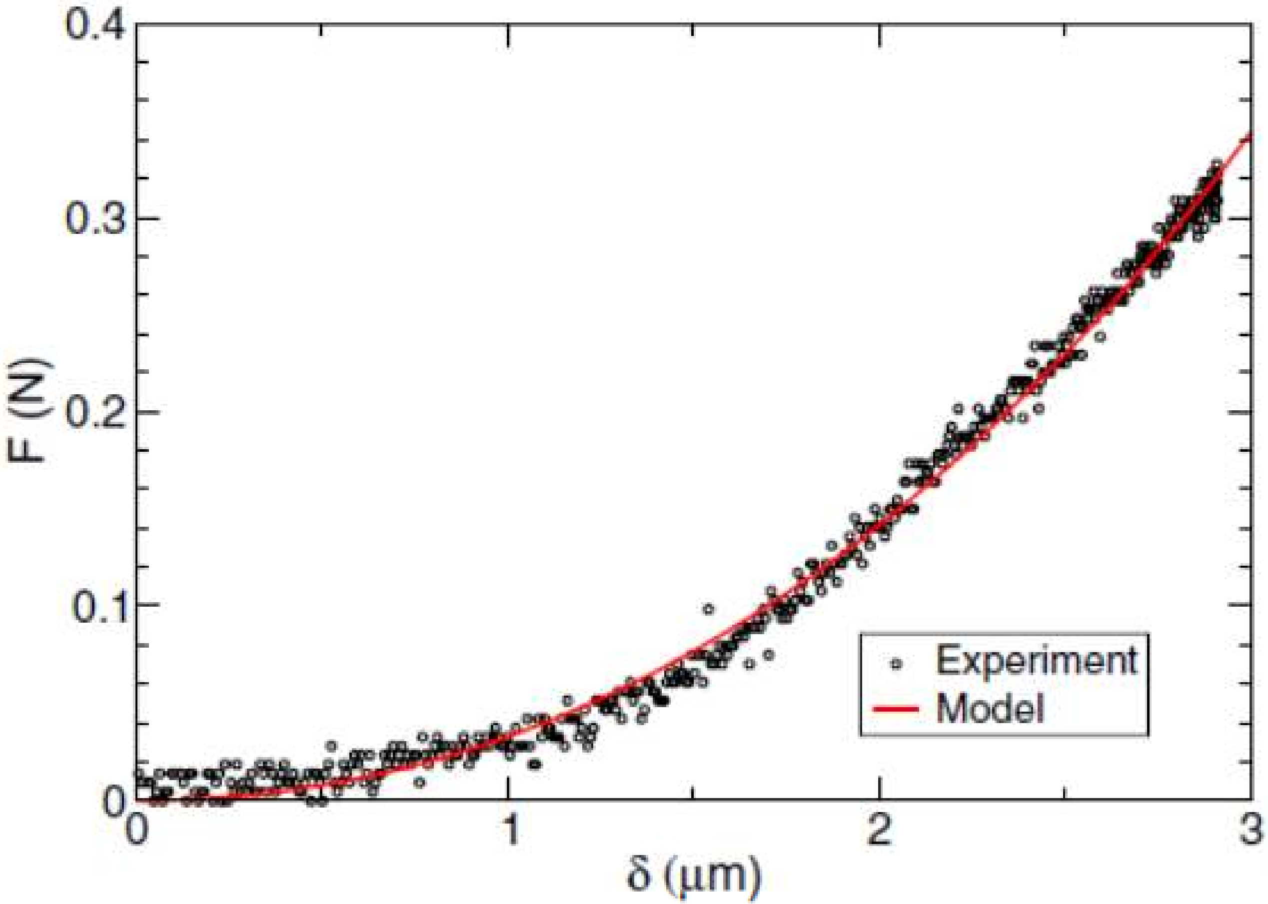
Não-linearidade!

Como?

$$N(\Delta) = N_T - \eta\Delta$$

Modelagem de nanoestruturas com *Física Básica*

Florestas de Nanotubos Helicoidais

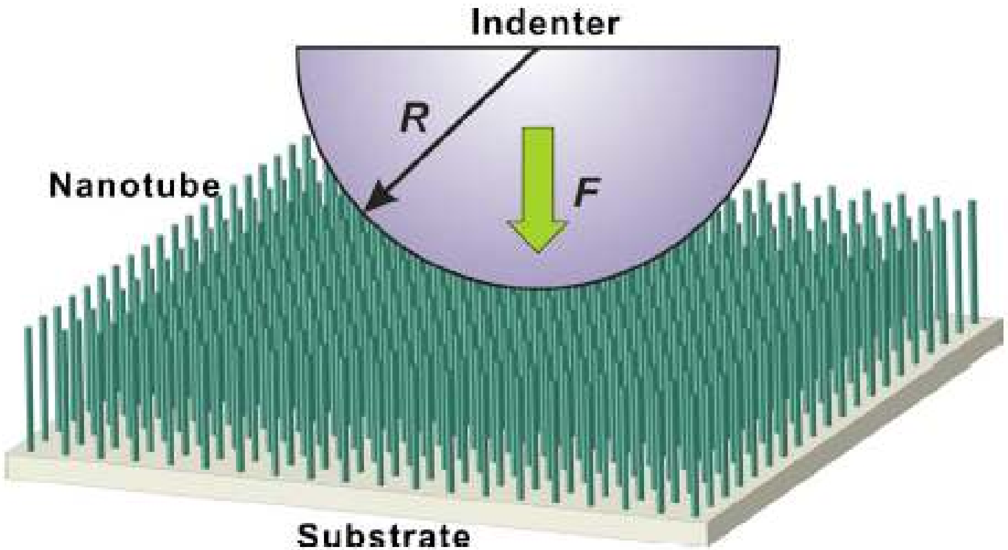


V. R. Coluci, **A. F. Fonseca**, D. S. Galvao and C. Daraio, *PRL* **100**, 086807 (2008).

$$F = k\frac{\pi R\delta^2}{4a^2[1-(\eta/N_T)\delta]}$$

Modelagem de nanoestruturas com *Física Básica*

Florestas de Nanotubos Helicoidais



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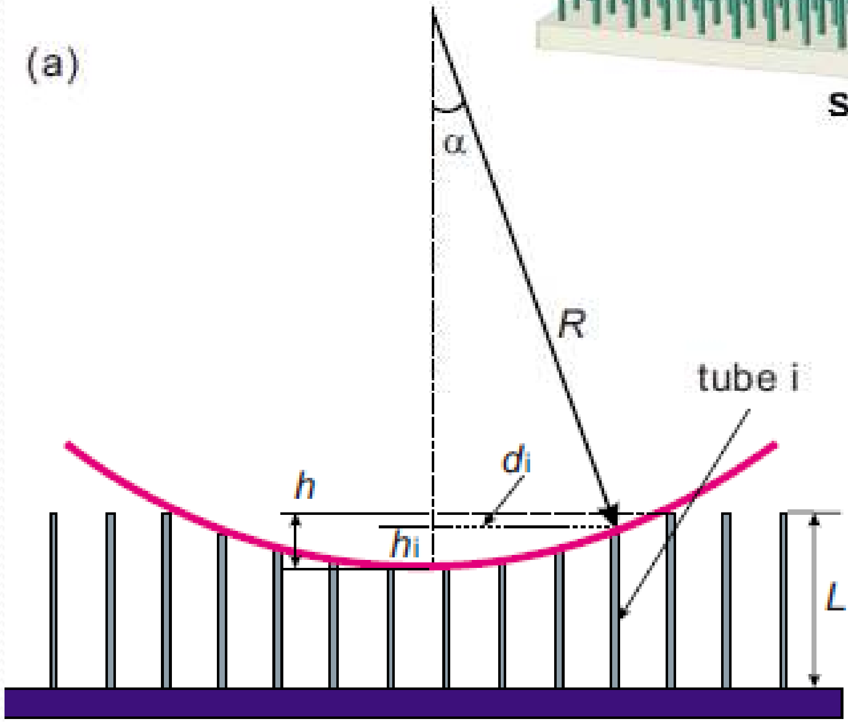
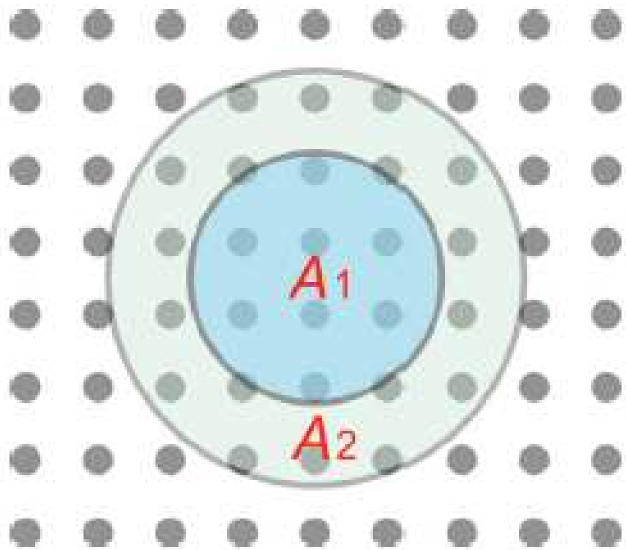




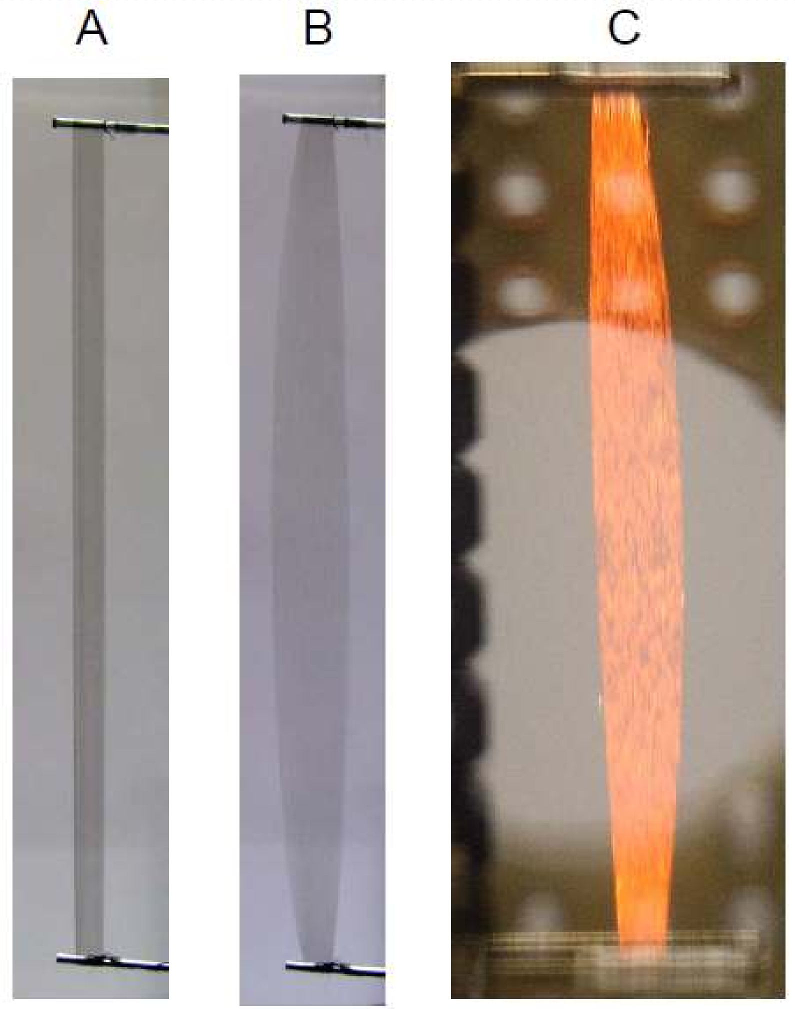
Journal of Engineering Materials and Technology JANUARY 2011, Vol. 133 / **011014-1**

Science
AAAS

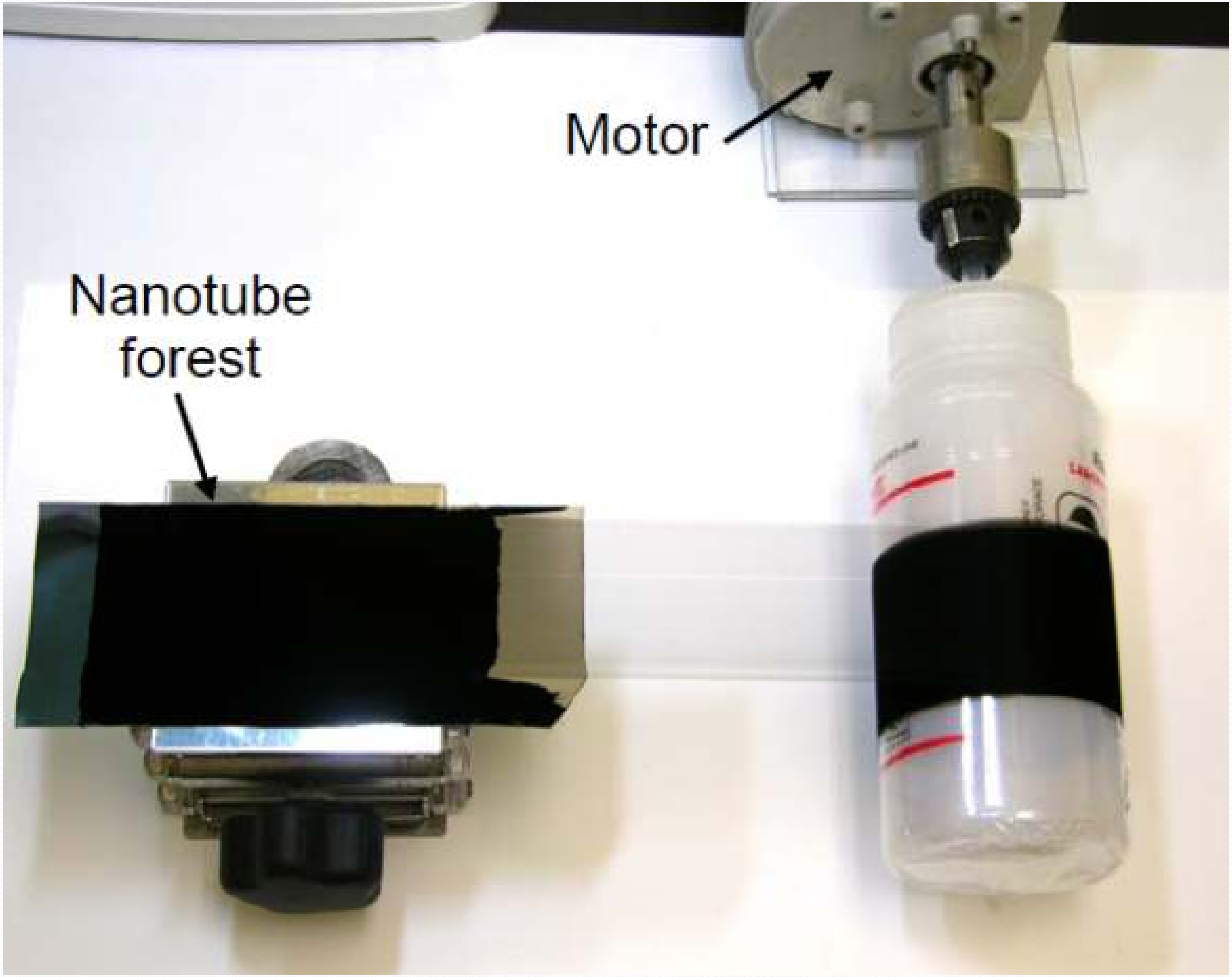
Giant-Stroke, Superelastic Carbon Nanotube Aerogel Muscles

