GDR CNRS International MECANO

« Mechanics of Nano-Objects »

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INP, Section 05
INP, Section 06
INC, Section 15
INSIS, Sections 08 et 09
Physique, Mécanique & Chimie

Outline

Foreword

For 4 years (2008-2011) the CNRS-funded Research network MECANO (GDR CNRS 3180 MECANO) [http://www.im2np.fr/GDR-Mecano] has been organizing scientific discussions on the issue of mechanical properties in small dimensions. 44 laboratories all over France have participated in scientific meetings, workshops and schools with lively discussions around this rapidly moving field. The MECANO network is a multidisciplinary one, which brings together physicists, mechanical engineers and chemists. The scientific questions raised by the issue of size effects on mechanical properties are many fold: one has – as always in nanoscience - to question how the basic theories we use at the macro- and meso- scales (plasticity, continuum elasticity, etc) apply at the nanometre scale. But studying mechanical properties of nanosize objects challenges also the experimental tools one needs to use: how to implement reproducible and controllable mechanical loading? How to measure fields (displacement, stress, strain, etc) with the required nano-resolution? Moreover nanoscience is often tackling the limits of continuum theories and thus simulation is an increasingly important tool to evaluate the different scale changes needed (from atoms to nano-objects). Finally most nano-objects are man made and the way they are grown or fabricated greatly influences their properties. Last but not least mechanics at the nanoscale is an important issue in various technologies. This concerns the reliability of the devices but also the enhancement of performances caused by strain: it is rather obvious when dealing with nanoelectronics or nanosystems but it is also important in coatings or in metallurgical alloys (nanoprecipitates are key for enhancing mechanical performances). This is therefore not a surprise that industrial partners (STMicroelectronics, St Gobain, Arcelor Mittal) have wished to join the network.

During the fall of 2010 MECANO's achievements and prospects have been analysed [http://www.im2np.fr/GDR-Mecano/rapport_MECANO_2008_2010.pdf]. Clearly the scientific questions raised are not exhausted. Moreover a clear need for formation of young scientists has appeared. On the other hand extending the network beyond French borders appears as an imperious necessity: our foreign colleagues have developed strong and complementary expertises. Moreover a number of MECANO members already have strong collaborations abroad and it would be extremely beneficial to share these partnerships. Such reflections have been submitted to the CNRS committees and the reports they gave have been very positive. This is the reason why we are submitting this proposal for an international CNRS research network focused on "Mechanics of Nano-objects".

The scientific project has been drafted by scientists from MECANO around four main themes:

1) Mechanics in small dimensions: elasticity, plasticity and fracture (*L. Thilly, E. Barthel, N. Combe, M. Legros*).

2) Experimental methods: local fields mapping and mechanical testing (*O. Robach, F. Amiot, MJ. Casanove, S. Labat, M. Verdier*).

3) Modelling and simulation: from angstroms to microns (*B. Devincre, H. Proudhon, L. Pizzagalli*)

4) Coupling between growth, stress and composition in nano-objects (*A. Ponchet, G. Grenet, F. Glas, P. Müller*)

These four topics are indeed strongly coupled but they offer a convenient way to organize the scientific life of the network.

Marseille, July 27 2011.

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SCIENTIFIC OBJECTIVES

I. Mechanics in small dimensions: elasticity, plasticity and fracture

References are listed in paragraph I.5

I.1. Context: why do we need to quantify and understand the mechanical response of small scale objects?

a) Technological impact

During the last 60 years, the continuous miniaturization of electronic devices has paved the way to the fabrication of small scale objects. Major improvements have resulted from new techniques for deposition, lithography and etching. Micromachining has also emerged as a powerful tool. For example, the focused ion beam (FIB) microscope offers both high-resolution imaging and flexible microfabrication in a single platform [1].

Small scale components are now used in a large number of applications in the form of thin films and multilayers. Small-scale structures, which lie at the core of microelectronics devices, are presently being developed for a much larger diversity of applications such as nanocomposite materials for wetting and adhesion control. Miniaturized and even nanoscale electro-mechanical systems (MEMS and NEMS), with micro- and nano- actuators and sensors are used increasingly for microelectronic and micro-optical applications. It can be anticipated that a growing number of applications will rely on small-scale structures generated at surfaces or interfaces or individual small scale objects. Enabling these emerging technologies requires full knowledge of the mechanical response of small scale objects which is still poorly understood. Indeed the materials these nano/microstructures are made of may strongly depend on the deposition/fabrication process. For example, due to the use of fast elaboration processes at moderate temperatures, thin film materials are often in metastable states, with no equivalent bulk structures; temperature, applied stress or strain, etc., are driving forces that possibly lead to strong relaxation processes; additionally, the mechanical properties are very much dependent upon the size of the structure. Therefore, in order to ensure proper fabrication, functionality and durability, an advanced knowledge of the mechanical response in relation to deposition and fabrication processes is needed.

b) Fundamental knowledge

For well-identified material structures, understanding the mechanical response of small scale structures is still a scientific challenge. Indeed the concept of “size effects” has been introduced nearly 60 years ago, first with “intrinsic size effects”, when it was observed that a reduction of the size of the materials microstructure (e.g. grain size) leads to increased yield strength [2, 3]. Several models have been developed to explain this so-called “Hall–Petch behavior” in terms of spatial confinement of dislocation against grain boundaries (pile-ups) but the debate on the origin of the Hall–Petch strengthening is still vivid [4, 5]. Other mechanical properties are modified by the reduction of the microstructure size such as fatigue and fracture strength [6, 7].

Size effects can also be induced by reducing the dimension of the probed structure: such “extrinsic size effects” have been evidenced also 60 years ago by the pioneering work of Brenner on whiskers [8]: when the diameter of these single-crystalline and defect-free filaments is decreased down or below the micrometer, the yield strength increases and approaches the theoretical strength of perfect crystal.

