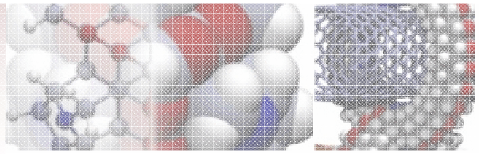

Strain engineering;
a new trend in nanotechnologies

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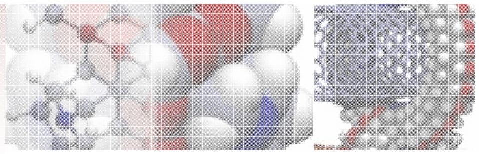


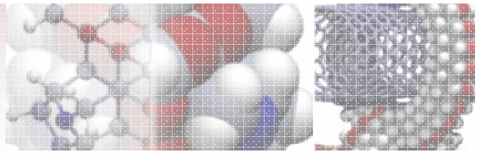
Synopsis

Strain Engineering Concept

Strain Engineering applications: thin films, nanomembranes, quantum dots, ultrastrength materials (graphene, nanowires, nanotubes, nanopillars, nanostrips), applications in mollecular biology

Fundamentals of ultra-strength: stress versus strain at nanoscale, inelastic strain, modeling

Experimental data about ultra-strength Ti based naostructured materials



Strain Engineering Concept is based on:
- material's physical and chemical properties are functions of the lattice parameters of the underlying crystal lattice, or - the elastic strain, $\varepsilon_{elastic}$, with respect to the stress-free reference state;
- fundamentally, electronic structure changes with $\varepsilon_{elastic}$.

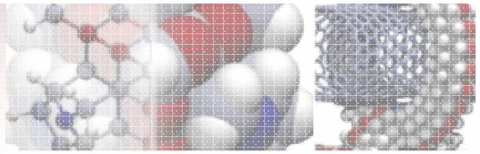
Physical and chemical properties depending on $\varepsilon_{elastic}$: electronic and phononic band gaps open or close with $\varepsilon_{elastic}$, thermal, spin, magnetic, transport, and electro-optical characteristics, catalytic activities of metal surfaces vary sensitively with $\varepsilon_{elastic}$

Definition: Elastic strain engineering is defined as achieving the desired functional properties by controlling $\varepsilon_{elastic}$ (x), where x denotes position vector in a material. The properties could be electronic magnetic optical, plasmonic, ionic or phononic, thermoelectric, catalytic etc.

Conceptually: given any material property, A, that one wants to optimize
>>> its derivative with respect to the elastic strain $\delta A/\delta\varepsilon_{elastic}$ is non-zero at zero strain
>>> gradient $\delta A/\delta\varepsilon_{elastic}$ can lead to the optimal property

Practically: there are specific particularities for each material and each application to manipulate by $\varepsilon_{elastic}$ a specific desired property

T. Zhu, J. Li, *Ultra-strength materials*, Progress in Materials Science 55, 710-757, 2010

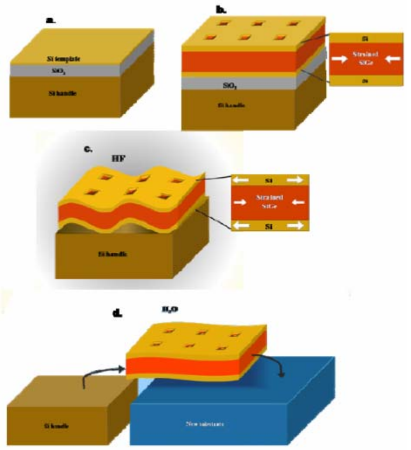


Strain Engineering applications

Various materials and applications:

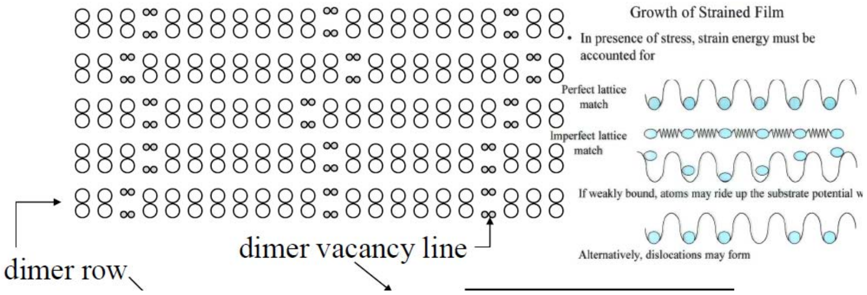
- thin films;
- nanomembranes;
- quantum dots;
- **ultra-strength materials** (graphene, nanowires, nanotubes, nanopillars, **ultra-thin strips**);
- applications in mollecular biology;
- etc.

Strain Engineering applications
thin films & nanomembranes;



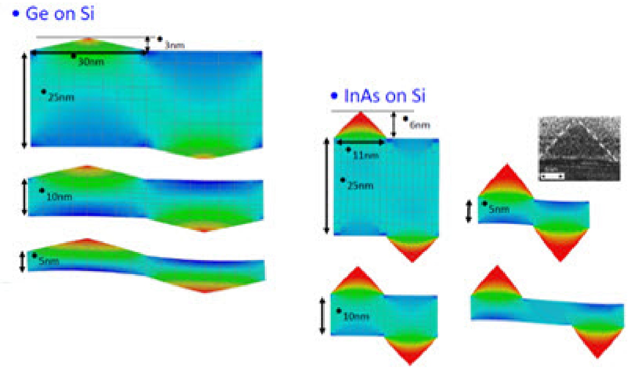
Applying strain to Si >> breaks the crystalline symmetry >> electronic band structure modifications. Band structure contributes to the magnitude of charge carrier mobility

D. M. Paskiewicz, S. A. Scott, D. E. Savage, M. G. Lagally, *Elastic Strain Engineering in Si Nanomembranes*, Abstract #1938, 218th ECS Meeting

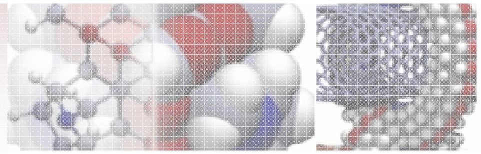


- Strain acts as an energetic term
- Is possible to control strain balance
- Strain controlled by nanostresors

C. Carter-Coman, A. S. Brown, R. Bicknell-Tassius, N. M. Jokerst, M. Allen, *Strain-modulated epitaxy: A flexible approach to 3-D band structure engineering without surface patterning*, Applied Physics Letters 69 (2), 257-259, 1996

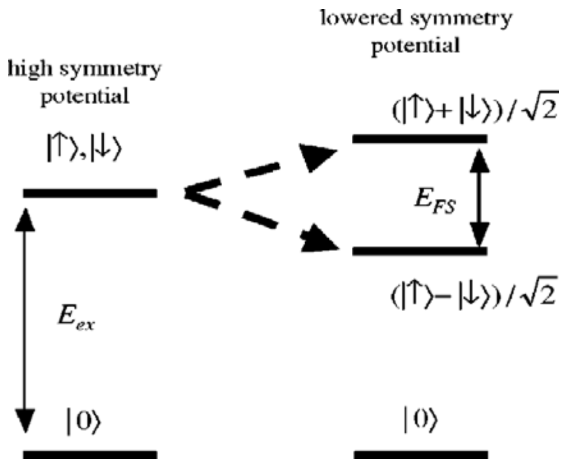


F. Liu, P. Rugheimer, E. Mateeva, D. E. Savage, M. G. Lagally, *Nanomechanics: Response of a strained semiconductor structure*, Nature 416, 498, 2002



Strain Engineering applications

quantum dots;



Ouantum dot exciton states in the case of the confining potential of a high (left) and low (right) symmetry. Fine structure splitting of the linearly polarized eigenstates in the low symmetry case is denoted E_{FS}. E_{ex} denotes exciton energy.

Strain reduction influences the magnitude of the fine structure splitting of quantum dot excitons(thermally annealed InGaAs quantum dot (QD) samples with differing degrees of In/Ga.