Ali E. Aliev, *et al.*

Science **323**, 1575 (2009);
DOI: 10.1126/science.1168312



Modelagem de nanoestruturas com *Física Básica*
Formação de Fios e de Nanotubos de Carbono

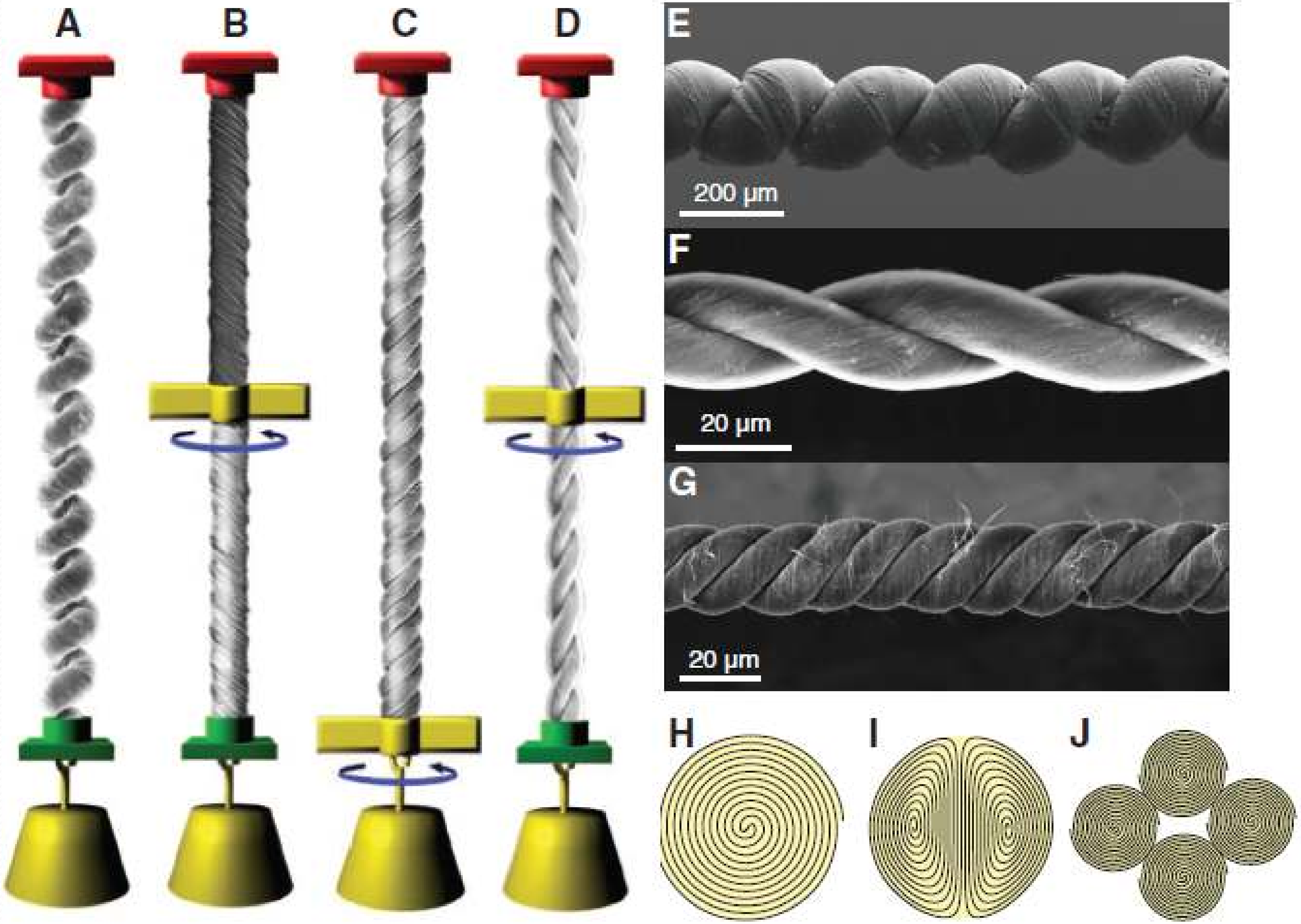


Science AAAS

Electrically, Chemically, and Photonically Powered Torsional and Tensile Actuation of Hybrid Carbon Nanotube Yarn Muscles

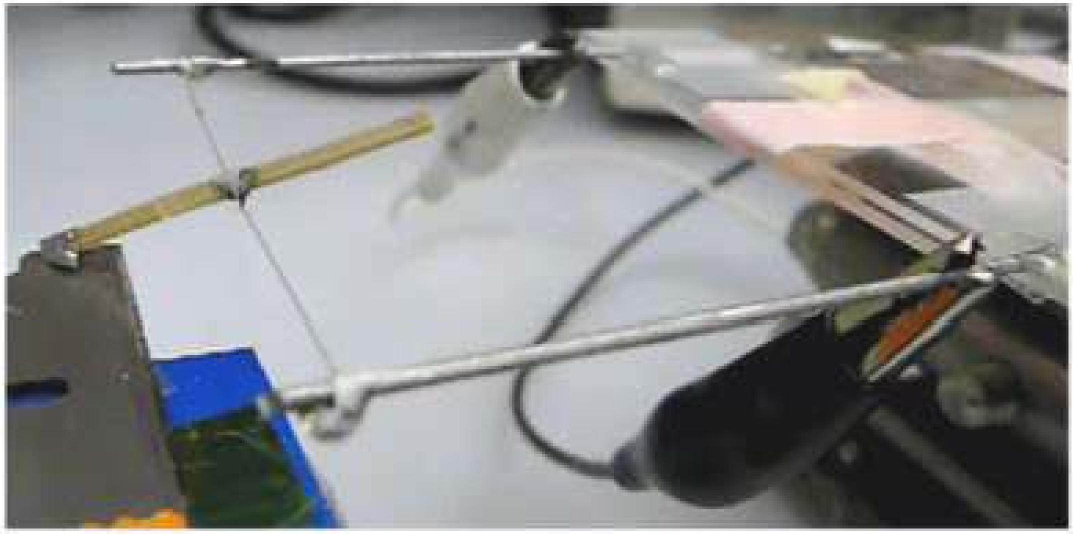
Márcio D. Lima *et al.*

Science **338**, 928 (2012);
DOI: 10.1126/science.1226762



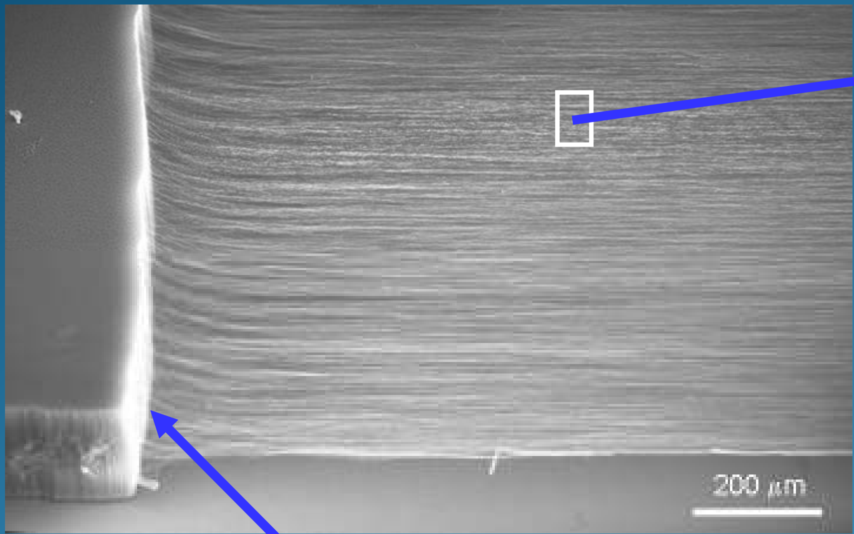
Miniature Greco-Roman style catapult

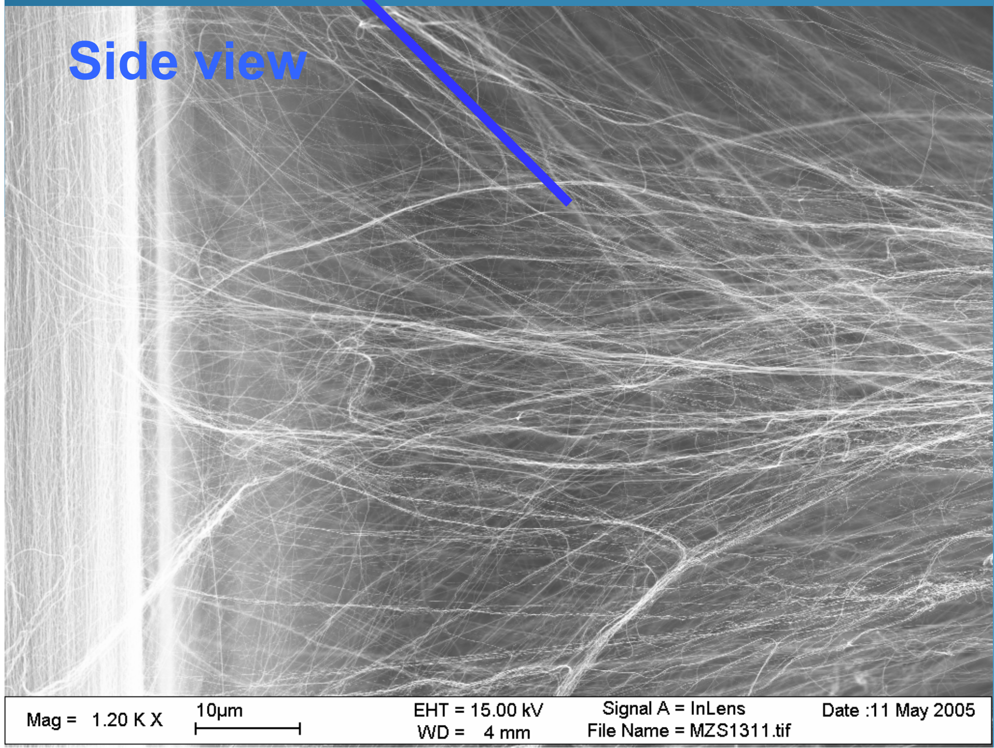
By electrical heating, fully infiltrated heterochiral yarn untwist and the arm of a miniature Greco-Roman style catapult rotates 300° and hurl a projectile.

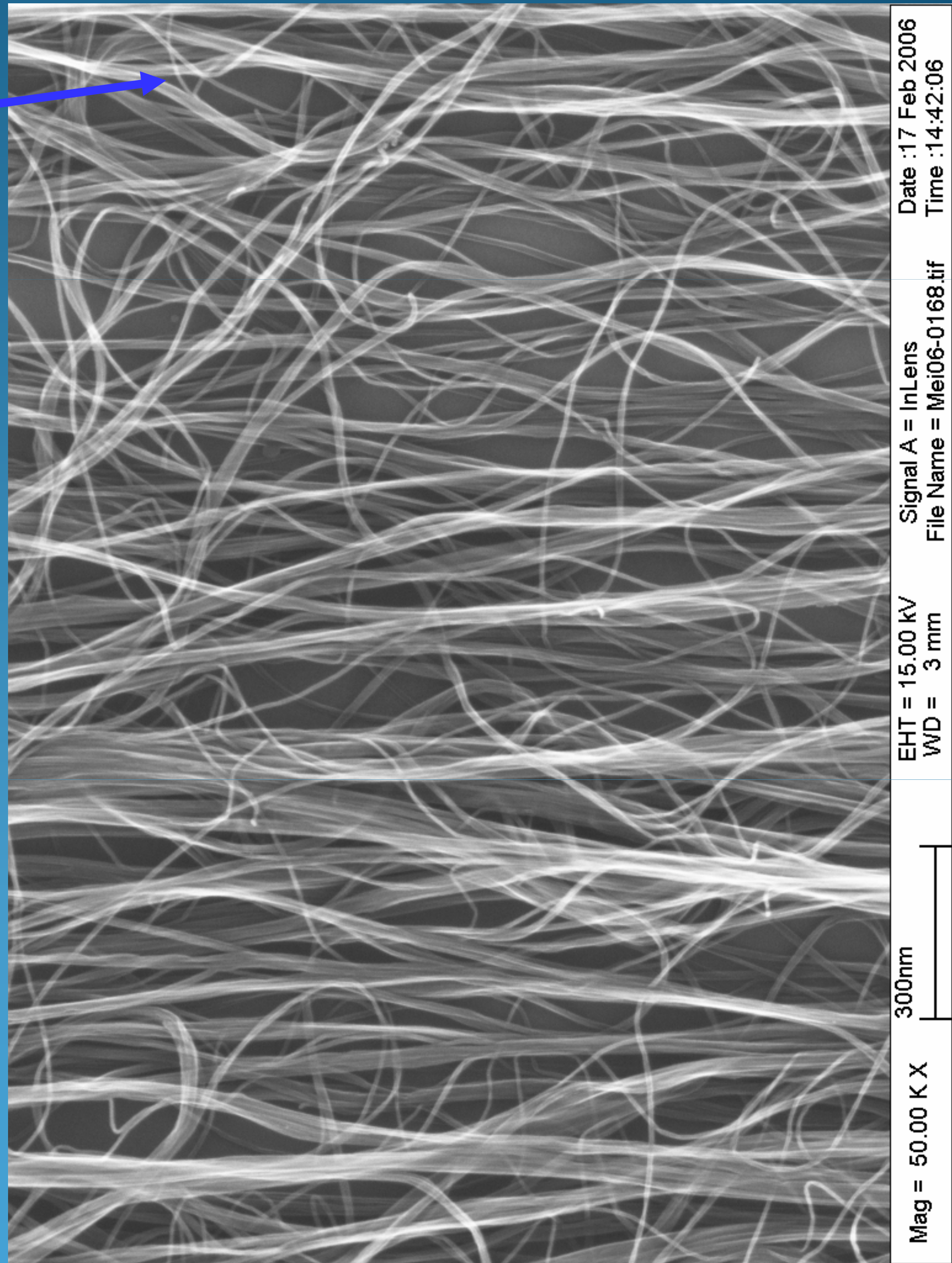


Forest Structure and CNT Sheet Structure are Correlated!