Small scale deformation is thus becoming a mature field of investigation for i) applications in MEMS and NEMS (MEMS can also be used as fundamental test platforms - see below), ii) uncovering fundamental aspects and elementary deformation processes in crystalline or amorphous materials that cannot be studied in macroscopic samples (e.g. dislocation nucleation processes, critical scale under which the linear elasticity theory fails to describe systems, etc.) and iii) targeting specific microstructure features (e.g. specific crystallographic orientation, grain boundary, etc.) and their individual impact on macroscopic mechanical properties.

I.2. Outstanding recent experimental results (techniques are developed in topic II, modeling in topic III)

The main questions that have recently been addressed by the community aim at a better understanding of how a system responds mechanically when its size becomes on the order of the defects responsible for its bulk properties. The defects are the surface relaxation extension for elasticity, dislocations for crystal plasticity, critical volume for plastic instabilities in glasses or cracks for toughness. Challenges originate from the experimental need to create specimen and test them at the relevant scale with state-of-the-art techniques, each of them being dedicated to probe a particular property.

a) Elasticity, residual strain

The case of elasticity is peculiar: since there is no characteristic length in linear elasticity theory, no size effects are expected. However, beyond the linear elasticity model, the surface or interface introduces a characteristic length of the order of few nanometers (order of magnitude of the penetration of the structural perturbation induced by the surface/interface): size effects on elasticity are thus expected for structures of the order of one to a few nanometers. And indeed, most of the theoretical (often numerical) studies predict some size effects under few nanometers [9].

The validity of linear elasticity at small scale can be probed through direct measurements of strain-stress curves, by measuring confined or resonant acoustic vibration frequencies directly in a microscope [10], or through vibration (Raman or time-resolved) spectroscopy [11-13]. Surprisingly, experimental results are very sparse. While the two first types of techniques report some size effects for objects up to hundred of nanometers [14, 15], vibration spectroscopy experiments report no effects even for structure size down to 2nm [12] and have up to now never evidenced any difference with the predictions of the linear elasticity theory. The size of the probe remains however a problem to capture the response of individual objects and to avoid the broadening of the results by the distribution of a collection of nanoparticles. Some recent developments in vibration spectroscopy experiments have enabled probing single nanoparticles in the range of tens of nanometers.

Besides these techniques, x-ray beams produced by synchrotrons have become sufficiently small and intense to detect variations of the lattice parameter in tiny structures (hundreds of nanometers) [16, 17], and even to reconstruct strain maps in 3D [18].

It is also worth noting that residual strains in coatings may be a major source of reliability in industrial products. On the one hand, relaxation of the ensuing stress during fabrication or service results in unwanted cracks [19], delaminations or shape distortions. On the other hand, shape distortions can be harnessed to fabricate specific devices [20]. In this area, understanding the build-up of residual strain has made significant progress in polycrystalline structures using white beam X-ray micro-diffraction [17].

b) Plasticity

Nanoindentation of surfaces is a versatile technique used to obtain mechanical properties at the nanometre scale [21] and is especially useful to study the very early stages of plasticity. Combined with FIB machining, this approach out sprung the pillar test that consists in the uniaxial compression of FIB-made micrometer size pillars using a flat-ended tip nanoindenter [22, 23]. This methodology provides stress–strain information of the sample, supposedly without strain gradients. The now famous experiment from Uchic et al (2004) triggered a renewed interest in the field of small scale plasticity as it pointed too very strong size effects without any apparent confinement of defects. It lead to an impressive mass of publications around pillar testing (for a recent review, see [24]) and the supposed new mechanical properties and plasticity mechanisms imposed by the size reduction of any material (single and polycrystals [25-27], pure metals [28], alloys [22], nitrides [29], semiconductors [30], glasses [31]). Several observations were reported from such compression tests:

i) the yield strength rises significantly when the pillar becomes smaller (in particular for pillar diameters below 20 µm);

ii) the plastic deformation proceeds intermittently via serial strain bursts.

An international effort was undergone to explain the observed size effect: in particular, the early model of “dislocation starvation” [32] associated to defect-free micro-pillars was revisited and arguments on the stochastic nature of plasticity are still being debated [33-36].

The mechanisms responsible for pillar and small-scale objects can be revealed by transmission or scanning electron microscopy (TEM, SEM), and especially in-situ SEM/TEM that allows one to follow dynamically a given micro-or nanostructure being deformed**.** Miniaturization of actuators and sensors lead to the implementation of true mechanical tests (establishment of a complete stress-strain curve) inside SEM and TEM, combined with structure evolution monitoring. This will to adapt the test structure to the sample size is also followed by researchers designing MEMS aiming at performing complete tests (strain and stress measurement) on free-standing thin films [37, 38] and wires [39-41] inside electron microscopes or synchrotrons.

A common ultimate goal pursued by all these studies is to capture in a single experiment the mechanical response with sufficient precision to measure the elastic and/or plastic properties and at the same time monitor the changes at the atomic scale imposed by the external stress. This combination has only been partly reached so far, in very particular cases. Minor et al. were able to record a compression stress-strain curve on 200 nm pillars inside a TEM, but the image resolution did not allow fully following the evolution of the dislocation structure [42]. Those mechanisms were followed more precisely in another experiment, without being able to record a stress-strain curve [43].

The mechanisms that are currently tracked therefore address the nucleation or the multiplication of dislocations [44, 45], a field where simulations have gained a true edge [46, 47]. To reach such a precision, experimental investigations are still fighting possible artifacts, such as the structure modifications induced by FIB machining [48], or the internal stresses resulting from growth in thin films for instance.