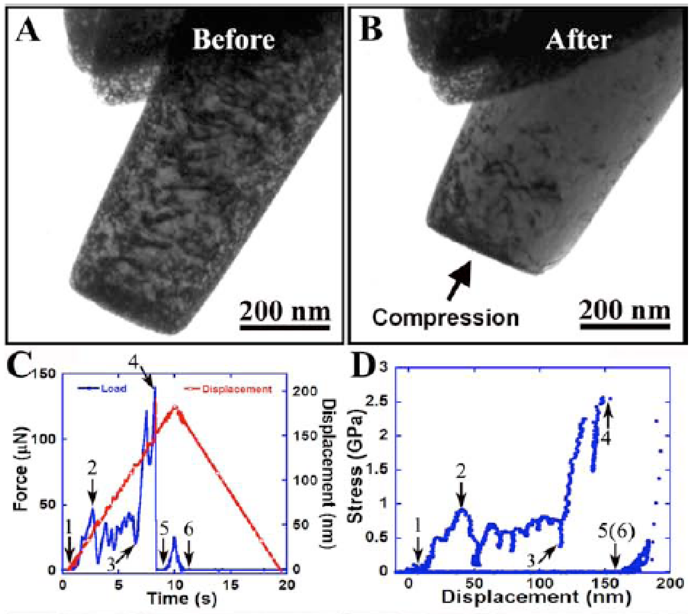
A. I. Tartakovskii, M. N. Makhonin, I. R. Sellers, J. Cahill, A. D. Andreev, D. M. Whittaker, J-P. R. Wells, A. M. Fox, D. J. Mowbray, M. S. Skolnick, K. M. Groom, M. J. Steer, H. Y. Liu, M. Hopkinson, *Effect of thermal annealing and strain engineering on the fine structure of quantum dot excitons*, Physical Review B 70, 193303, 2004.

mollecular biology;

Strain Engineering in mollecualr biology -Engineering a strain is integral to modify the host and its properties towards improvising quantitative and qualitative presence of desired products in a given biological system (***Syngene/ http://www.syngeneintl.com/)***

Strain Engineering applications

ultra-strength materials (graphene, nanowires, nanotubes, nanopillars, **ultra-thin strips**);



Single-crystal Ni pillars between 150 and 400 nm in diameter-micromachined using an FEI 235 Dual Beam focused ion beam (FIB)

T. Zhu, J. Li, S. Ogata, S. Yip, *Mechanics of Ultra-Strength Materials*, MRS Bulletin, 34, 167-172, 2009

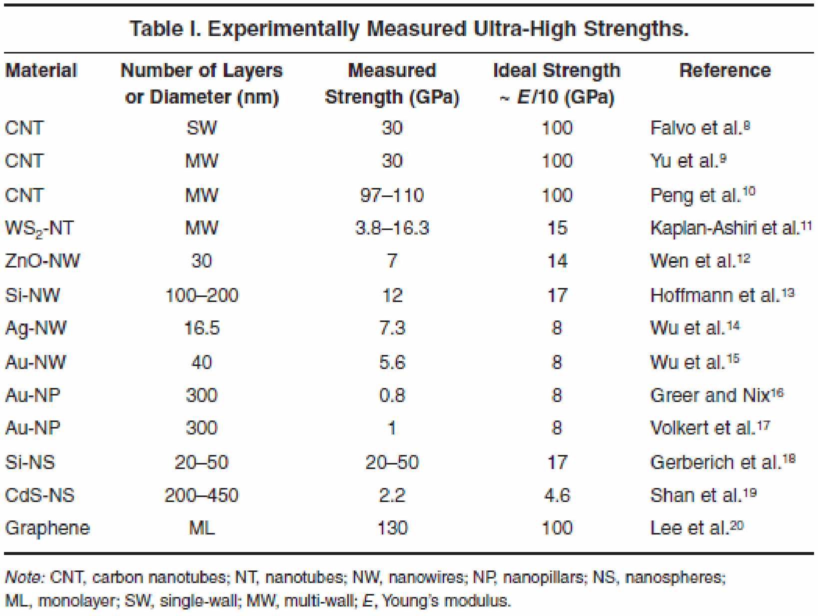


Table I. Experimentally Measured Ultra-High Strengths.