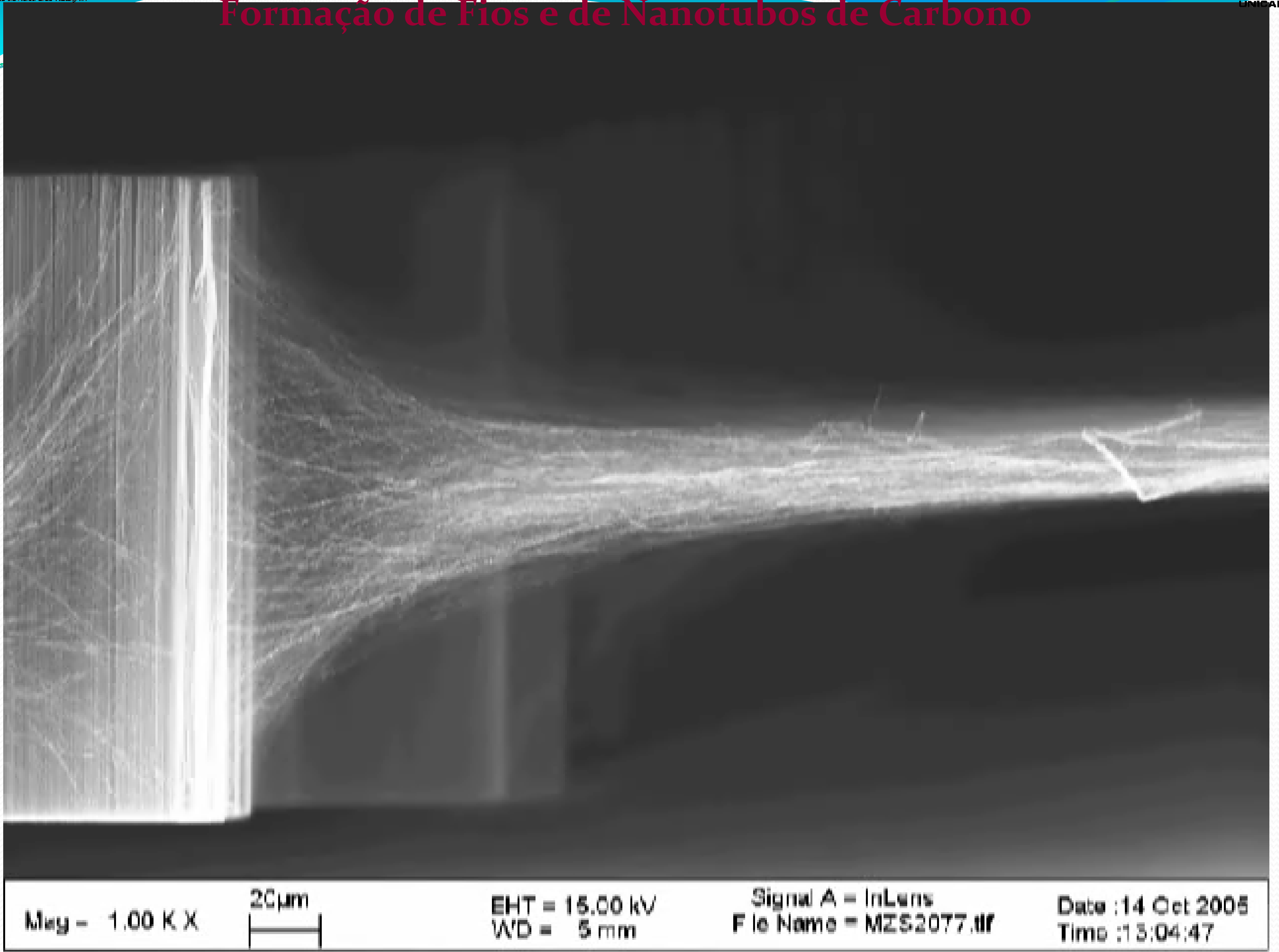
Fibril branching continues throughout the sheet, thereby making a laterally-extended, inherently interconnected fibril network.



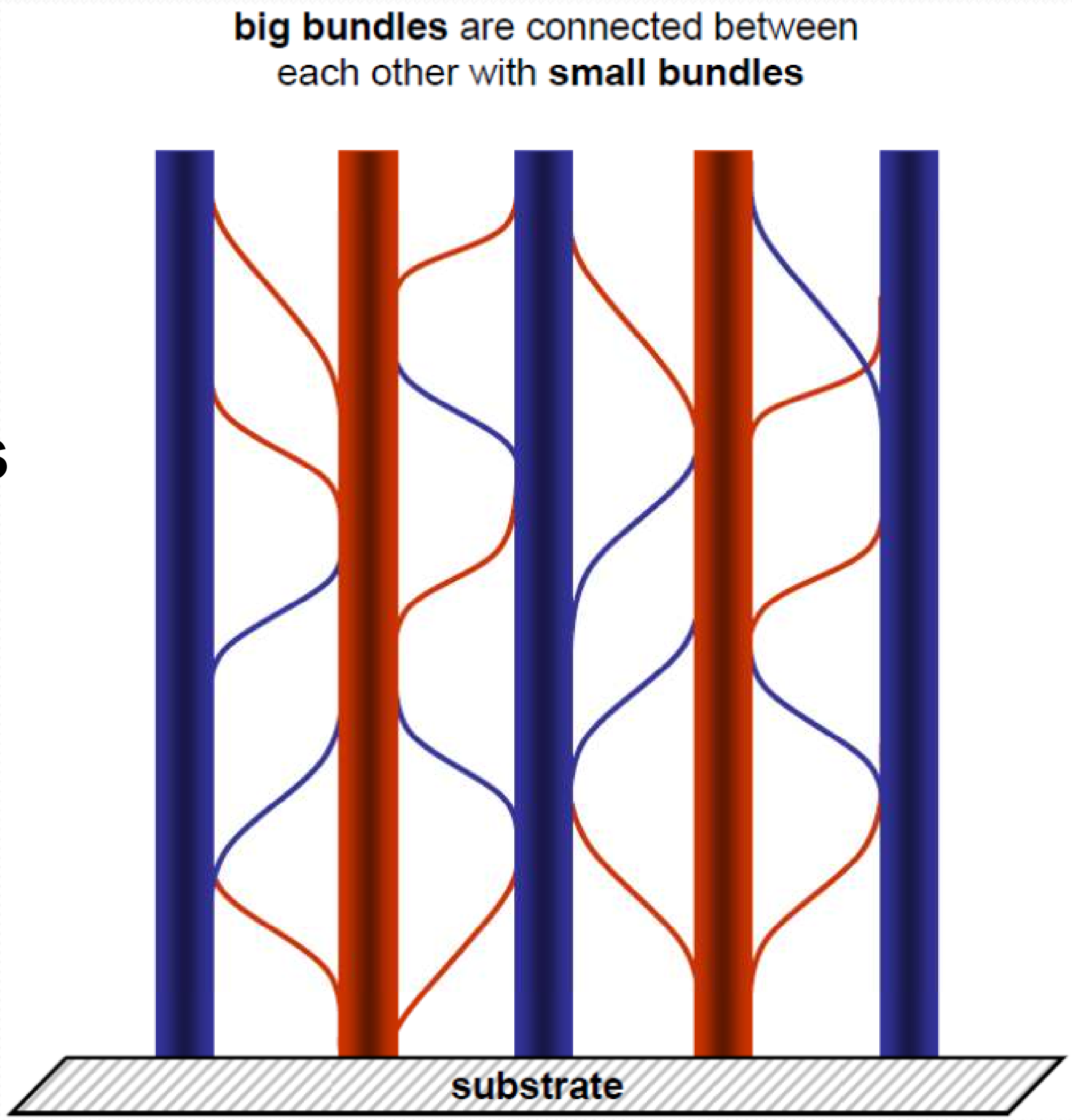




Formação de Fios e de Nanotubos de Carbono



Mecanismo de formação das sheets

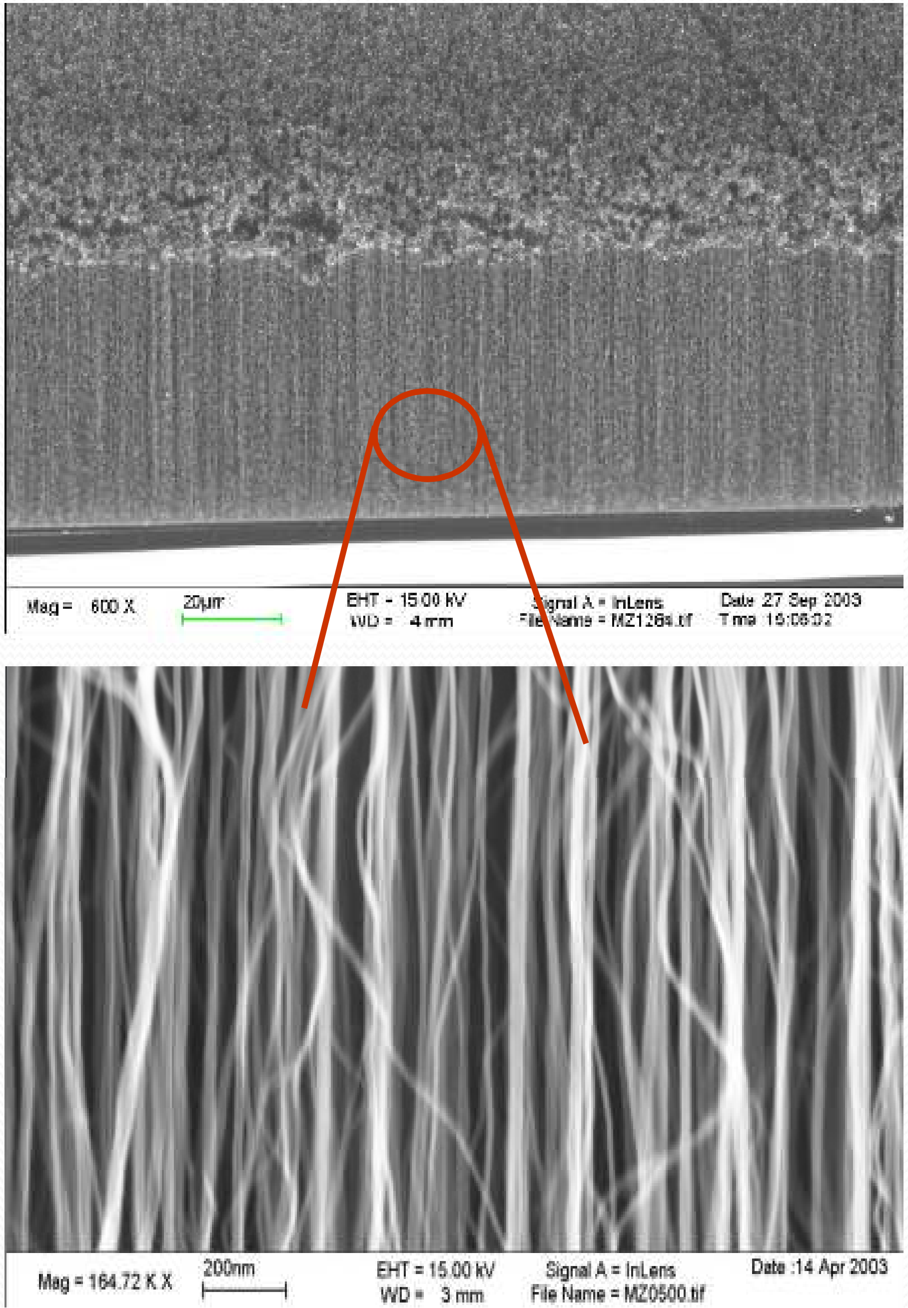


A. A. Kuznetsov, **Alexandre F. Fonseca**, R. H. Baughman *and* A. A. Zakhidov

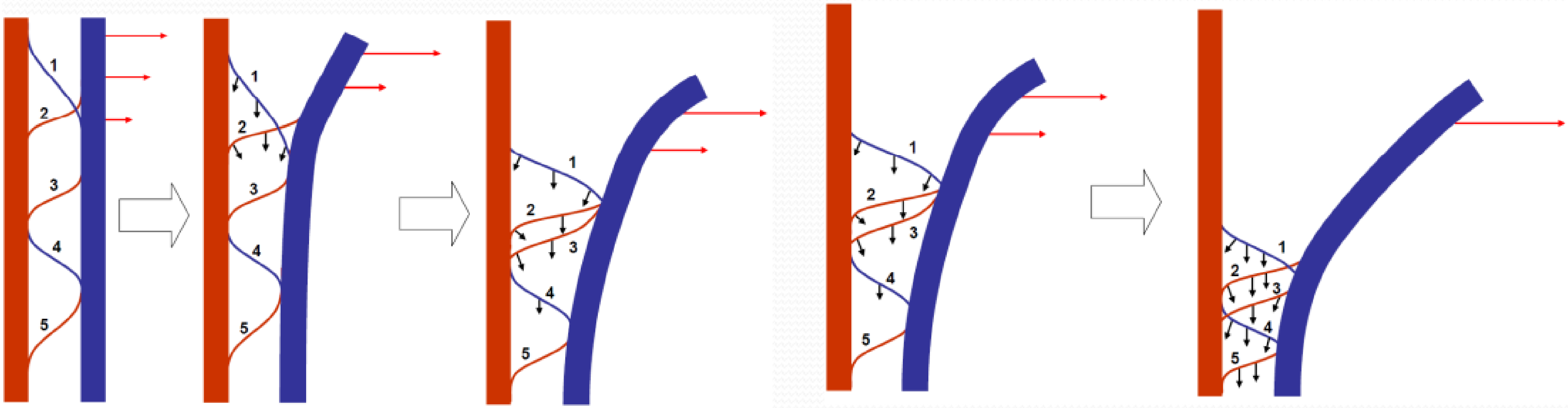
Structural Model for Dry-Drawing of Sheets and Yarns from Carbon Nanotube Forests *ACS Nano*, 2011, 5 (2), pp 985-993