In nanocrystals, the interplay between grain boundaries and dislocations produce extremely complex responses and the variety of investigation techniques, processing routes and characterization tools have lead to different interpretation of the role of this interplay. Grain boundaries and especially twin boundaries are alternatively supposed to block or nucleate fresh dislocations, depending on the grain or the twin size [49]. There too, simulations are necessary to discriminate the main processes at responsible for the onset of plasticity [50].

c) Toughness

These recent experiments have emphasized the seminal and early work from Brenner on whiskers, where the absence of initial defects lead to stress close to theoretical ones for Copper, Gold or Nickel micro wires [51]. Such theoretical stresses have been attained recently in nanowhiskers [52] and underlined the critical importance of the initial defect structure. Whiskers, deform elastically before failing abruptly, without any evidence of plasticity. These observations confirm that the nucleation of the first dislocations in a crystal free of any internal defect occurs at stresses much higher than in FIB-made structures [53, 54]. Similarly for amorphous materials, 2-point bending experiments on pristine fibers have revealed rupture strains as large as 18 % for silica [55]. This is certainly unexpected for a reputedly brittle material, and points to our poor understanding of the intrinsic deformation mechanisms of these amorphous materials. In particular it is not yet possible to assess whether intrinsic failure is purely brittle or if it occurs through mechanisms related to small scale plasticity.

Interfaces and surfaces also play a significant role in this area: it has been shown recently that surface effects couple to the mechanical response of the bulk in non-trivial ways. The case of metal film adhesion is exemplary: if the film thickness is reduced, adhesion drops because of the limitation of the plastic dissipation through confinement ("size effect") [56, 57]. Interestingly, the system geometry can lead to more complex loadings: it has been shown how a film resistance to cracking can be improved if the film is elastically decoupled from the substrate by an adequately chosen interlayer [58].

I.3. MECANO 2008-2011: contributions to the field and scientific locks

During the past 4 years, the MECANO network has organized several workshops and schools where different issues in relation with small scale deformation mechanisms were discussed. In particular, the present topic has been in depth discussed at the winter school “Mechanics of nano-objects” (14-19 March 2010). More specialized workshops were devoted to this thematic, in particular i) workshop “surface elasticity” (13-14 November 2008), ii) workshop “modeling, characterization and functionalization of surfaces for micro-nano-manipulation” (15-16 June 2010), iii) workshop “Adhesion and wetting” (scheduled 6-7 october 2011), iv) workshop “vibrational properties of nano-objects” (scheduled november 2011).

During these meetings the latest findings (listed in paragraph I.2) were presented. Clearly these results are promising but also show that there is still a long way to go before a full understanding of the mechanical response of small structures. The discussions brought new ideas/new approaches to nail down the following open questions and initiate some answers as developed in paragraph I.4.

I.4. Perspectives for the next years

Concerning elasticity, on the one hand vibration spectroscopy experiments on nano-objects show no size effects and theoretical results predict rather accordingly size effects only below very few nanometers; on the other hand, experiments performed on nanowires reveal size effects under tens or hundreds nanometers. The discrepancies between all these results need to be clarified. Especially, the interpretation of experiments performed on nanowires needs further investigations to uncover the respective role of the nanowire surface/interface and the one of the experimental set-up. In this context, vibration spectroscopy experiments need to be extended to nanowires to probe the properties of single nanometer scale characterized objects.

Concerning plasticity (including fracture) of nano-objects, hot questions deal both with the preparation/characterization of the samples and the investigation of the elementary deformation mechanisms. The role of the initial microstructure and defect density on the experimental results need to be revealed, and notably, the effect of the small scale samples preparation methods, e.g. FIB milling or growth technique. The role of surface/interface, especially for dislocations nucleation, need to be quantified with respect to the internal sources of dislocation. Of course, such role shall depend on the precise surface/interface state and/or on the boundary conditions in small scale tests. Besides, nanostructured materials also reveal plasticity by grain boundary motion that needs further characterization.

The resolution of these controversies will rely on the design of specific experiments to uncover particular aspects of i) material structure and ii) deformation at the local scale. Concurrently the experimental results need to be related to simulation studies to uncover the elementary deformation mechanisms at the atomic scales. Plasticity mechanisms under mechanical stress and thermal stress must be also compared. Note that a more explicit description of interfaces (extending beyond the mere free boundaries they are often restricted to), will also be needed at least for proper inclusion of rupture effects at the relevant scales. Finally, both elasticity and plasticity investigations need to be completed on well known crystalline structures (fcc, bcc, hcp, etc.) and extended to amorphous materials or glasses. The latter extreme case will surely benefit from and, in some cases, drive research in these areas.

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II. Experimental methods: local fields mapping and mechanical testing

II.1. Context

The experimental techniques of interest for the GdR are numerous. Among them are those that allow:

- to characterize the internal or near-surface structure of an object

- to apply a mechanical load to it

- to measure the object's response to the load, either global or local (field measurement), possibly in situ.

Experimental techniques were addressed during several specialized workshops of the MECANO GdR, in particular “white beam micro-diffraction” (24-25 September 2009); workshop “measuring fields at small scale” (9-10 December 2010), “characterization and functionalization of surfaces for micro-nano-manipulation” (15-16 June 2010), and during the winter school “Mechanics of nano-objects” (14-19 March 2010).

The aim was, not so much to offer a catalogue of examples of application, but rather to "open the black-boxes", in order to allow non-experts to grasp the hypotheses used to convert the results of raw measurements into physical results.

A summary of the current trends and prospective for the next years is given below for several approaches.

II.2. Mechanical testing techniques and their applications to nano-objects

II.2.1. Goal of the measurements

Mechanical tests are designed to allow for identifying the mechanical behavior of the object, that physically describe its strain response to applied stress or temperature. Measurements fall into two classes:

- the ones at low strain (a fraction of the interatomic distance, exploiting atomic vibrations), that aim at establishing elastic properties

- and the ones at higher strain, that allow to characterize irreversible behaviors (plasticity and rupture).

For these measurements, both the dimensional metrology of the samples and the type of applied load are critical. Indeed, boundary conditions (the object's morphology and its clamping to the loading system) need to be established and validated. For appropriate identification of behavior laws, simple tests are the best adapted, the first two tests on the complexity scale being tensile and bending uniaxial loads.