Material	Number of Layers or Diameter (nm)	Measured Strength (GPa)	Ideal Strength ~ *E*/10 (GPa)	Reference
CNT	SW	30	100	Falvo et al.[8]
CNT	MW	30	100	Yu et al.[9]
CNT	MW	97–110	100	Peng et al.[10]
WS_2-NT	MW	3.8–16.3	15	Kaplan-Ashiri et al.[11]
ZnO-NW	30	7	14	Wen et al.[12]
Si-NW	100–200	12	17	Hoffmann et al.[13]
Ag-NW	16.5	7.3	8	Wu et al.[14]
Au-NW	40	5.6	8	Wu et al.[15]
Au-NP	300	0.8	8	Greer and Nix[16]
Au-NP	300	1	8	Volkert et al.[17]
Si-NS	20–50	20–50	17	Gerberich et al.[18]
CdS-NS	200–450	2.2	4.6	Shan et al.[19]
Graphene	ML	130	100	Lee et al.[20]

Note: CNT, carbon nanotubes; NT, nanotubes; NW, nanowires; NP, nanopillars; NS, nanospheres; ML, monolayer; SW, single-wall; MW, multi-wall; *E*, Young's modulus.

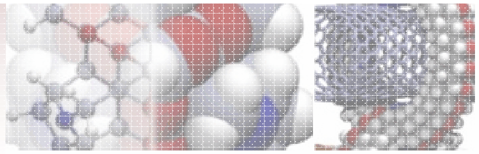
Z. W. Shan, R. K. Mishra, S. A. Syed Asif, O. L. Warren, A. M. Minor, *Mechanical annealing and source-limited deformation in submicrometre-diameter Ni crystals*, Nature materials, 7, 115-119, 2008

Fundamentals of ultra-strength - stress versus strain at nanoscale, inelastic strain, modeling

Ultra-strength phenomena definition:

The material's sample-wide stress has reached a significant fraction of its ideal strength and this state persists for a considerable period of time (seconds till years) without significant stress relaxation; "significant fraction" to be > 1/10 irrespective of shear, tensile or compressive stresses, unless otherwise specified

T. Zhu, J. Li, *Ultra-strength materials*, Progress in Materials Science 55, 710-757, 2010



Ultra-strength phenomena characteristics:

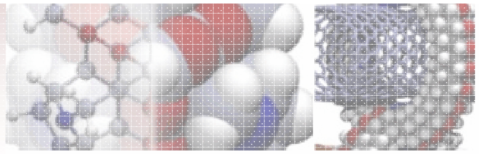
- broader than that of high-pressure physics - large non-hydrostatic stresses due to shear, tension and compression may be sustained;

- in **conventional materials**: the applied non-hydrostatic load tends to be relaxed by plastic deformation and fracture;

- in **ultra strength materials** the relaxation is posible by **inelastic deformation mechanisms**;

- **in nanostructured materials** a much larger range of non-hydrostatic stresses can be achieved, >>>> controlling the physical and chemical properties of materials (by **strain engineering - SE**).

T. Zhu, J. Li, *Ultra-strength materials*, Progress in Materials Science 55, 710-757, 2010



The inelastic strain is physically attributed to: dislocation glide, deformation twinning, crack formation and growth phase transformation, mass transport by diffusion etc; in an ideal defect-free structure at T = 0 K: $\varepsilon_{\text{inelastic}}$ stays zero unless the ideal strength is reached

$\varepsilon_{\text{elastic}}$ depends locally on stress in a one-on-one correspondence,
$\varepsilon_{\text{inelastic}}$ depend on stress with a highly non-linear, and temperature and history dependent relation.