ACS NANO

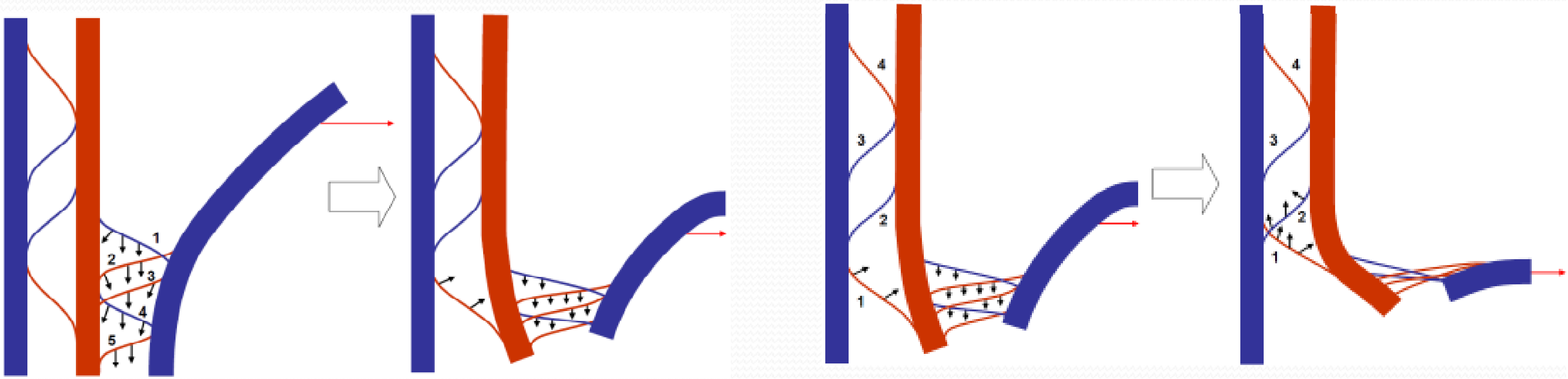
SEM of oriented forests



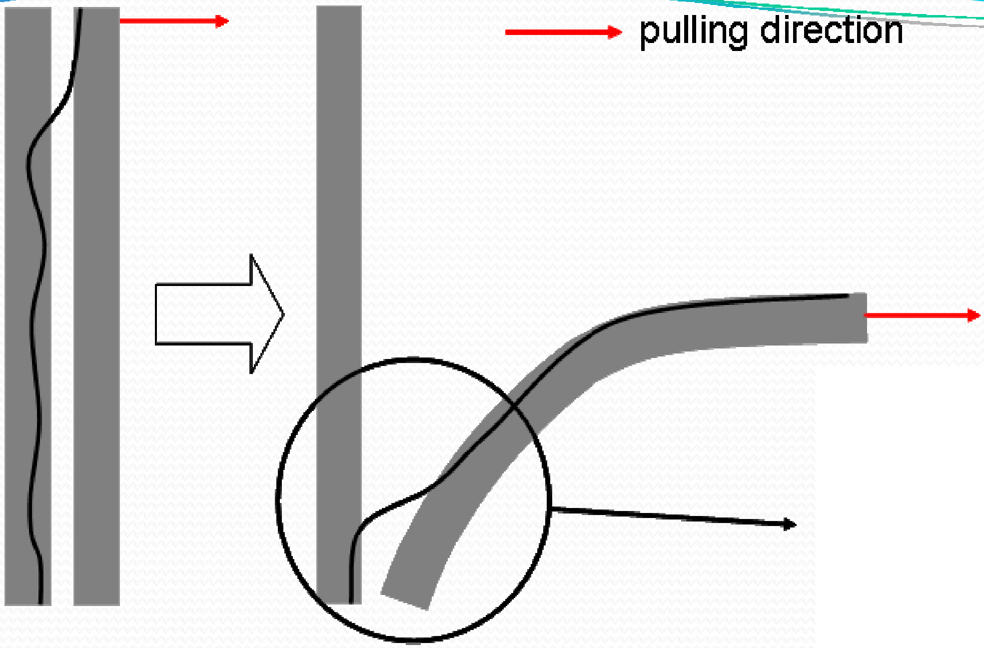
Esquema do processo de "pulling out"



Mas que forças estariam atuando? Como encaixar isso no modelo?



Forças entre conexões e big bundles



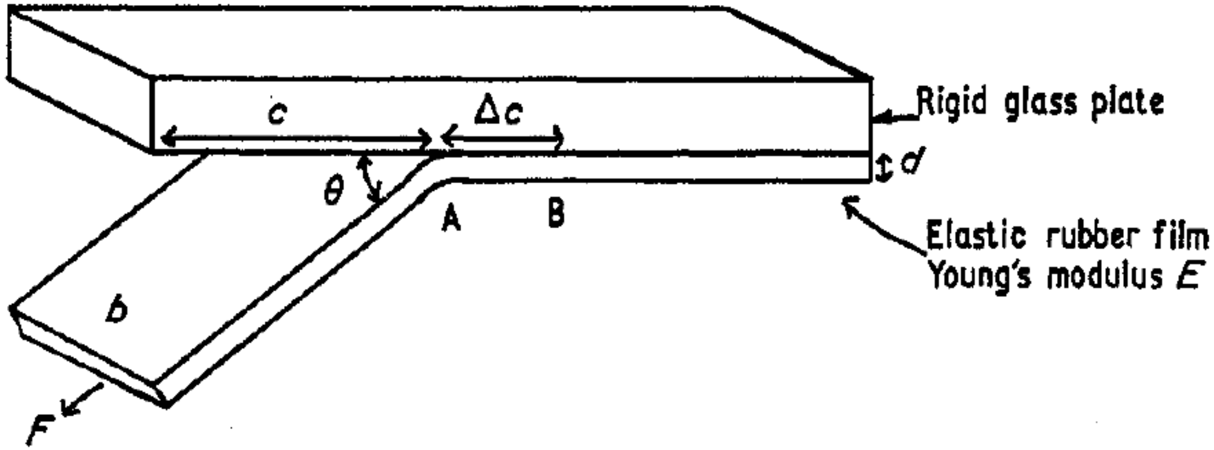
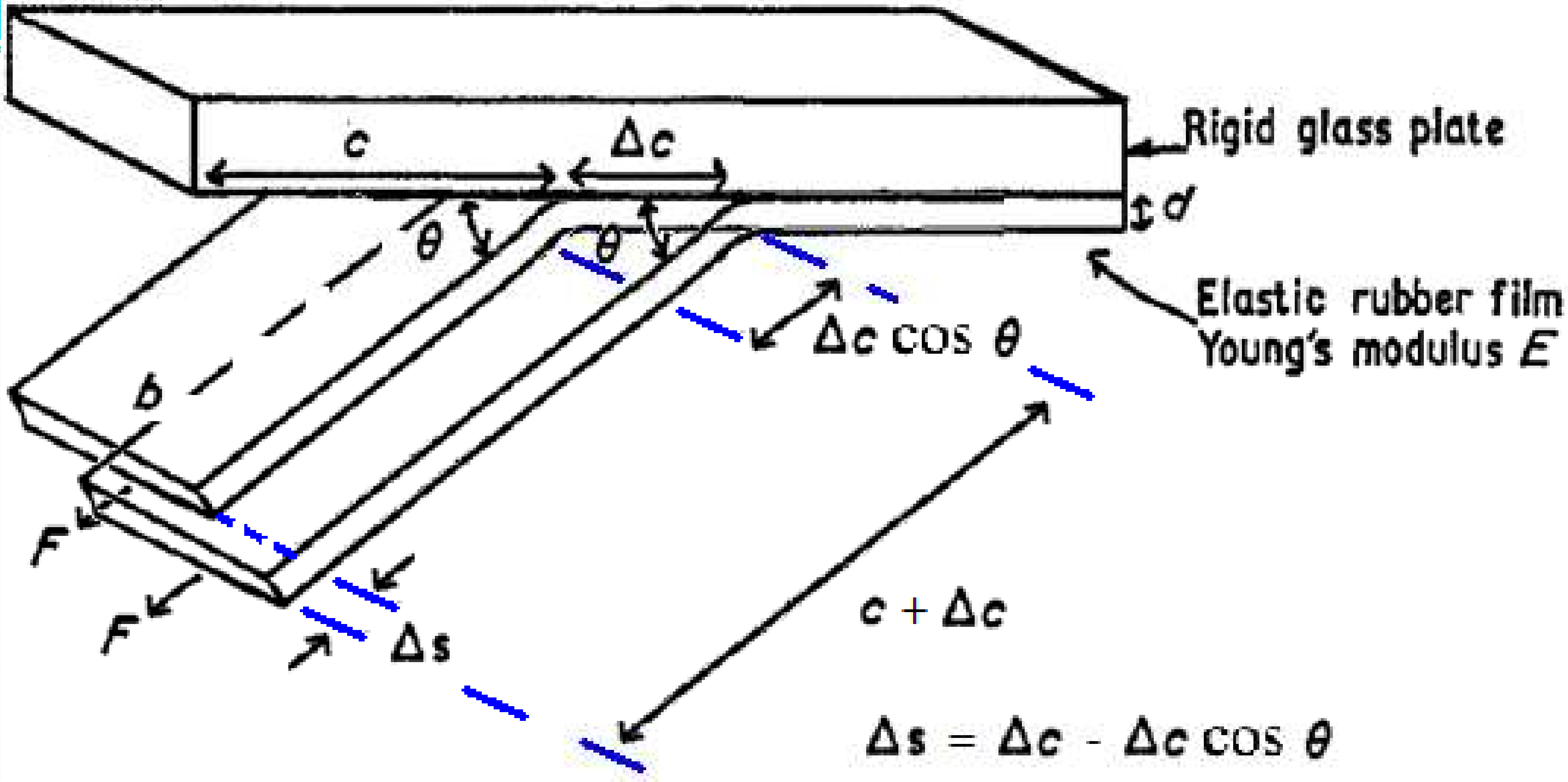


Figure 1. Elastic film peeling from a rigid substrate.