II.2.2 Contribution of the MECANO GDR 2008-2011

A first overview of the different methods for mechanical testing was drawn by the GDR during the plenary meetings and workshops ("characterization and functionalization of surfaces for micro-nano-manipulation" 15-16 June 2010), and during the winter school "Mechanics of nano-objects" (14-19 March 2010). It highlighted the small number of complete studies of mechanical properties, the frequent apparent contradiction between results (e.g. ZnO nanowires whose elastic properties change with the technique, either Raman (small strain) or bending/tensile testing), the lack of fine structural characterization of the tensile test specimens and the lack of variable-temperature studies (almost all the tests are carried out at room temperature).

Recent measurement techniques were described, in particular, for the elastic domain, Raman, Brillouin and picosecond ultrasonics measurements (IEMN), whose advantage is the absence of contact with the sample, and, for large strains, the use of integrated devices (UC Louvain la Neuve).

II.2.3. 4-5 year perspectives

The need for comparative Round-robin tests, measuring the same sample by different techniques, was clearly identified. Structural characterization (for instance by the means of electron microscopy or synchrotron radiation) should ideally be performed in situ, during elaboration and during testing. The effect of the method used for transferring the sample onto an integrated experimental setup should be established.

Bringing in the discussion specialists of experimental techniques of contact mechanics and adhesion should give ideas to better control the contact between the loading device and the sample, for sample shapes that can not be optimized to limit the influence of this contact. A step in this direction was taken with the "Robotics" workshop ("characterization and functionalization of surfaces for micro-nano-manipulation" 15-16 June 2010), and will be continued in September 2011 with the "adhesion-bonding" workshop.

The need was also highlighted to perform a large number of tests to obtain results that are statistically significant. This calls again for closer collaboration with high-technology platforms, to develop methods allowing to parallelize the tests.

II.3. Local structural characterization: field measurements

For the present description, the local characterization techniques are separated (arbitrarily) between the ones analyzing **a single object** (ex: grain, bicrystal, transistor, single nanowire or quantum dot…), and the ones analyzing a large and complex **collection of objects** (polycrystal, collection of nanoparticules…). Several of the current developments aim at increasing the overlap between techniques in terms of the range of samples that can be studied. This in order to allow coupled studies by two different techniques (ex : extending

Digital Image Correlation to high spatial resolution combined to low strain, and extending diffraction to high accuracy on elastic strain for large plastic strains).

The ultimate aim is to map both irreversible and reversible atomic displacements, as well as the composition, and the state of stress.

II.3.1. Contribution of the GDR 2008-2011

Workshops were devoted to “white beam micro-diffraction” (24-25 September 2009); “measuring fields at small scale” (9-10 December 2010), “characterization and functionalization of surfaces for micro-nano-manipulation” (15-16 June 2010). Specific lectures on X-ray diffraction and TEM were also given during the winter school “Mechanics of nano-objects” (14-19 March 2010).

The interaction between specialists of the different techniques gave rise to several projects aiming at:

- comparing quantitative results obtained by different techniques (ex: micro-Laue, TEM, EBSD)

- simultaneously coupling two or more types of measurements (ex : Digital Image Correlation (DIC) and micro-Laue, AFM and microdiffraction)

- applying new mathematical procedures for data analysis, inspired from the ones routinely used for another technique (ex : for stress measurements by micro-Laue in strain-hardened samples).

- introducing new data analysis methods stemming from much broader signal processing theories (ex: coherent diffraction and "restoration" methods)

The discussion between the "surfaces and nano-objects", "mechanics", "physical metallurgy" and "plasticity" scientific communities enabled the participants to better grasp the physical objects "seen" by each technique, and the associated filtering that artificially enhances one particular structural phenomenon among the several simultaneously present in the sample (ex of the dislocations that are barely visible in classical x-ray diffraction and highly visible in TEM or coherent diffraction).

The GDR also allowed to reinforce starting collaborations between experimentalists and theoreticians / "simulators" by making the first more familiar with the language of the latter and the other way round.

II.3.2. Multi-object techniques: state of the art and prospective

The techniques for ***numerical digital image correlation*** (DIC) developed during the last decade allow to measure the 2D displacement field induced by a plastic or elastic strain (> 10^{-4}). They provide a wealth of information on the kinematics of the mechanical test, with high data collection speed. The fastest version uses 2D optical images (with or without a microscope) (best spatial resolution 5 microns), while more elaborated versions allow 3D measurements (x-rays + tomography) or better spatially-resolved 2D measurements (using SEM images).

The information that is obtained is used to check boundary conditions, to perform heterogeneous tests [1] or to identify material properties or constitutive models [2-5].

The techniques for identifying behavior laws from macroscopic scale measurements are already well developed. In recent studies, the reference / strained image pair is analyzed using a finite-element type grid for discretizing the displacement field. This lowers the noise on the measured displacements by forcing them to comply with the continuity conditions imposed between the elements. This type of irregular mesh allows to correctly grasp the phenomena occurring on very different scales (ex: progress of a crack-tip, large discontinuities of displacements at the interface between two Portevin-Le Chatelier bands), and to easily compare the results with numerical simulations. User-defined basis functions can be introduced to add a priori known specificities of the mechanical behavior into the analysis. The parameters of the model (ex: x,y position and stress intensity factor K of a crack tip) may be directly adjusted on the raw data.

This contrasts with the still relatively "visual" comparison between experiment and theory for "crystallographic" field measurements on polycrystals. A perspective would be to adapt the identification techniques originally developed to exploit displacements field data, in order to allow them to exploit crystallographic fields data. The use of DIC on SEM images for better spatial resolution is also an ongoing development.

"Crystallography" field measurements have significantly developed recently, with the progress of x-ray Laue microdiffraction [6], of 3DXRD [7], and of diffraction contrast tomography [8] (on synchrotrons), and the development of high-angular-resolution EBSD [9, 10] and Kossel microdiffraction [11, 12] (in the SEM). These techniques provide a measurement of the local average crystalline unit cell (and consequently the orientation and the elastic strain tensor), and for some of them the deviations of the unit cell with respect to the average, inside the small probe volume (due to orientation and elastic strain gradients, related to plastic defects and elastic lattice curvature).

