

# Accelerator Enabled Nano-Nuclear Materials Development

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#### Abstract

Nuclear renaissance isn't possible without the development of new nano-hetero-structured materials. A novel micro-hetero structure, entitled "cer-liq-mesh", nuclear fuel that self-separates the fission products from nuclear fuel, makes fuel reprocessing easier, allowing near-perfect burnup by easy fast recladding, being prone to improve the nuclear fuel cycle. Fuel heating analysis led to development of new direct energy conversion nano-hetero structured meta-materials resembling a super-capacitor loading from nuclear particles' energy and discharging as electricity, prone to remove 90% of the actual nuclear power plant hardware, increasing the energy conversion efficiency. Usage of ion beam recoil analysis is used to measure and prove the nano-grains' and nano-clusters' special properties, such as shape-enhanced impurity diffusion and self-repairing in cluster structured fractal materials. The nano-grain liquid interface is studied by ion beam simulation in order to develop a new generation of nuclear fuels with enhanced breeding and transmutation properties, able to directly separate the transmutation products, thus reducing the need for hard, hazardous chemical processes. Ion-beam channeling in material may be extended to neutrons and gamma rays, and using hybrid NEMS structures new applications may create novel solid-state nuclear reactor control reactivity system, radiation modulators for gamma, neutrino communication systems and ultra-light radiation shielding.

#### 1. Introduction

Nuclear era debuted in the spring of 1945, with a military application, that ended the WWII, and was subject for cold war arms race, that ended with MAD (Mutually Assured Destruction) [1]. Nuclear Power, far from being the most important application, appeared as a byproduct of this MAD race, when U.S. President Dwight D. Eisenhower gave a speech to the UN General Assembly in New York City on December 8, 1953, entitled [2] "Atoms for Peace" that was followed by program that supplied equipment and information to schools, hospitals, and research institutions within the U.S. and throughout the world, followed by NPT (Non Proliferation Treaty) of 1970s[3], scrapped de facto by the end of 2016 by Russia and China.

Since 1950s to 1990s Nuclear power thrived, starting from 1945, up to 1985, the number of operational nuclear reactor grew, up to about 440 operational nuclear reactors[4], as square dotted pink line with corresponding values showed on the right ordinate, but due to INES-7 nuclear accidents of Fukushima and Chernobyl, and other accidents plotted with orange diamonds, with the name of the location attached nearby in red for INES-7- high severity accident, brown for INES-6 - severe accident, and pink for INES 5 – accident - and dark pink for INES 4 – minor accident- the nuclear power development stagnated, and its decline followed post-Fukushima, as Fig. 1 shows.

Due to continuous safety improvements, the probability of an accident [4] declined by 2 orders of magnitude from 1950s to 2000, but still remained significant, as orange continuous zigzag



line shows, and its trend line plotted over with corresponding values on the right ordinate.

The accident probability that next INES-7 nuclear accident to take place by 2050s as the stair thick orange line shows that is scary for many governments, as Germany Japan which took steps to phase out nuclear power. On the plot, one may see with thin, blue dotted zigzag line commercial aviation fatality rate, with corresponding values on the left ordinate in blue, that is orders of magnitude higher than total causalities in nuclear power industry, the only difference is that by the radioactive releases nuclear accidents affects larger populations with invisible, hard to understand for them threats. On the right, overlapped is a pie, showing the main results of the nuclear accidents, and the meltdown and criticality dominates, showing that are real issues with nuclear materials.

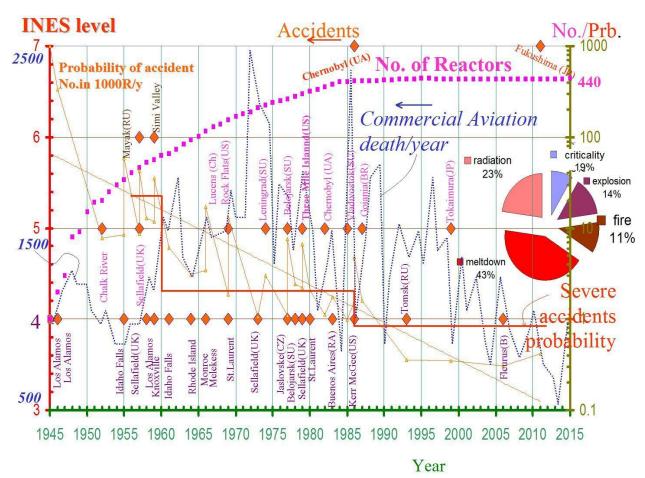


Fig. 1 Nuclear power development and accident probability compared to aviation

Therefore, now nuclear power is dying under economics hits, due to costly safety and security that makes nuclear power more expensive than fossil fuel power, politics under the pressure of bad public opinion, and nonproliferation paranoia. In this context people start to talk about nuclear renaissance, in spite the fact that actual nuclear power is not completely dead yet but seems to be in critical condition, in its last thoughts, and talk



about renaissance is inappropriate, and have to be replaced by "reinvigoration".

A hidden factor was the freeze of the technology and minds of nuclear developers and regulators. In fact, Nuclear Power was born too early, under the pressure of war, and was not in synchronism with appropriate material technology to support its development.