- specific items: mechanical annealing, length scale effect; time scale effect; image force for the force experienced by a dislocation in the vicinity of a free-surface (**a hypothetical negative dislocation** is assumed to exist on the other side of the boundary)

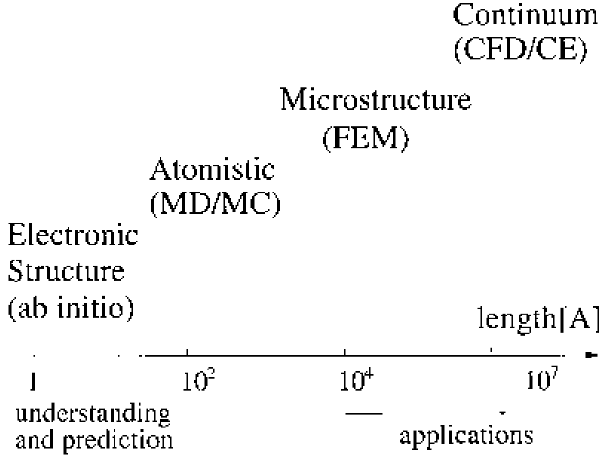
T. Zhu, J. Li, *Ultra-strength materials*, Progress in Materials Science 55, 710-757, 2010

Modelling

-**four distinct levels of microstructural complexity**: electronic-structure, atomistic, mesoscale, and continuum;

- at each level: **corresponding methods of simulation**, first-principles quantum mechanical calculations, classical molecular dynamics and Monte Carlo simulations, finite-element methods, and continuum mechanics;

- **multiscale modeling**: a particular challenge, especially the connection between atomistic and the mesoscale.

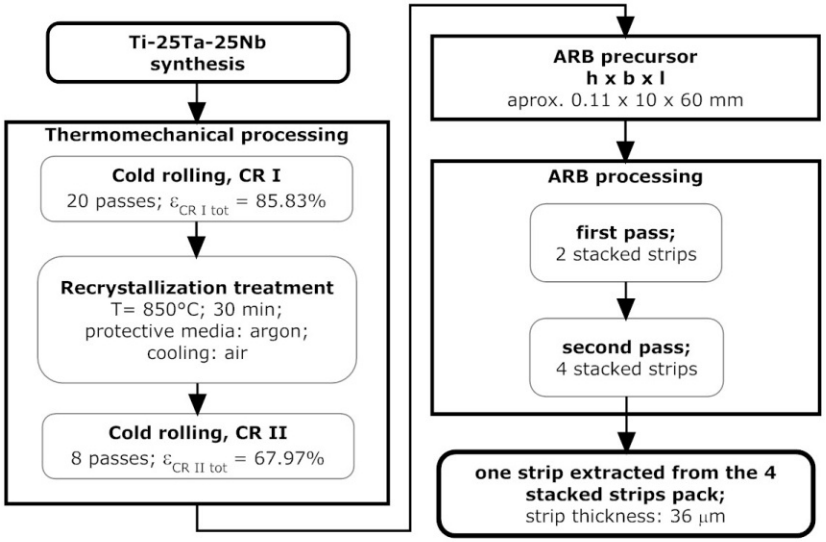


The four characteristic length scales in multiscale materials modeling.

S. Yip, J. Li, W. Cai, J. Chang, D. Liao, *Atomistic measures of mechanical deformation and thermal transport processes*, Computational Fluid and Solid Mechanics: Proceedings, First MIT Elsevier, New York, 2001. ISBN: 0080439446.

The *in-situ*, quantitative nanoscale compression tests - inside a JEOL 3010 (300kV) transmission electron microscope (TEM). The holder has a nominal force and displacement resolution of 0.1 N and 0.5 nm, respectively. (*National Center for Electron Microscopy, Lawrence Berkeley National Laboratory,Berkeley, California)*

Experimental data about ultra-strength Ti based naostructured materials



Ti-25Ta-25Nb synthesis

Thermomechanical processing

Cold rolling, CR I
20 passes; $\varepsilon_{CR\ I\ tot}$ = 85.83%

Recrystallization treatment
T= 850°C; 30 min;
protective media: argon;
cooling: air