Laue microdiffraction (with local measurements at the submicron scale) benefited of several developments: - the adding (ongoing at ALS and ESRF) of in-depth spatial resolution (initially only available at APS), - the writing of an open source data analysis code (ESRF) which contributed to open the discussion on analysis and uncertainty sources (see : LaueTools on SourceForge web site), - the setting up of a technique to measure 2D maps of the full strain tensor (and not only the deviatoric) (ESRF). The technique also benefited from the collaboration with specialists of plasticity, with ongoing projects to directly calculated Laue patterns from dislocation dynamics simulations (Capolungo et al, Daveau et al, TMS 2011), and from the discussion with the specialists of DIC, to apply the differential method used in EBSD to the measurement of elastic strain gradients in crystallites too damages to apply the "absolute strain" version of the technique (Castelnau et al TMS 2011).

Conversely, HR-EBSD may benefit from geometry calibration procedures developed for Laue microdiffraction, in the quest to render elastic strain measurements absolute.

The extension of accurate stress measurements to materials with strongly damaged grains, which represent most industrial materials, is still in progress. The discussion between the members of the GDR about the current restriction to very well crystallized materials clearly favored the emergence of ideas to make the technique evolve.

The coupling with the measurement of composition fields is still in need of development. In alloy polycrystals, the conversion of the "unit cell" field into a stress field requires an hypothesis on the reference state and on the elastic properties. The existence of composition gradients (linked for example to segregation to grain boundaries), and of the associated gradients of lattice parameters and elastic / plastic properties will affect this hypothesis, and therefore the stress results. The workshop on "coupling between growth, composition and elasticity" (16-17 june 2011) allowed to start the discussion on this theme, mostly at the nanometric scale, based on studies of epitaxial structures. In the future it is desirable to extend the discussion to polycrystals, in particular by developing the practice of coupled field measurements (mechanics + composition).

Compression of results is also a crucial issue, in particular the question of which formalism to use to compress results from maps of complex fields (ex : tensors), to reduce them to a small number of scalar quantities, as can be done in fluid mechanics or optical image analysis (ex : D. Jeulin, Mathematic morphology laboratory in Meudon). The data compression is a key point to attempts to quantify the comparison between two complex samples, or between a sample and a simulation. Collaboration with mathematicians and numerical simulation specialists will be crucial.

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II.3.3. Single-object techniques: state of the art and prospective

These crystallographic techniques, which include coherent x-ray diffraction imaging and TEM / STEM, provide intra-object field measurements with a very high spatial resolution.

X-ray coherent diffraction [1-6] provides the field of 3D positions of the atoms (and therefore their displacements) and the occupancy field of the atomic sites (object's shape) in an "isolated" nano-object (its diffraction signal needs to be isolated from the one coming from the rest of the sample). The information on the displacement field is therefore similar to the one obtained in 2D by TEM, but with a spatial resolution around 2 nm. The determination of the displacement field is recent, the earlier experiments providing only the object's shape (imaging). A recent experimental advance is the use of energy scans instead of angular scans to obtain the 3D signal, which facilitates the data acquisition, the sample motion not being necessary anymore.

Future developments point towards the analysis of signals coming from less perfect nano-objects that may contain several plastic defects, and possibly composition gradients. A possible opening toward a method for data analysis alternative to the Gertchberg-Saxton algorithm emerged during the "field measurements" workshop (9-10 december 2011) (cf. talk by D. Brie).

One of the greatest interests of **TEM/STEM techniques** is their ability to analyze single objects down to the atomic scale, and this goes from a single dislocation, interface or grain boundary to a single particle, nanowire or nanopillar. Well known for enabling the combination of structural and chemical information using the same instrument and on the very same spatial region, TEM/STEM techniques have included during the last decade more and more quantitative analyses of the images and spectra in order to provide more and more reliable mapping (elemental or chemical mapping, strain fields…) at the nanometer scale [7-14].

One question that still generates developments is the conversion of measured strain fields into "initial strain fields" (before sample cutting) [15]. A specificity of TEM analyses is the need for specimens transparent to electrons accelerated at medium voltages (typically 200 or 300keV), which often implies sample thinning likely to provide additional strain relaxation (thin foil effect including surface relaxation) [16]. Such effect can be taken into account provided a suitable modeling (typically finite element modeling) is simultaneously performed for comparison [17, 18]. Nevertheless the specimens after thinning are rarely fully characterized and more realistic sample geometry and boundary conditions (free surfaces, clamping…) should be considered in the modeling [19].

For alloys, the effect of composition gradients due for instance to segregation effects ("initial" or "cutting-induced") still needs to be included in the simulation of TEM images or spectra. Here atomic simulations may help to predict the presence of such gradients. Here, as in mechanical testing, a more accurate definition of the model (gradients, environment…) is mandatory, because we are dealing with nano-objects, thus largely influenced by surfaces and environment, but also because in the case of TEM different effects can produce the same kind of contrast in the images.

An important development is given by in-situ experiments from which highly valuable information can be expected. Indeed, progress in instrumentation (in particular enhanced mechanical and thermal stability) now gives access to in situ experiments with much higher resolution. Different solicitations can be applied, mechanical, chemical or even electrical ones.

In parallel to TEM, large efforts are now dedicated to analyses of single objects using **Raman and microRaman spectroscopy**. This technique will be particularly valuable to probe internal strains in single nano-objects [20].

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III. Modelling and simulation: from angstroms to microns

References are listed in III.3.

III.1. Context

Nowadays, numerical simulations have become an essential tool for investigating and modeling deformation mechanisms (both elastic and plastic) at small scale. Although simulation has been initially developed as a stand alone theoretical approach, it is increasingly used as a tool for interpreting experiments. It is especially important in the case of nanomaterials, where the experimental limits are often reached. As highlighted by the development of multiscale modeling approaches during the last decade, the various available simulation methods have different application domains.