$$\left(\frac{F}{b}\right)(1-\cos\,\theta)-R=0.$$

K. Kendall, J. Phys. D: Appl. Phys. **8**, 1449 (1975).

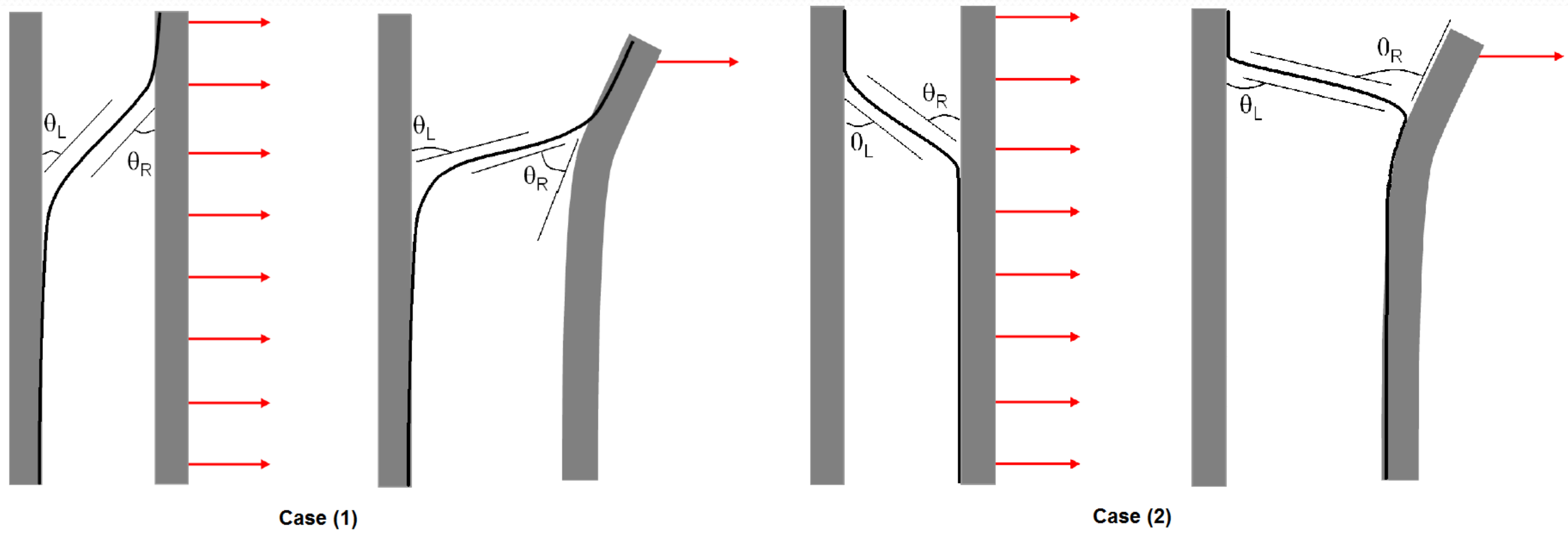
Forças entre conexões e big bundles



$$\left(\frac{F}{b}\right)(1-\cos\,\theta)-R=0.$$

K. Kendall, J. Phys. D: Appl. Phys. **8**, 1449 (1975).

Forças entre conexões e big bundles

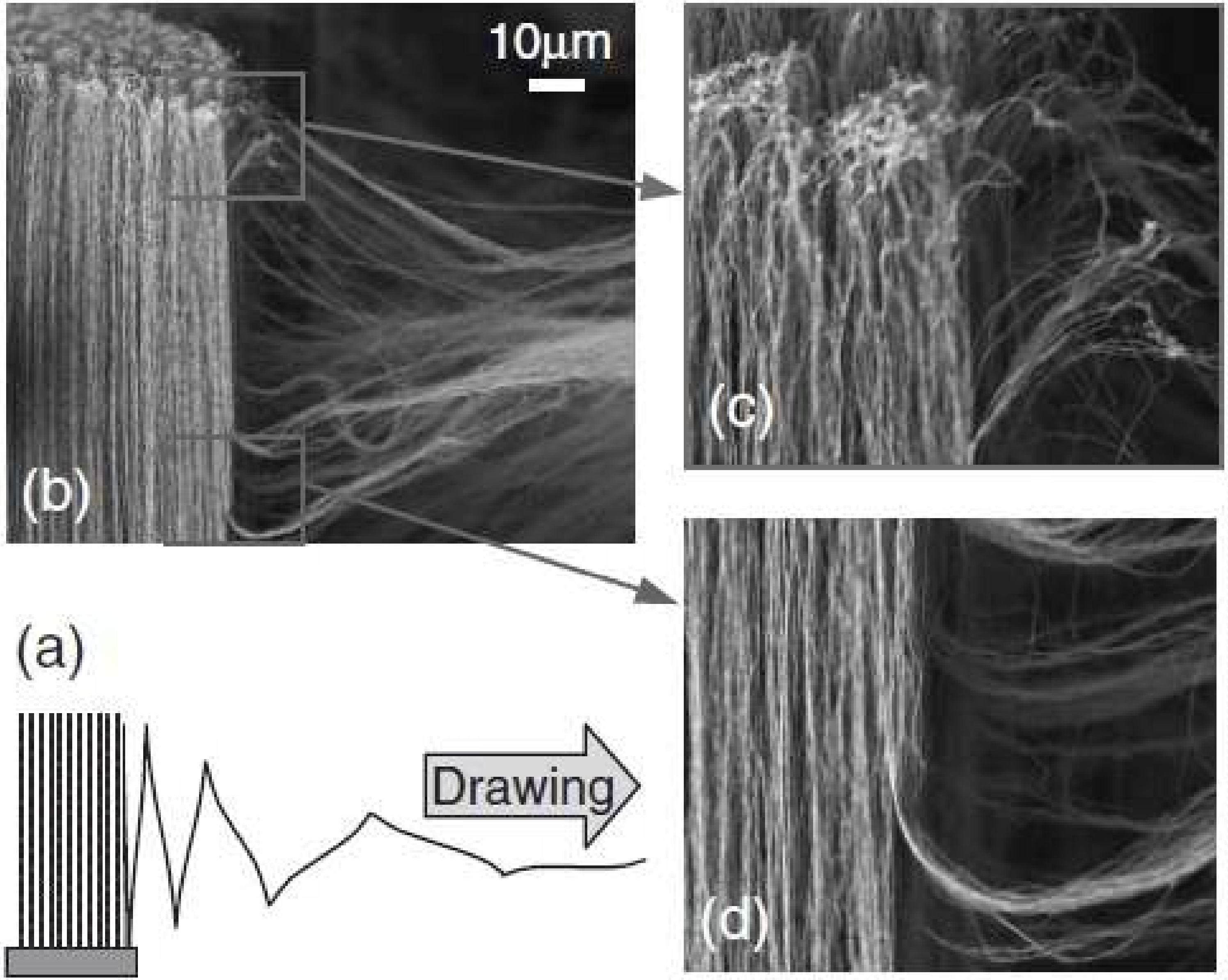


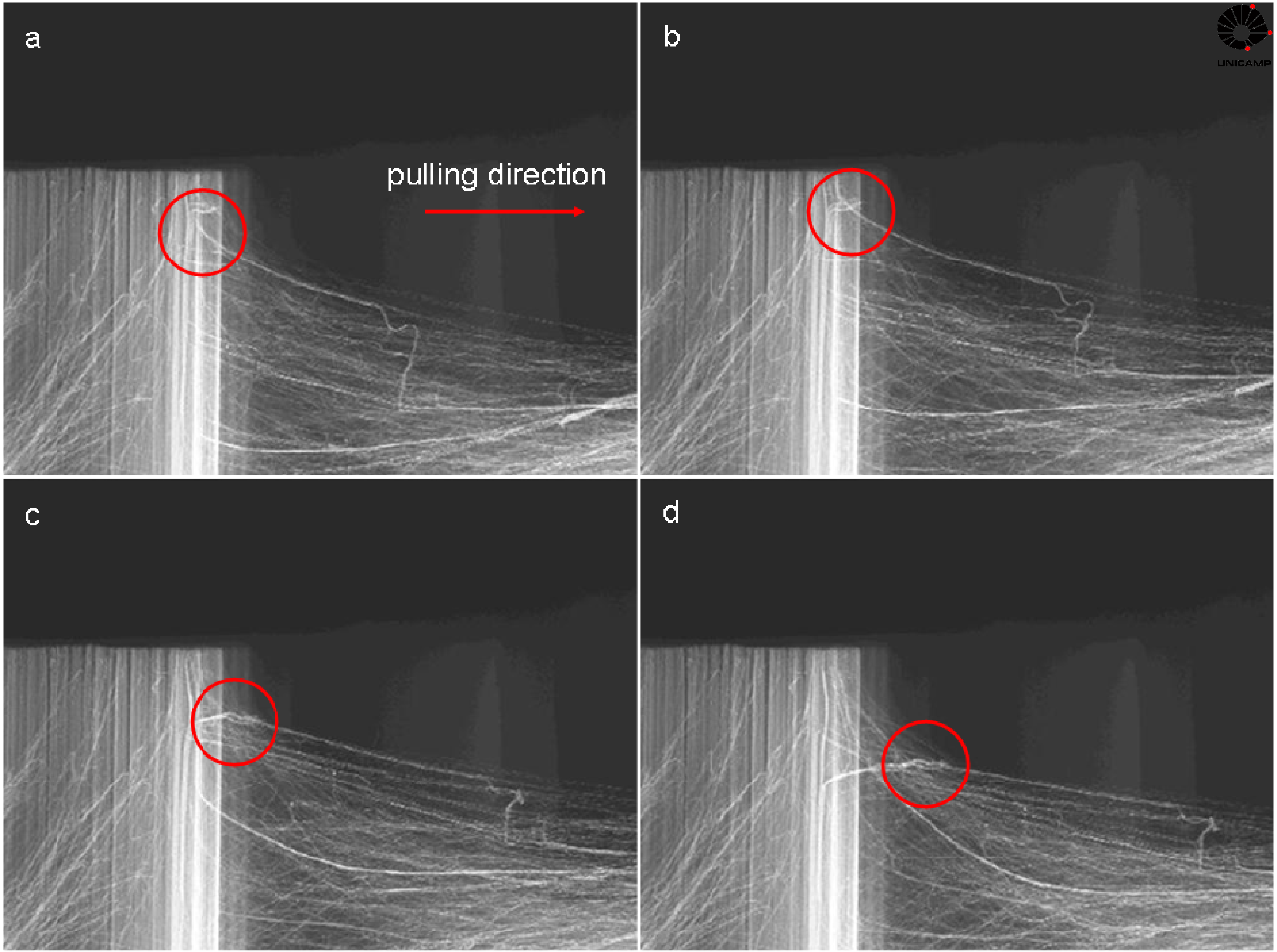
"Unzipping" and bending of the big bundles

Synthesis, Nanoprocessing, and Yarn Application of Carbon Nanotubes

Yoshikazu NAKAYAMA[1,2]
Osaka University, Suita, Osaka 565-0871, Japan

Japanese Journal of Applied Physics
Vol. 47, No. 10, 2008, pp. 8149–8156




a
b
c
d
pulling direction
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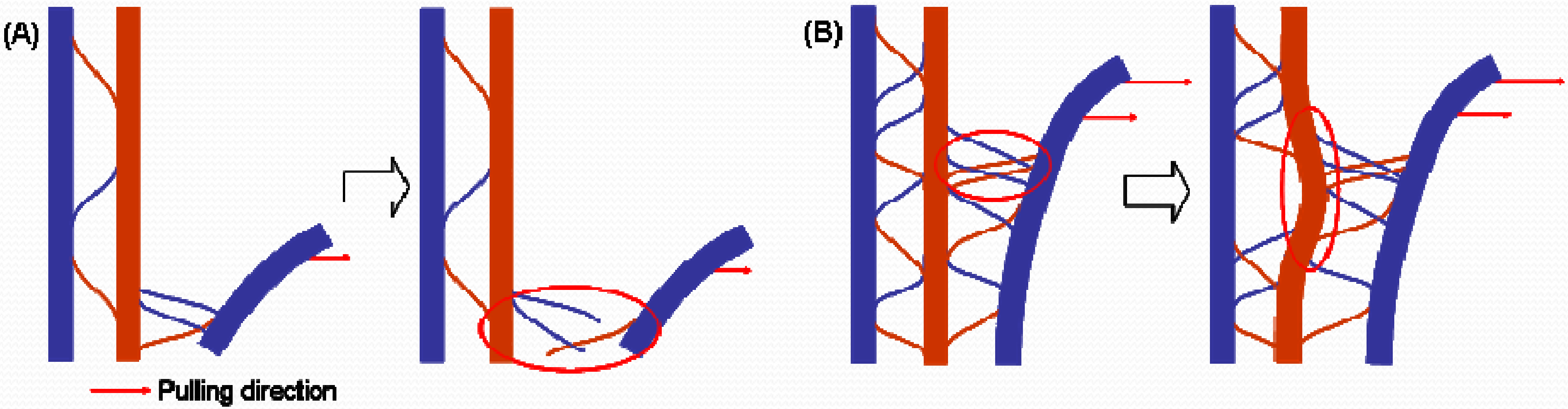
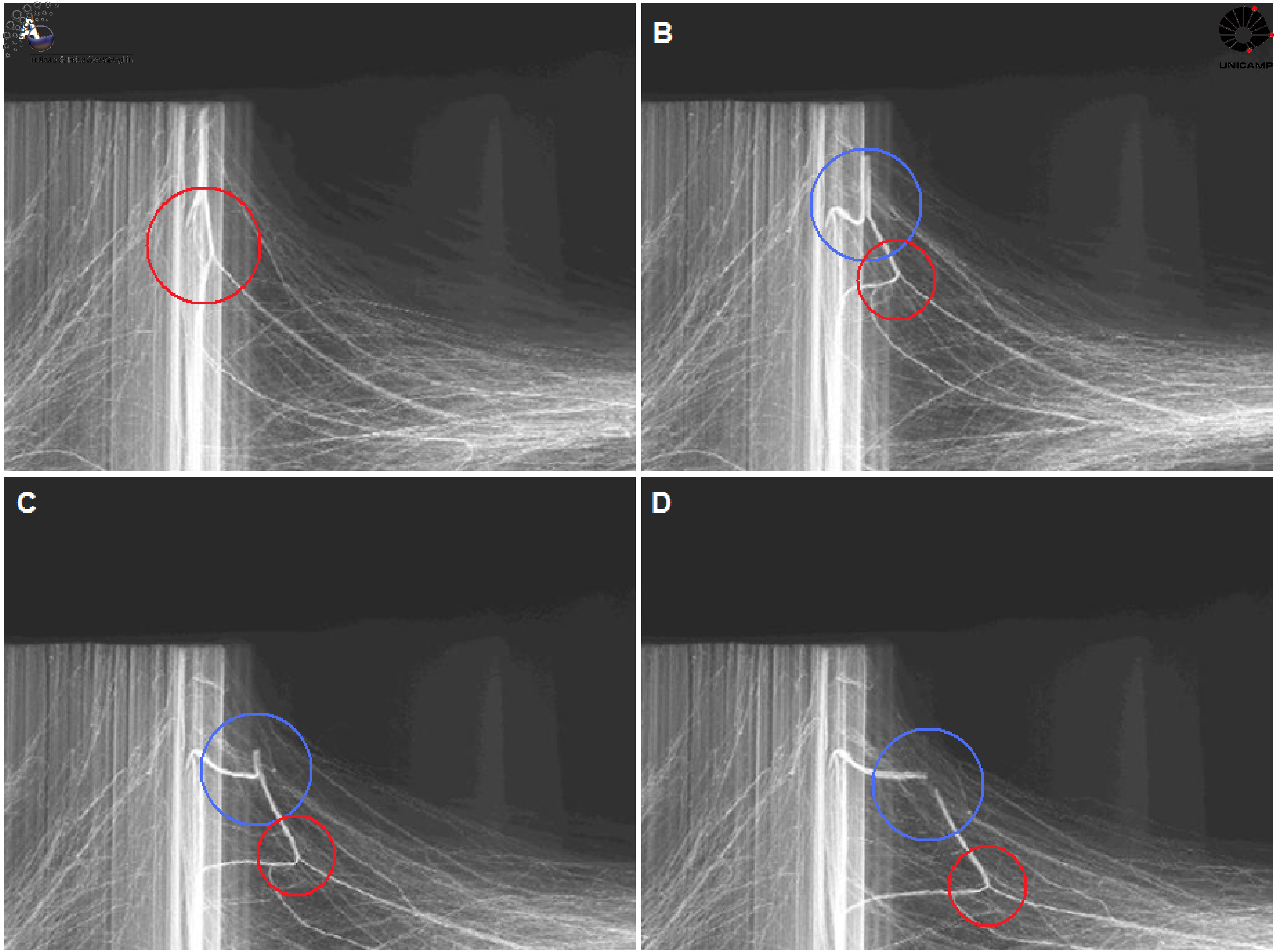
Efeitos da concentração BAIXA e ELEVADA de conexões.