Cold rolling, CR II
8 passes; $\varepsilon_{CR\ II\ tot}$ = 67.97%

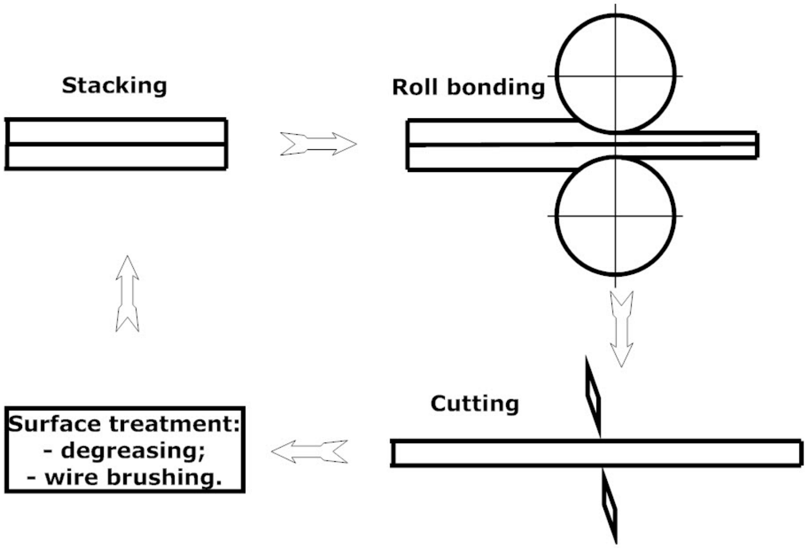
ARB precursor
h x b x l
aprox. 0.11 x 10 x 60 mm