Atomistic simulations (ab initio, MD, etc..) are the main tool for studying nanomaterials and are usually employed in the determination of elementary properties of solids (crystalline or amorphous), and their defects. Elasticity theory can be used for all materials, but the observed differences of mechanical properties between various systems will depend on the fine structure of dislocation cores or on different diffusional mechanisms, for instance. This is especially true for nanomaterials. Numerical simulations at the atomic scale are usually performed with a description of matter based on semi-empirical interatomic potentials. Although a more accurate description taking into account the electronic structure is possible (e.g. DFT, tight-binding), the computational cost of these methods prevents the use of models comparable to experimental systems, i.e. with dimensions larger than ten nanometers. Those approaches are however well suited for the study of elementary properties directly linked with the fine structure of defects [1-2]. A combination of molecular dynamic and interatomic potentials is therefore mainly employed in current investigations. It allows for investigating the system evolution in time considering the temperature and various stress states [3], thus making feasible "numerical experiments". Nevertheless, the time scales that can be reached with atomistic simulations are far from the experimental ones. This explains why the results of atomistic simulations are often used for fitting larger scale models, or to feed mesoscopic approaches better suited for a direct comparison with experiments.

Mesoscopic simulations, such as Kinetic Monte Carlo (KMC) or Dislocations Dynamics (DD) methods, have been more and more used in the last years. They are well suited for the modeling of nano-objects or nanostructures with complex boundary conditions (of morphology and/or loading). Space and time scales that can be reached with these simulations are much larger than for atomistic simulations [4-5]. Then a simple comparison with measured mechanical properties and microstructural observations is obtained. The discrete nature of these simulations allows for studying collective properties associated with localization and self-organization phenomena.

Finally, continuum simulation methods such as Phase Fields (PF) and Finite Elements (FE) methods can be used for fast and multiphysics calculations. With these methods, it is possible to perform studies taking into account simultaneously chemical (e.g. phase transitions) and mechanical (e.g. plastic deformation) processes, at submicron scales.

For domains of interest for the GDR MECANO, one can mention that simulations are mainly employed for the study of mechanisms and properties associated with a decrease of the material dimensions. A key issue is the influence of the system size on elastic and plastic properties, and the understanding of the associated mechanisms. For fragile bulk materials (semiconductors, ceramics, etc...), there is a growing interest for the study of a size-dependent brittle-ductile transition. More specifically, issues such as the determination of the onset of plasticity (dislocation nucleation, fracture activation,...), and plasticity propagation (dislocation avalanche, fracture mobility) are the focus of many studies. It is noteworthy that it is sometimes possible to compare the results from different simulation methods for the same phenomenon (a good example is the investigation of dislocation avalanches in micro-pillars [7-9]).

The simulated nano-objects are typically 1D, nanowires or nanopillars, because of the large number of dedicated experiments. There is also a research activity, albeit less important, concerning the mechanical properties of nanospheres. Finally, in a more general perspective, one could mention ongoing studies on the relation between interfaces and plasticity, which is at the heart of the mechanical properties of nanostructured materials.

III.2. Prospective for the next years

Important simulations problematic which are relevant to the GDRI project and for which there is still relatively few investigations, can be gathered in three categories. First, simulating realistic systems closer to the experiment is of interest. For instance, an important issue is an investigation of the influence of implanted species following a FIB fabrication on the properties of nano-object. Also, the development of more realistic boundary conditions in the simulations is essential. Secondly, one is interested in the modeling of systems dedicated to possible applications. For instance, in domains linked with the semiconductors industry, important issues could be the determination of the influence of the oxidation or passivation of nano-object surfaces on their properties. Besides, plastic relaxation processes in self-assembled monolayers is an emerging subject. Third, the need for new or optimized properties is in favor of more complex and innovative systems development, such as core-shell nanowires.

Furthermore, there will be an increase of the number of simulations dedicated to experiments interpretation in the next years. A characteristic example of such activity is the simulation of X-ray coherent diffraction measurements. Those experiments allow in principle to determine the strain fields of a crystal with a spatial resolution of 20 nanometers. Such a resolution requires complex calculations of inverse reconstruction that are difficult to realize without using numerical simulations [10]. Another example of simulation-experiment coupling is expected in relation with the recent progresses made in field measurements methods (see the proceeding of the “Atelier Mesures de champs aux petites dimensions” Besançon 9-10 décembre 2010). In fact, it is now possible to perform simulations with initial conditions reproducing many details of the material microstructure and the corresponding internal loading state [11]. Such simulations can then be directly compared to experiments to validate or fit theoretical models.

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IV. Coupling between growth, stress and composition in nano-objects

The bibliography can be found in IV.5.

IV.1. Context

Large efforts are devoted worldwide to fabricate new types of nano-objects, for fundamental studies as well as for applications (active zones in nano-devices and nano-systems). These objects often undergo internal stresses[1], but assessing the impact of stress on physical properties (magnetic, electronic, optical…) remains a difficult issue, because strain, chemical composition and morphology are intimately imbricated. Nano-objects will also increasingly be used as nanogenerators or sensors due to their remarkable properties, such as piezoelectricity, which are very directly related to their mechanical properties *[Yang 2009].* Numerous studies are also devoted to study size effects on the mechanical properties of nano-objects.

A main issue is that an actual nano-object cannot be described simply as a sampling of bulk material bounded by a surface or an interface. Nano-objects result from complex fabrication methods which make them different from bulk: (i) **Nanostructuration from bulk material** using electron beams, ionic beams, chemical etching… is likely to generate defects (implantation, crystalline defects, preferential etching, defect revelation, etc…). (ii) **Self-assembly methods** include a wide variety of approaches allowing the construction of the nano-objects from basic arrangements of atoms or molecules: growth processes, chemical synthesis, metallurgy….. As these methods are generally conducted far from equilibrium, the nanostructure differs from the equivalent nominal bulk structure, which in some cases does not even exist *[Glas 2007, Le Bouar 2011 and ref. therein, Ponchet 2011 and ref. therein]*.