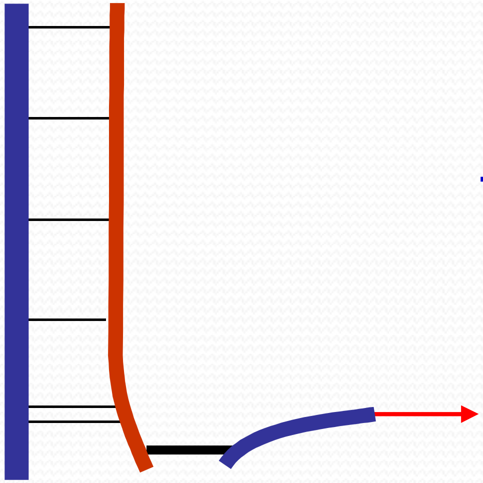




A
B
UNICAMP
C
D

Mínima and Máxima alturas da Floresta de CNTs: L_{MIN} and L_{MAX}

Smallest length: L_{MIN}

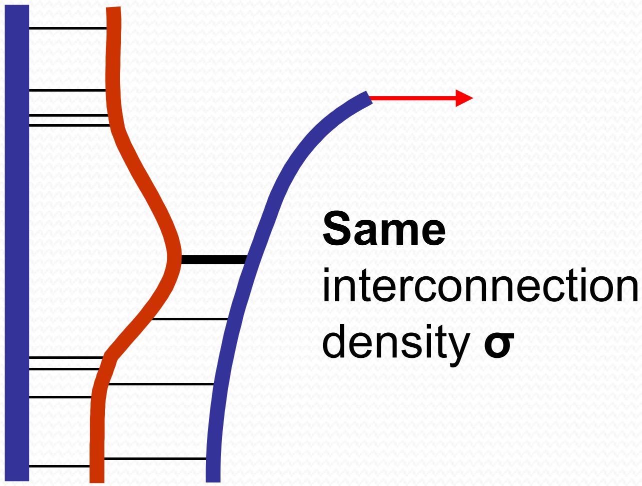


$f_{MIN} \leftrightarrow L_{MIN}$ $\quad f_{MIN} = N_{MIN} * f_1$

$f_{MIDDLE} \leftrightarrow L_{MAX}$ $\quad f_{MIDDLE} \sim 2N_{MIN} * f_1$

Using $\sigma = N_{MIN} / L_{MIN} \rightarrow$ $L_{MIN} = (f_{MIN} / f_1) * (1/\sigma)$

Largest length: L_{MAX}



Considerando $\sigma = N_{MAX} / L_{MAX}$

$L_{MAX} \leftrightarrow f_{MIDDLE} \sim 2N_{MIN} * f_1$

Então, $N_{MAX} = 2 * (2N_{MIN})$!

e, portanto: $L_{MAX} = 4 L_{MIN}$

f_1 – força entre “big Bundle” e interconexões

Mínima and Máxima alturas da Floresta de CNTs: L_{MIN} and L_{MAX}

$$r \equiv L_{max} / L_{min}$$

NanoTech CNT forests: $r \sim 4$ ☺

Nano Lett. **8**, 700 (2008) { $r \sim 5.1$; $r \sim 3.4$

Carbon **48**, 2855 (2010): $r \sim 3.5$

NANO **5**, 31 (2010): $r \sim 8.8$ ☹

Não se pode ganhar todas!

Instituto de Física Gleb Wataghin

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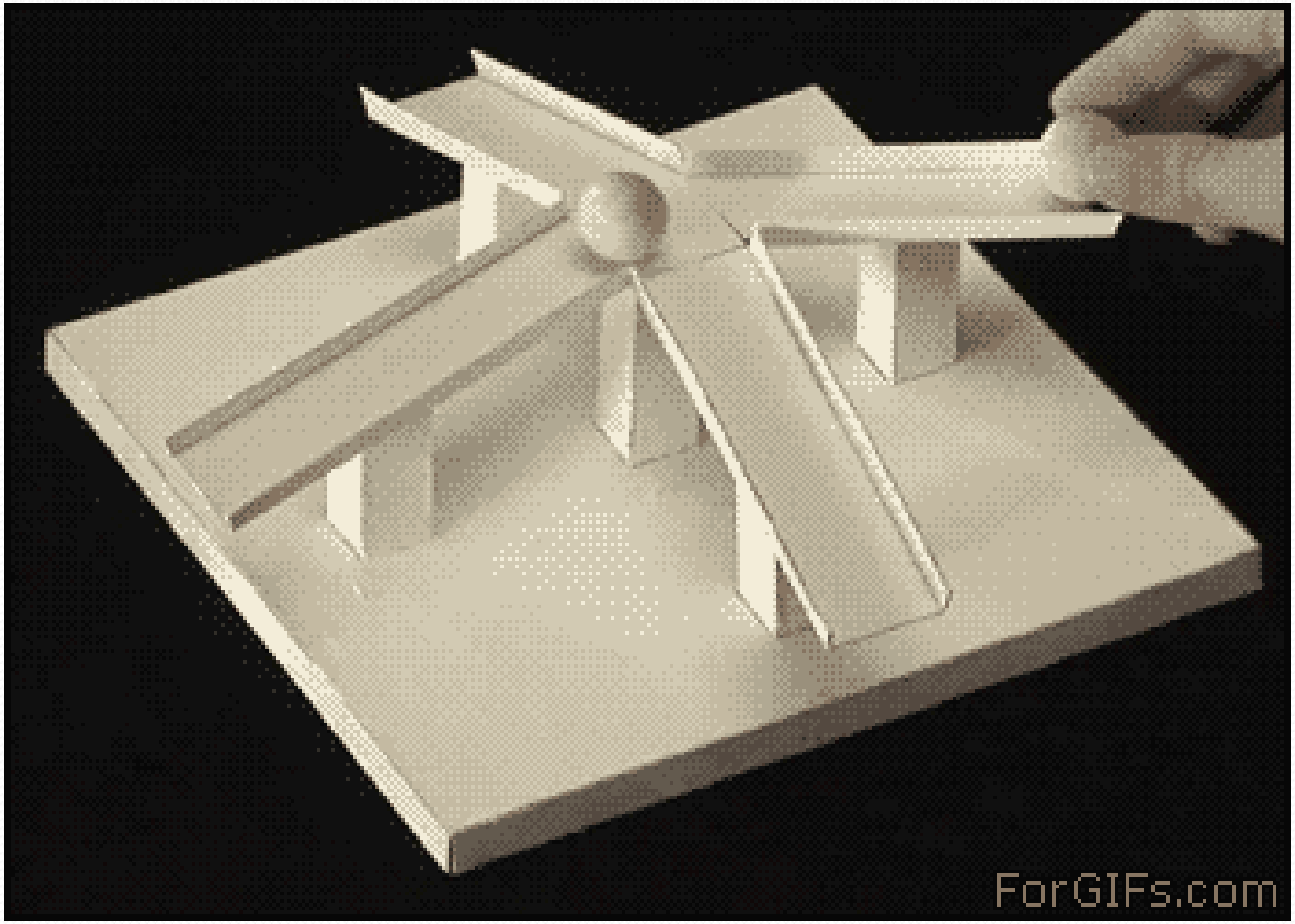
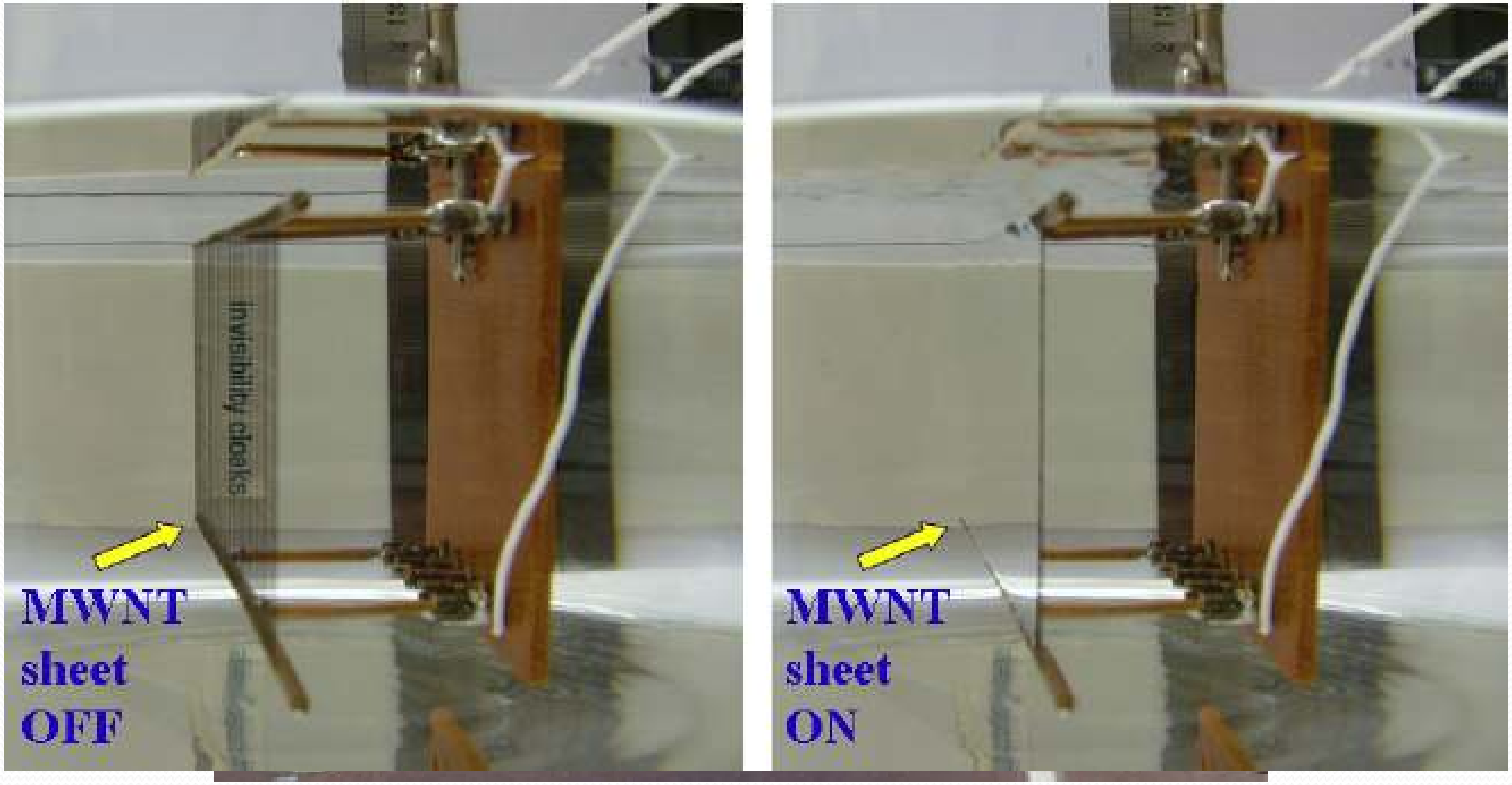
Comentários

Muitos problemas requerem o ponto de vista certo!

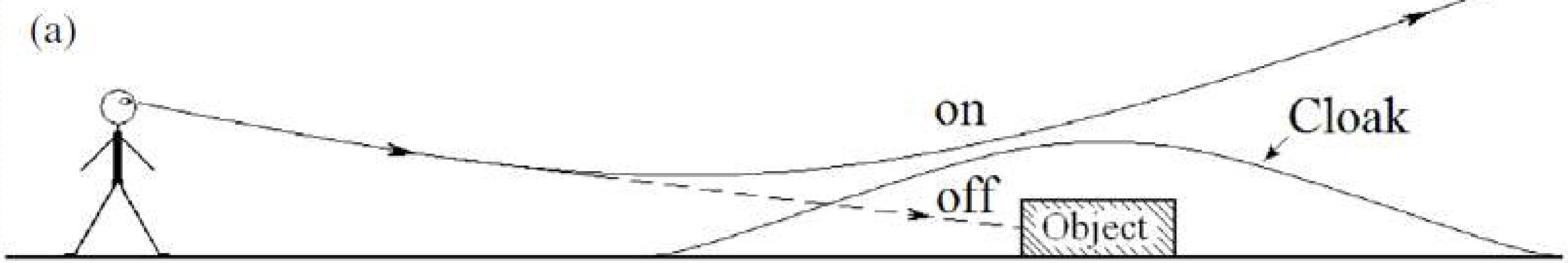


O segredo do *manto da invisibilidade*

O segredo do *manto da invisibilidade*



Ali E Aliev, Yuri N Gartstein and Ray H Baughman, Nanotechnology 22, 435704 (2011).