ARB processing

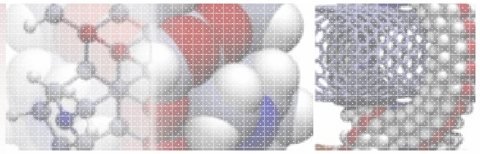
first pass;
2 stacked strips

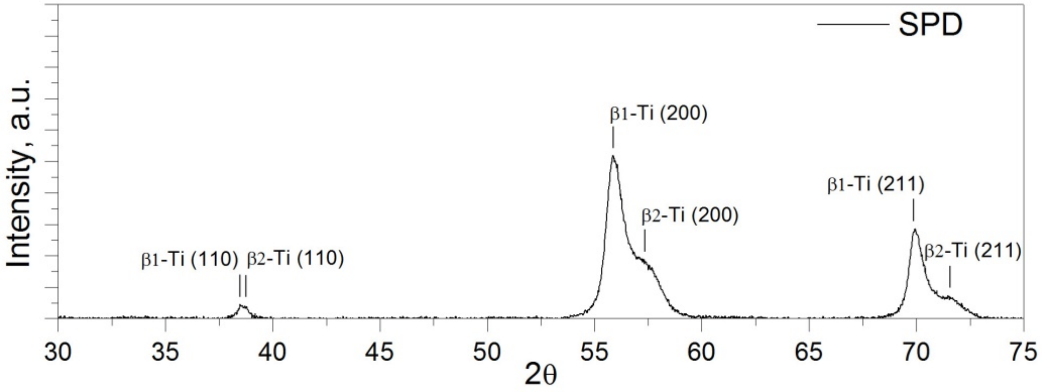
second pass;
4 stacked strips

one strip extracted from the 4 stacked strips pack;
strip thickness: 36 μm



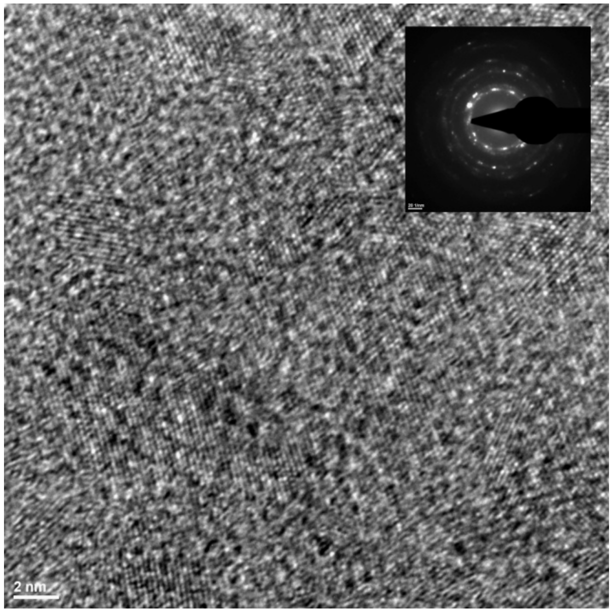
Surface treatment:
- degreasing;
- wire brushing.



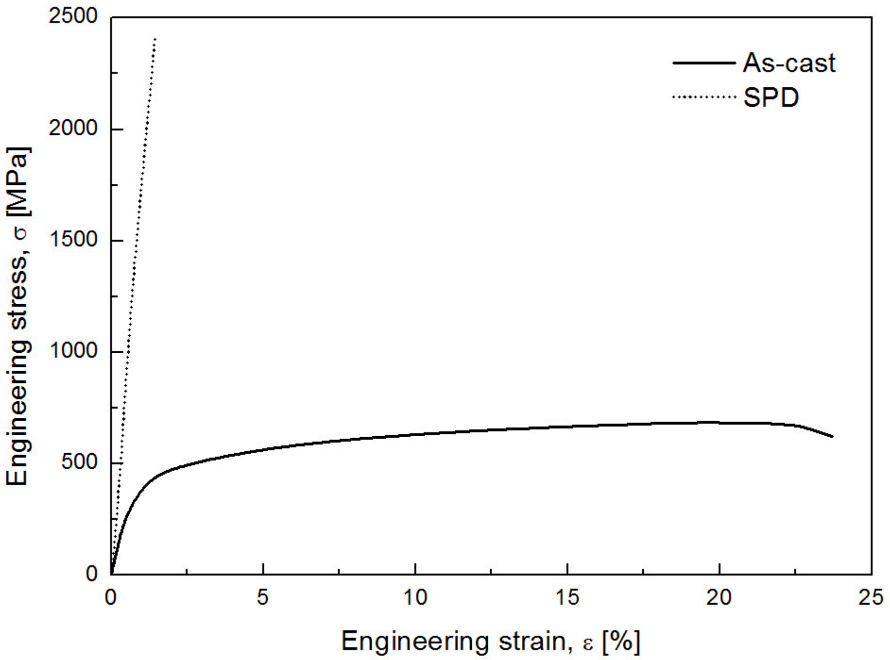


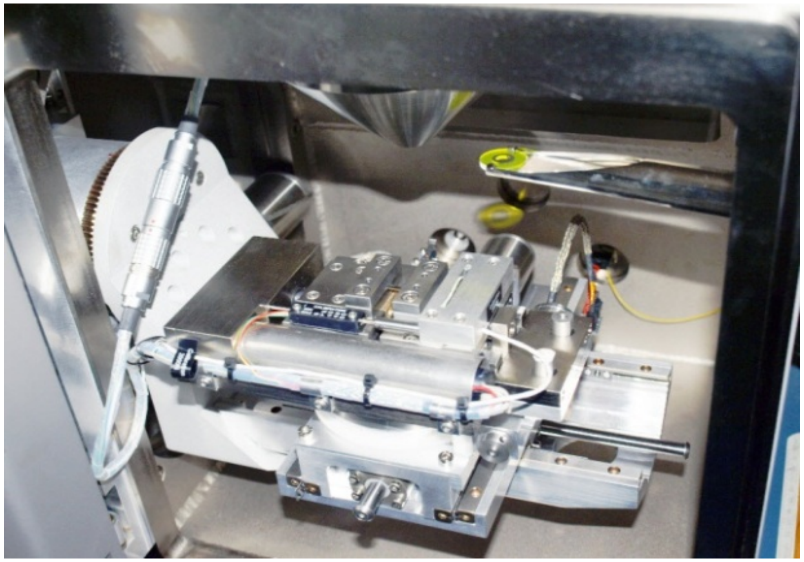
In the case of SPD processed alloy the XRD analysis showed the presence of the β-Ti phase. Two sub-beta phases were identified:
β1-Ti phase quantity 55.75±2.59%;
β2-Ti phase quantity 44.25±1.61%.