As a consequence, there is a strong coupling between fabrication, internal stresses and mechanical properties.[2] Internal stresses, defects and elastic properties are intimately related to the structure and the chemistry, which are rarely fully characterized. The understanding of the elementary mechanisms involved in fabrication processes is therefore essential.

In this respect, it is necessary to evaluate quantitatively the influence of stress on the basic physical properties of nano-objects that have an impact on their formation, such as surface energy, chemical potential, attachment energies, diffusion lengths....

In addition, internal stresses play a role in many methods developed to organize nano-objects or structure the matter at the nanometric scale: either the internal stresses are generated by the structuration, or they are exploited as a driving force for structuration.

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[1] Internal stresses can be defined as the stresses existing without external mechanical solicitation and resulting from the fabrication process. Internal stresses are generated by any process inducing a crystalline heterogeneity (heteroepitaxy, non-epitaxial formation or deposition of another material (oxide, nitride, metal...), implantation, annealing…) or a structural discontinuity (surface stress).

[2] Mechanical properties of a material (Young modulus, yield stress…) can be defined as their elastic or plastic responses to an external solicitation.

Another important practical issue is to design and fabricate of nano-objects having specific mechanical properties (wires, structured membranes, MEMS, MOEMS....)

To summarize, the following topics are being investigated by the scientific community:

- Role of internal stresses in the formation of nano-objects and in their final configuration (size, shape, structure, inhomogeneities)

- Use and tailoring of stress to fabricate nano-objects

- In particular, possibility of fabricating nanostructures from materials which it would be impossible to assemble in bulk form

- Design and fabrication of nano-objects having specific mechanical properties, or else specific stress-induced physical (optical, magnetic...) properties (wires, structured membranes, MEMS, MOEMS....)

- Influence of stress on the basic physical properties of nano-objects that have an impact on their formation (surface energy, chemical potential, diffusion lengths, attachment energies....)

IV.2. Recent developments of nano-objects fabrication

At the international level, large efforts have been devoted to the development of new types of nano-objects. Let us mention in a non exhaustive list:

- Nanowires are now grown by various methods (vapor-liquid-solid epitaxy, evaporation, electrochemical synthesis...). Semiconducting nanowires allow a novel approach of strained heterostructures *[Glas 2007, Wang 2007, Landré 2010, Consonni 2011]*. Nanowires of various systems are also used for mechanical tests of size effects *[Park 2009 and ref. therein]*.
- Free-standing nanorods and nanoparticules of very small sizes (< 5 nm) are now currently fabricated by chemical synthesis. They can include a single phase or multiple phases *[Le Bouar 2011 and ref. therein]*.
- The so-called « origamis » 3D objects (roll-up, springs, cages, etc) are achieved by a stress relaxation mechanism of heterostructures induced by an etching process *[Songmuang 2006]*.
- Cage compounds, nanotubes and planar sheet structures (carbon, graphene, clathrates…).

IV.3. MECANO 2008-2011: contributions to the field

Several workshops organized by MECANO were very closely related to the issue of nano-object growth: « Elasticity of nano-objets » (Toulouse, November 2008), « Coupling between growth, stress and composition in nano-materials » (Marseille, June 2011), « Adhesion – bonding » (Lyon, September 2011).

During the scientific winter school “Mechanics of nano-objects” (14-19 March 2010), several lectures were directly devoted to the link between fabrication and mechanical properties.

Communications at the GDR meetings (for instance: Croissance de nanofils III-V: quelques mécanismes, Marseille 2008 ; Autogenèse de micro-nano-résonateurs photoniques 3D par relaxation de contraintes, Paris 2009).

MECANO has been a forum allowing specialists from various fields (physics, chemistry, mechanics….) to revisit the issues related to internal stresses and mechanical properties, through the role of fabrication processes.

It has been very clearly emphasized that size effects should be examined in the context of fabrication methods: one has to keep in mind that the actual nano-objects, as they results from fabrication and as they exist in functional devices, do not a priori obey to an ideal model.

This has been discussed in particular as regards the possible modification of elastic and plastic properties of nanowires and nanopillars compared to bulk material. It has also been underlined that the experimental studies of mechanical properties are most often conducted on nano-objects which have been specifically fabricated for this purpose and are somewhat simplified compared to those actually present in functional devices.

IV.4. Prospective for the next years

Some prospective issues have been identified for the next years:

- ***Investigating the role of internal stresses in the formation*** of nano-objects and in their final configuration (size, shape, structure, inhomogeneities)

The influence of the ***free surfaces and size effects*** on elementary mechanisms of growth should be investigated from a fundamental point of view *[Ross 2005, Chuang 2007, Schwarz 2011]*. This includes the stability of small-size systems *[Le Bouar 2011 and ref therein]*, the issue of competition between crystalline phases and the order-disorder transition *[Glas 2007, Patriarche 2008, Akiyama 2006]*, the order-disorder transition *[Alloyeau 2009],* the relation between elasticity, composition and growth in nanoalloys etc…

In addition, the modification of well-established mechanims (such as Volmer-Weber or Stanski-Krastanov *[Tersoff 1993]*) when growth occurs not on a bulk substrate but on a previously formed nanostructure is of great interest .

- ***Influence of stress on those basic physical properties of nano-objects*** that have an impact on their formation, such as surface energies, chemical potentials, attachment energies, diffusion lengths... These issues should orientate in this specific direction part of the work carried out in theme 3.

- ***Understanding the generation of internal stresses***

New or complex materials will be at the origin of new mechanisms of stress generation. Let us list for instance:

- heterogenous interfaces (oxyde/semiconductor, metal/semiconductor…) *[Saint Girons 2009]*
- nanostructured materials (nanocrystallites in glasses and amorphous oxides., porous materials…)
- structures with very large free surfaces ; in particular in nanowires and nanoparticles, it is expected that core-shell effects, phase demixing and misfit stress relaxation will be quite different than they are in "classical" (hetero)structures *[Glas 2006, Laneuville, 2011, Langlois 2008, Schmidt 2008, Raychaudhuri 2006].*

Another interesting issue is the subtle impact of fabrication on stress generation at very small scales, particularly in the vicinity of interfaces. Is it possible to modify the elastic energy excess associated to a particular interface, and modify its repartition (stress gradient across the interfaces), by the means of the fabrication process?