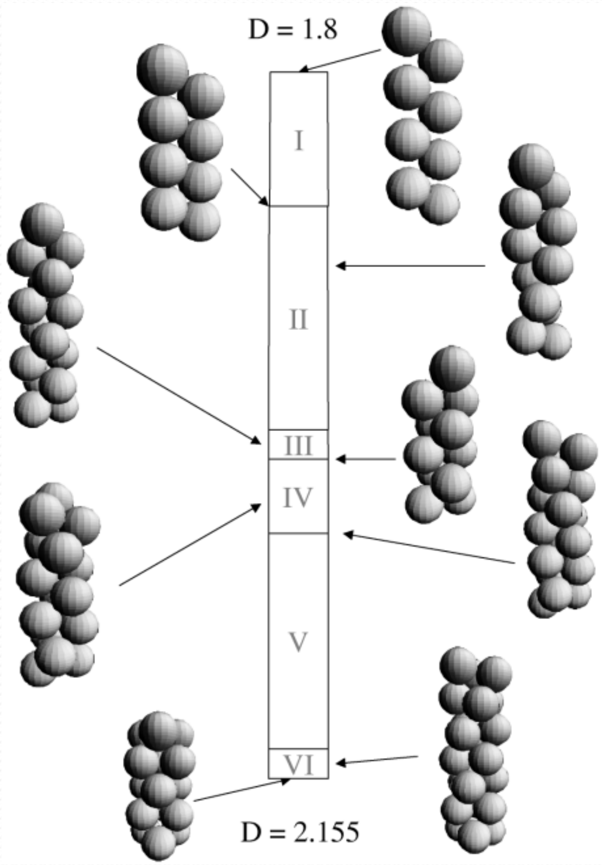


Ideias e Projetos

Extensão & Pesquis

Investigating Chirality in Closely Packed Confined Spheres

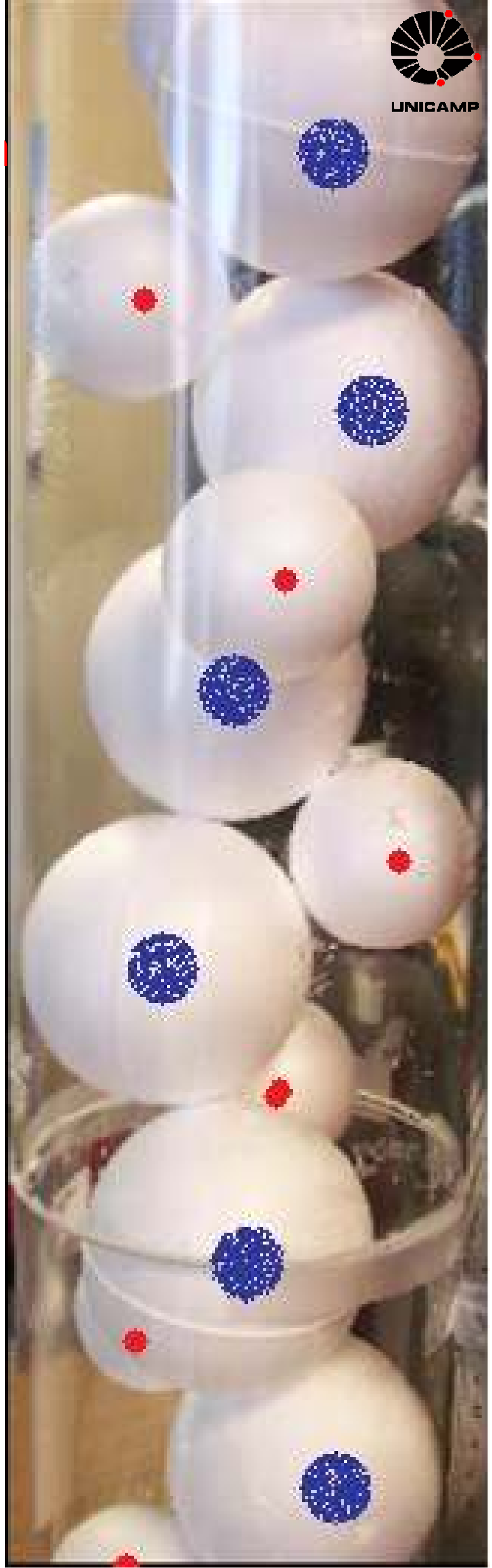
Vivek Menon, Mitu Bhattatiry, Srishti Goel, and Peter Cha



$$\rho_n = \ldots$$

$$z_n = \ldots$$

$$\phi_n = \ldots$$



Pickett *et.al*, PRL **85** p. 3652 (2000)

Projetos Atuais: Expansão Térmica de Grafenos

Linear thermal expansion of mono, by and trilayer – graphene

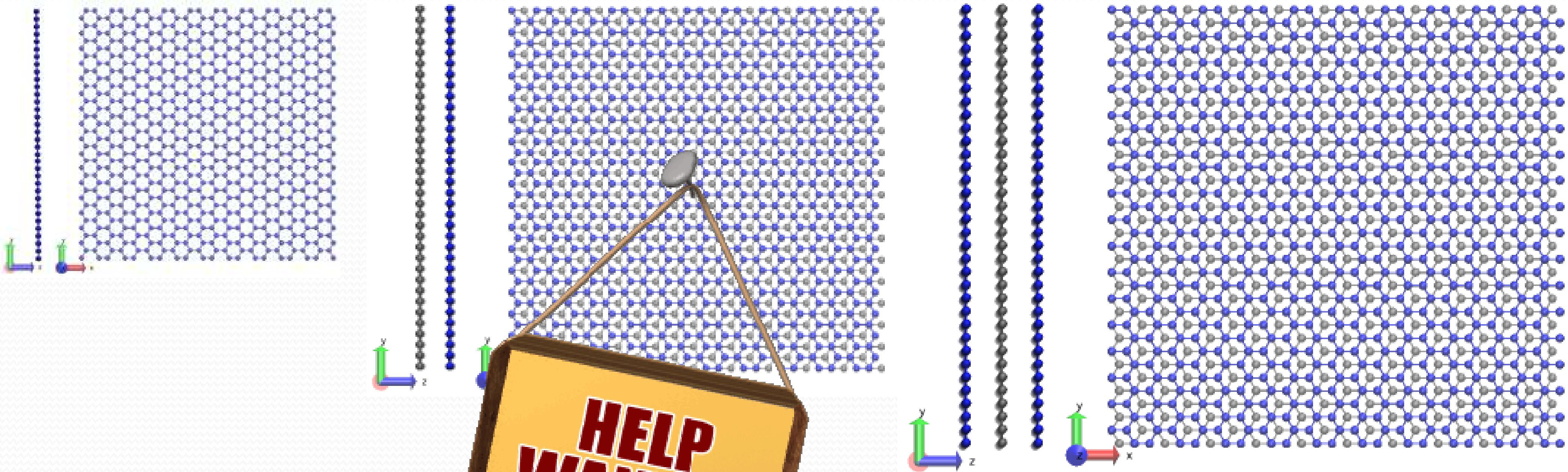


Table: Averagem coefficie… sion of graphene (x 10^{-6} K^{-1}) at 300K obtained by different methods for compa…

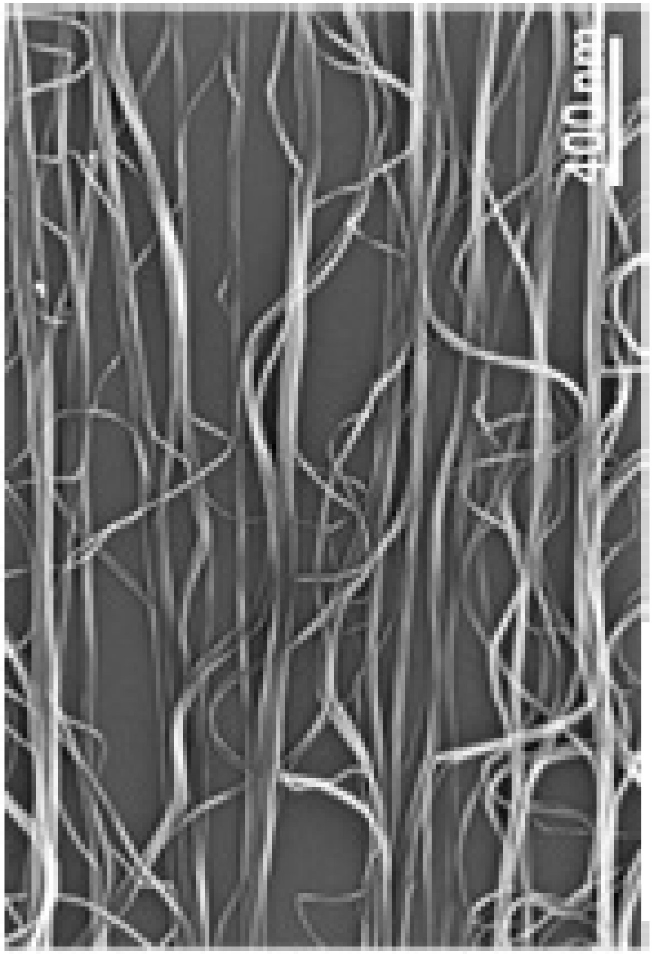
Experimental [1]	DFT [2]	REBO* [3]	Our results with REBO
-7	-3.5	-90	-3.8

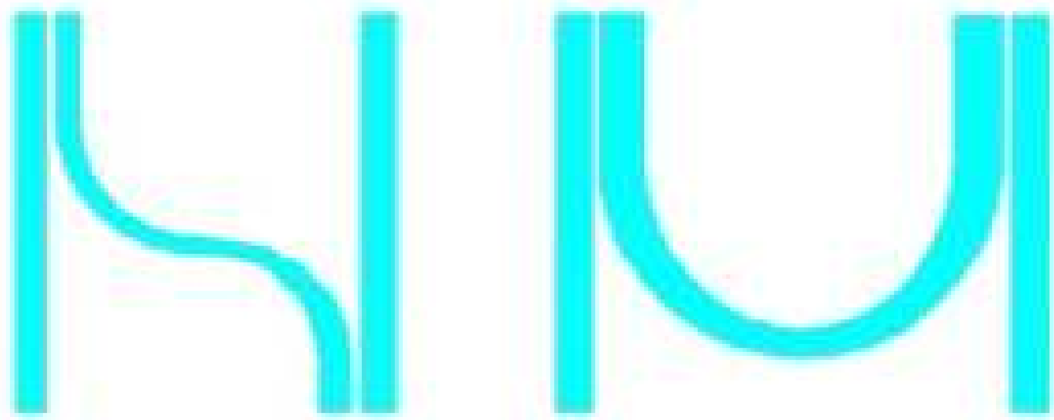
* **Strange result.**

[1] W. Bao, F. Miao, Z. Chen, H. Zhang, W. Jang, C. Dames and C. N. Lau, *Nature Nanotechnology* **4**, 462 (2009).
[2] N. Mounet and N. Marzari, *Physical Review B* **71**, 205214 (2005).
[3] M. Neek-Amal and F. M. Peeters, *Physical Review B* **83**, 235437 (2011).

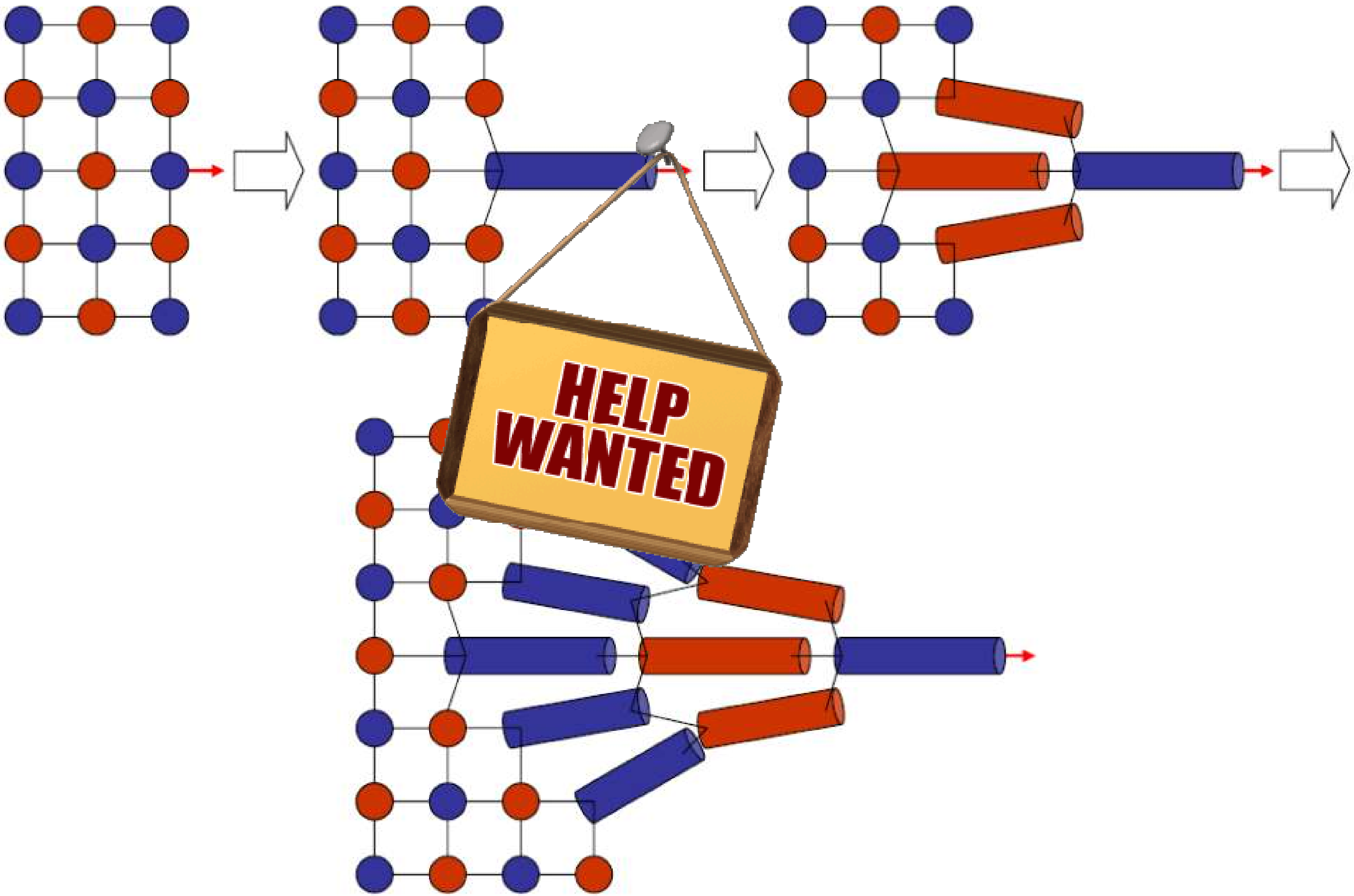
Projeto de Iniciação Científica – Virgilio UFF, e Prof. R. Capaz UFRJ