Calculated crystallite size (coherent crystalline domains) for both b-Ti phases were :
β1-Ti phase about **6 nm;**
β2-Ti phase about **4 nm**.



Precursor HRTEM image
Tecnai G2 F30 S-TWIN
(UPB)



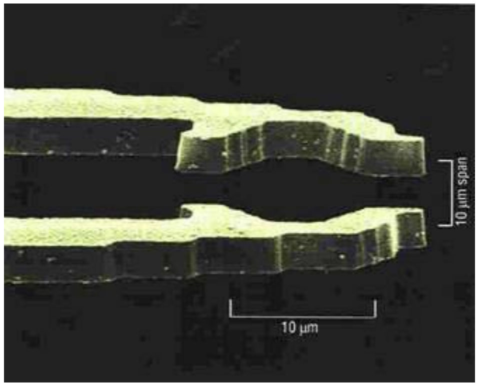


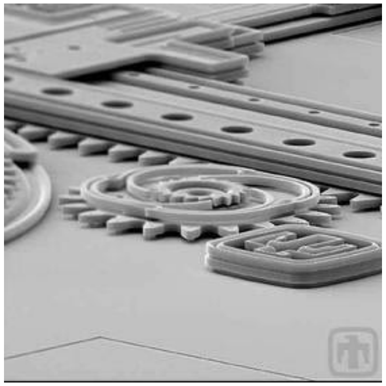
TESCAN Vega II-XMU SEM fitted with a micromechanical testing module GATAN MicroTest 2000N

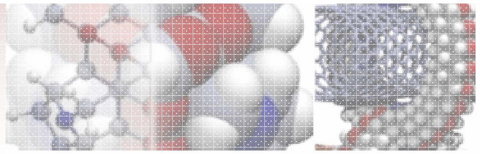
Mechanical investigations in the case of SPD processed alloy, in comparison with as-cast state, **show a steep increase in ultimate tensile strength from 682 MPa to 2423 MPa**, a high decrease in elongation to fracture from 24% to 1.5%. For this alloy, in SPD state, is difficult to achieve high strength and high ductility at the same time.

Possible applications of ultra-thin – ultra-strength Ti-based strips **in MEMS applications**:

- ultra-thin mechanical parts (gears);
- cantilevers;
- micro-gripers;
- strain-gages;
- etc.







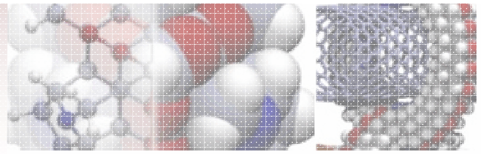
Experimental data about ultra-strength Ti based naostructured materials

- **the physical mechanism**: a competition between the dislocation germination rate and the mobile dislocation annihilation rate - **an atypical strain hardening;**

- progressive activation and subsequent exhaustion of dislocation sources- dislocations in ultra-thin can travel only very small distances before annihilating at free surfaces >>>> reducing the overall dislocation multiplication rate;

- concept of dislocation starvation - gliding dislocations leave the crystal more rapidly than they multiply >>>> very high stresses to nucleate new/mobile dislocations;

- the strength is defect nucleation controlled rather than propagation controlled.



Conclusions

- **ultra-thin nanostructures** structures contain a high density of initial defects after processing; **can be made dislocation - free by applying purely mechanical stress.**

Perspectives

- strain rate and temperature sensitivity investigation in ultra-strength materials domain;

- temperature-controlled nanomechanical testing is a direction for future growth;

- ultra-high stress correlation with diffusive and hybrid displacive - diffusive processes.