- ***Nanostructuration exploiting stress effects:***

The general aim is to use and tailor stress to fabricate nano-objects. Beyond the nowadays well established methods (Stranski-Krastanov growth, dislocations network…), new original methods will be developed; examples include:

- Tuning the so-called « origamis » objects ; it is noted that tuning the size and shape of the resulting *micrometric* objects will require a precise control of stress gradients in *nanometric* layers.
- Wetting/dewetting
- Self-organisation using surface acoustic waves *[Taillan 2011]*.
- Reorganization using post-growth process (annealing for instance): as the deposits are generally far of equilibrium, chemical reorganization induced by internal stress relaxation can be exploited to achieve new nano-objects *[Abellan 2011]*.

- ***Fabricating well-controlled objects to analyze size effects on mechanical properties***.

What is called "size effects" in these experiments should be discussed. Indeed, there are various effects which can be intrinsic in the size reduction or can be due to fabrication and manipulation *[Ponchet 2011 and ref. therein, Shim 2009]*. So the study of the surface as a possible actor of size effects – whether through the surface stress or as a source of defects – have to be carried out in well-controlled conditions of the surface state.

The actual boundary conditions which are related to elaboration and manipulation should also be determined carefully (rigidity of the clamping, free surfaces….).

- ***Design and fabrication of nano-objects*** having specific mechanical properties (wires, structured membranes, MEMS, MOEMS....)

To summarize, the following topics are considered worth investigating in the next 4 years :

- Role of internal stresses in the formation of nano-objects and in their final configuration (size, shape, structure, inhomogeneities)

- Use and tailoring of stress to fabricate nano-objects

- In particular, possibility of fabricating nanostructures from materials which it would be impossible to assemble in bulk form

- Design and fabrication of nano-objects having specific mechanical properties (wires, structured membranes, MEMS, MOEMS....)

- Influence of stress on the basic physical properties of nano-objects that have an impact on their formation (surface energy, chemical potential, diffusion lengths, attachment energies....)

- Design and fabrication of nano-objects having specific mechanical properties (wires, structured membranes, MEMS, MOEMS....)

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V. International partners in the GDRI project:

Based on the previous analysis and considering the existing collaborations as well as the complementarities between French labs and foreign ones the following list of European partners has been contacted:

- Gerhard Dehm et al. - Erich Schmid Institut , Montanuniversität, Leoben, Austria
- Johann Michler et al. - EMPA, Thun , Switzerland
- D. Raabe et al. - Max Planck Institute, Dusseldorf, Germany
- E. Mittemeijer et al. - Max Planck Institute, Stuttgart, Germany
- A. Wilkinson et al. – Oxford University, UK
- J. Boland et al. - Trinity College, Dublin, Ireland
- Helena Van Swygenhoven et al. - Paul Scherrer Institute, Switzerland
- H. Riechert et al. - Paul-Drude-Institut für Festkörperelektronik, Berlin Germany
- T. Pardoen et al. - Université Catholique Louvain, Belgique
- E. Bitzek et al. - Erlangen University, Erlangen, Germany
- L. Miglio et al., - University of Milano-Bicocca, Milano, Italy

They have given a positive informal answer to participate in the network. Considering the expertise available in Europe we have decided to confine the network within Europe.

PARTICIPATING INSTITUTES

As of July 24, 2011 28 French institutes and 11 European groups have expressed their interest for the network. They are listed below together with contact persons. The French partners were part of MECANO GDR 3180. Most of the European ones have already collaborations with French partners. They have been selected in order to bring complementary expertises in the 4 different themes, which have been described in the scientific project.

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ORGANIZATION

The network is aimed at promoting scientific discussions between the participants in order to spur research in the field of mechanics of nanoobjects.

To fulfil that purpose one general meeting and two specialised workshops will be organized per year. A school will also be organized every 2 or 3 years. All these meetings will be opened to scientists outside the network.

All these events as well as the proper circulation of information within the network will be organized by the network coordinator assisted by an executive committee.

Scientific Management Committee

The Scientific Management Committee is composed of representatives of the laboratories, and is limited to a single representative per laboratory.

The Scientific Management Committee is chaired by the Network Coordinator.

The Scientific Management Committee establishes a statement of the progress of the GDRI's work and assesses the budgetary resources to be requested by the Network.

The Coordinator may consult the Scientific Management Committee on any other question relating to the Network.

The Scientific Management Committee meets at least once a year, and whenever such is necessary, at the initiative of the Coordinator or of a third of its members. As necessary, with the unanimous agreement of the Scientific Management Committee members, these meetings may be held by teleconferencing or Visioconferencing.

Network Coordinator

The Network Coordinator of the GDRI is appointed by the Parties for a four (4) year term.

The Network Coordinator draws-up the annual scientific report and financial review of the GDRI to be sent to the Parties.

Executive committee

A small operational committee (around 10 persons) will be designated by the scientific committee on proposition by the network coordinator in order to assist the network coordinator in the day-to-day organization of the network. The executive committee shall meet at least twice a year. The executive committee shall comprise the 4 coordinators of the 4 topical groups: 1/Mechanics in small dimensions: elasticity, plasticity and fracture, 2/Experimental methods: local fields mapping and mechanical testing, 3/ Modelling and simulation: from angstroms to microns, 4/Coupling between growth, stress and composition in nano-objects.

FINANCIAL NEEDS

Taking into account the program aforementioned i.e.:

- One plenary meeting per year
- Two workshops per year
- One school every two or three years
- One meeting of scientific management committee per year
- Two meetings of executive committee per year

And considering that:

- some meetings can be organized on the same dates (e.g. plenaries and meetings of scientific committees).
- extra funding will be sought for schools

It seems reasonable to ask for a yearly funding of 50 k€, which amounts to 200 k€ for the duration of the GDR.