Projetos futuros

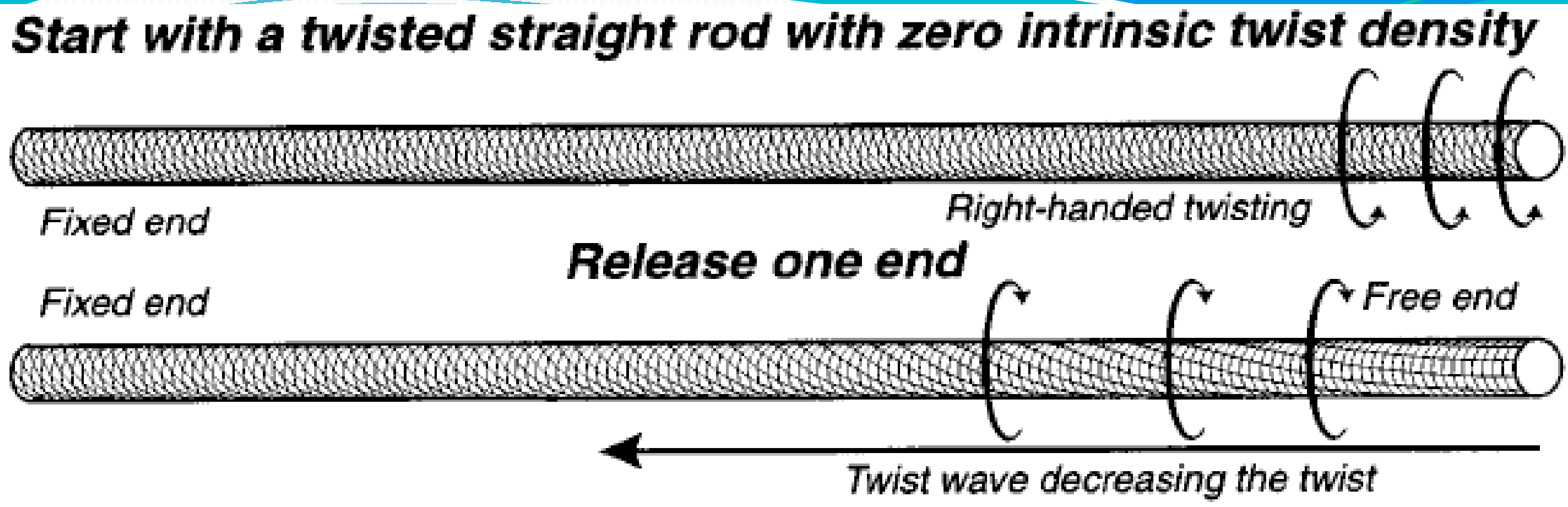


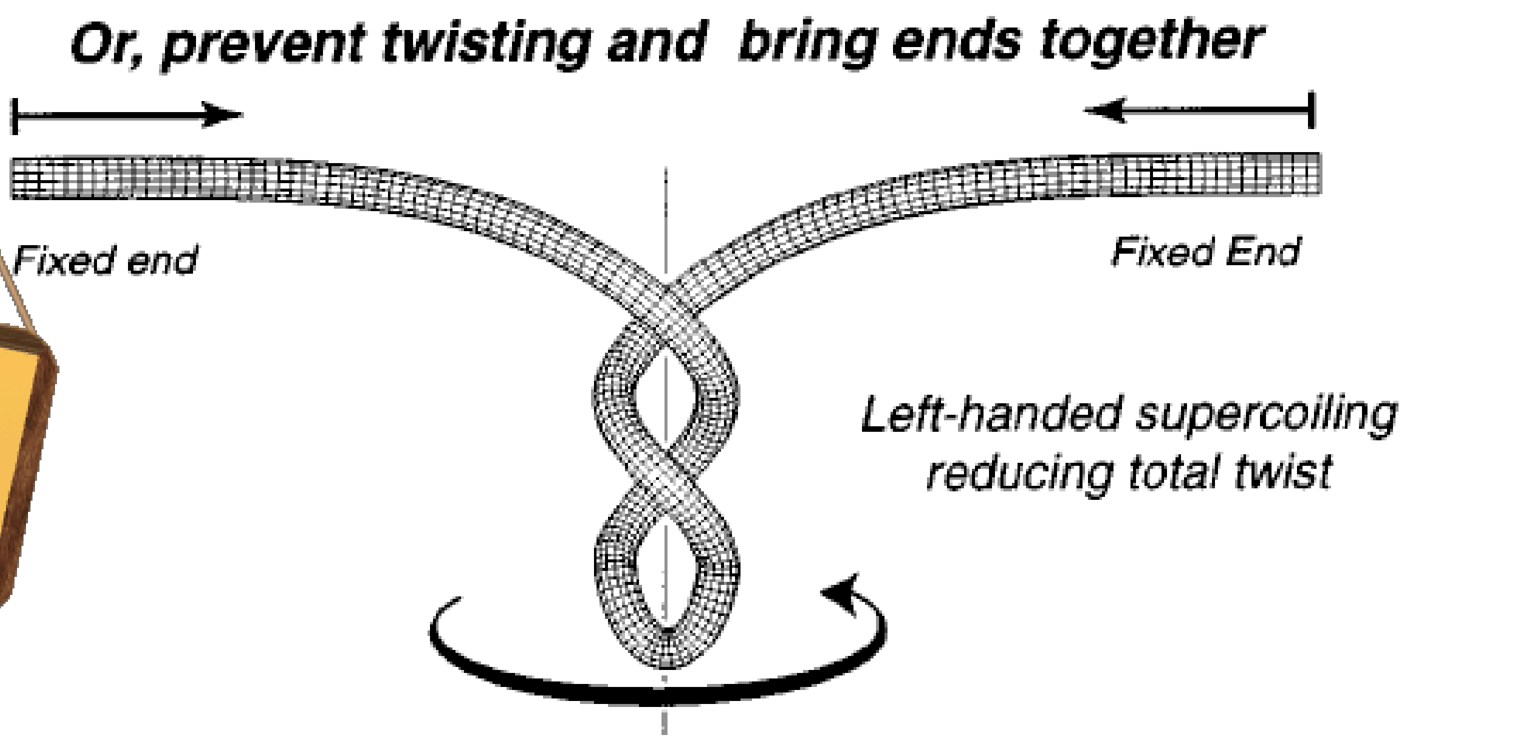


Projetos futuros



Projetos futuros



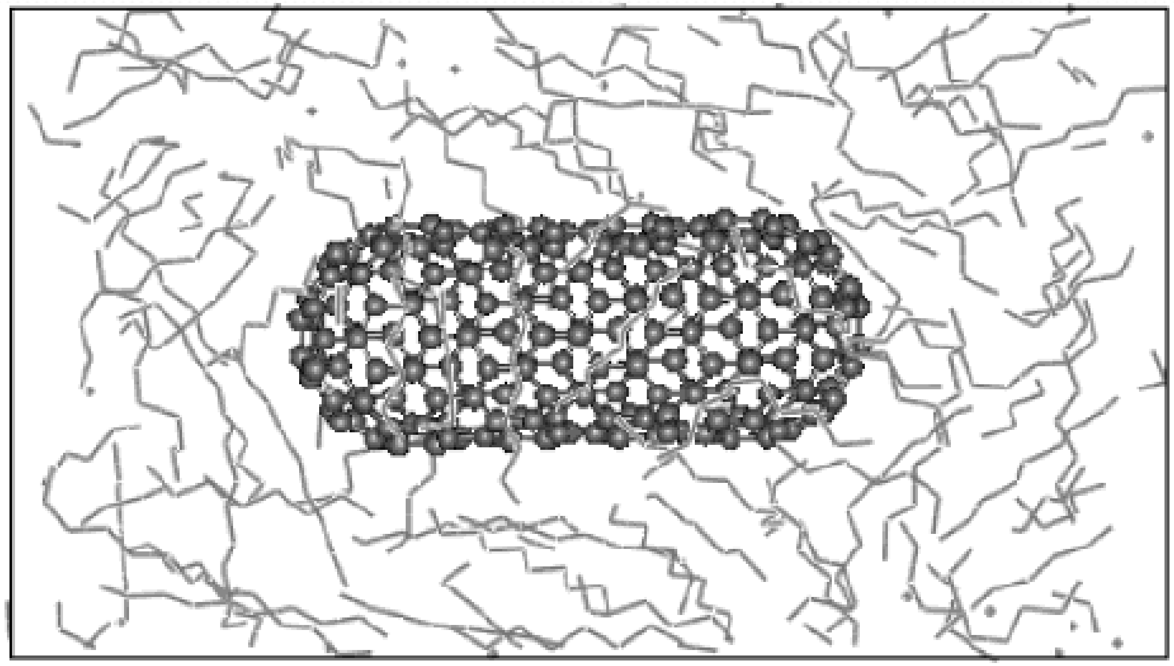


The Nonlinear Dynamics of Filaments

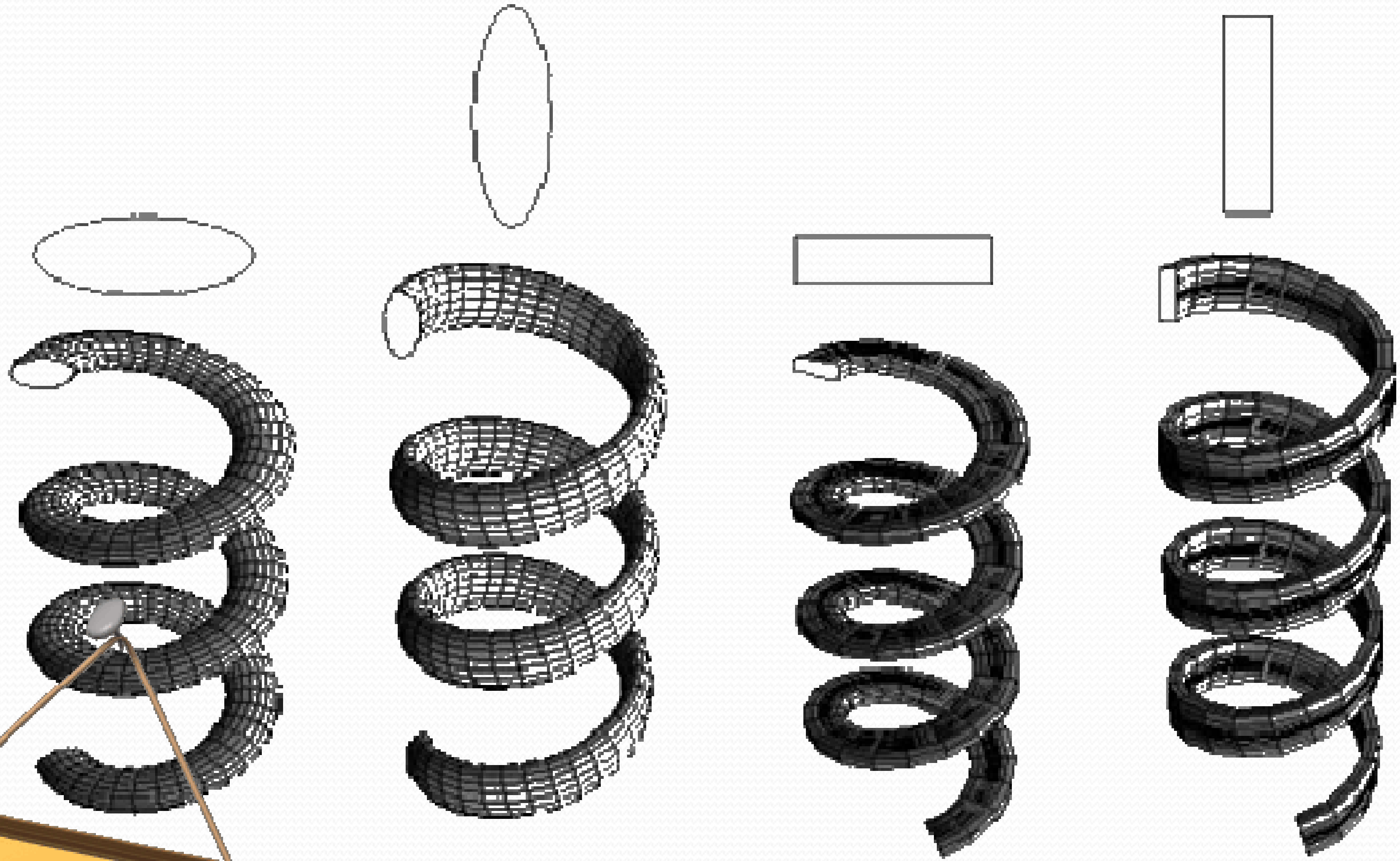
ALAIN GORIELY and MICHAEL TABOR

Nonlinear Dynamics **21**: 101–133, 2000.

Projetos futuros



Projetos futuros



MRS Symp. Proc., 0963-Q20-27 (2007).

$$k^{NORMAL} > k^{BINORMAL}$$

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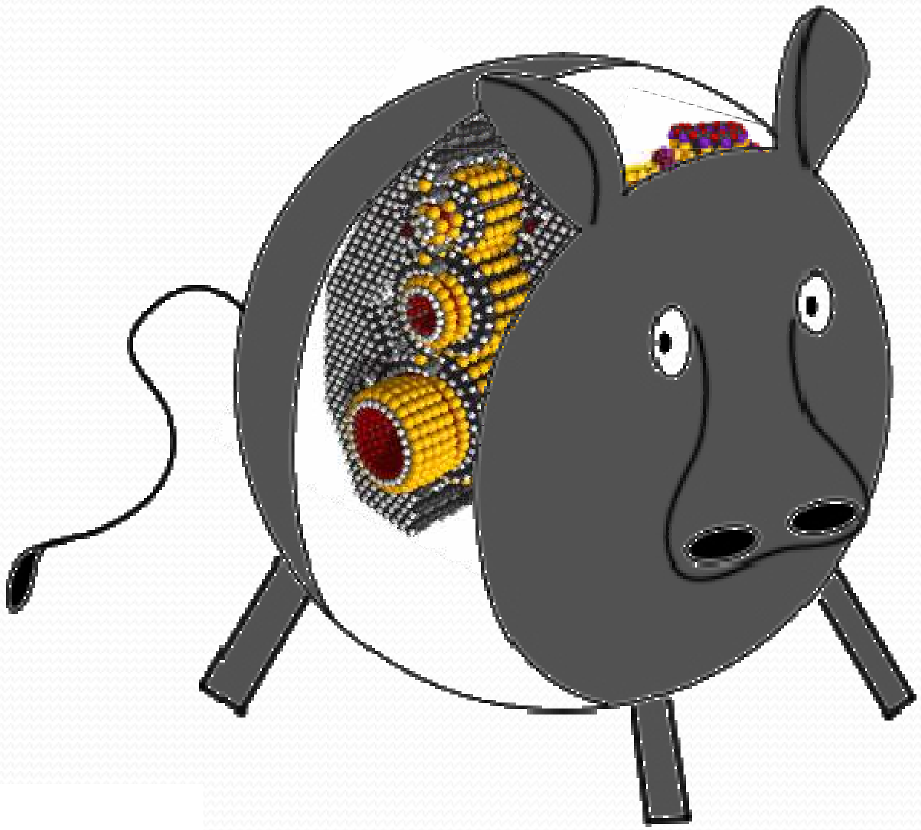
Precisa-se: alunos para projetos de IC e Pós!!

Obrigado!



FAPESP
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