The problems in actual nuclear reactor were long ago identified and various solutions have been developed, but the research palette was very large, and hard to evaluate. By 2004, DOE confronted with a wave of fund cuts, and pressure from the corporations to maintain and extend the operation period for the existing reactors, for profit, with minor changes, decided to create the "Road Map to Generation IV", and to concentrate the funding on low risk, minor gain, smooth spending, evolutionary developments from 1970 old designs, and in reality to defund all new game changing, evolutionary projects, [5], but up to now none of the selected for funding solutions gave any significant change of course from decay of nuclear electric power, in order to prevent the need for a "renaissance". The conservative approach, nonproliferation fears and over regulations, NRC slow action but aggressive regulations kept out private investments. To this dare situation, nuclear accidents disclosed to public hidden aspects of mismanagement and flaws hidden in various designs that increased public's fear and rejection of nuclear electric power.

The lack of consistent funding for advanced materials able to support a real nuclear application development proved again that without advanced materials it is impossible to have advanced applications and new nuclear reactor generations, better than those envisaged by DOE, in order to perpetuate the actual state of things far into 2060, driving in fact to an extinction of nuclear electric power by that time.

#### 2. Actual nuclear reactor weaknesses

The research in nuclear materials was aimed to eliminate the issues identified in nuclear power applications since the early beginning, and the solutions found over the time improved gradually the performances, but only in the recent times, when nano-technologies and accelerator studies come stronger into play, significant developments become possible, that finally may materialize in novel generations of nuclear power reactors.

Using a combination of accelerator and nanotechnology specific knowledge, it was possible to conceive, test and develop new nuclear materials designs that may solve some of the major problems in nuclear power applications.

In order to perform successfully, one needs to understand above and beyond the related process.

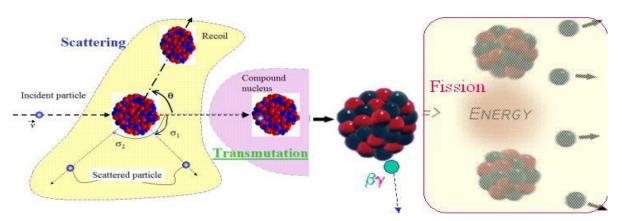
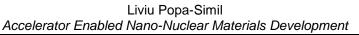


Fig. 2 Neutron induced nuclear reactions in Actinides





As Fig. 2 shows, Scattering, Transmutation and Fission are the main reaction possibilities for a neutron that collides with an actinide nucleus.

#### Nuclear Fuel damage by Fission products

Fission is the process happens mainly to actinides, where neutron capture triggers nuclear structure destabilization, which most frequently ends up with two radioactive isotopes and release of about 200 MeV (32 pJ) per fission act.

Fig. 3a shows neutron usage inside different type of components of a nuclear reactor at fuel at its midlife, with an average burnup factor. This neutron allocation makes difficult the breed and burn process, even inside travelling wave reactors, because in order to fission a fertile actinide as <sup>232</sup>Th or <sup>238</sup>U one needs about two neutrons, and as figure shows is a deficit of about 12% and a higher neutron multiplication rate that requires usage of <sup>239</sup>Pu, or another source of higher energy neutron is needed. The actual fuel performances, characterized by the red interpolation line, in Fig. 3b, have improved very little since 1960s, when those measurements were performed, and our goal is to move it towards the green dashed line. In the actual conditions no "near-perfect" burnup is conceivable without recladding, or novel radiation damage robust structural materials.

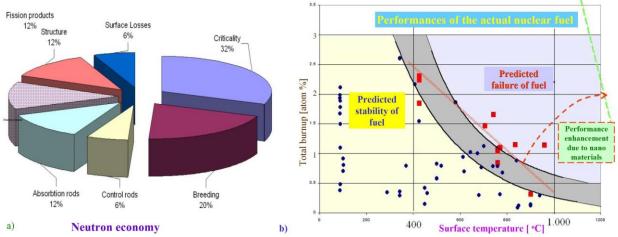


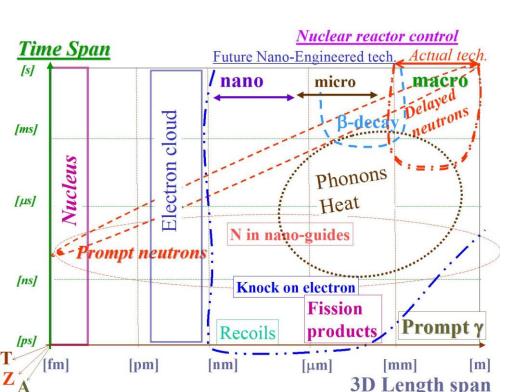
Fig. 3 Neutron balance and fuel performances; a) Neutron economy; b) Fuel performances.

### Fission products space-time features

Fission process basically performs inside five main places:

- Close neighborhood of the actinide nucleus that fissions, involving several atomic diameters, affected by the prompt products;
- Electronic stopping range of the fission products, taking several thousands of atomic diameters/size,
- End of the stopping range of the fission products, also called Bragg peak zone, characterized by a high dislocation density;
- range of fission products migration, characterized by frequent chemical structure changes following the FP decay
- range of FP decay by products effects





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Fig. 4 Multiscale-multidimension domain of main nuclear fission participant entities

Old "harmony" concepts may be applied to nuclear power too, but one needs the usage of nano-micro engineered nuclear materials in order to achieve a higher level of "harmony" among the process hosting structure and the agents of fission depicted in Fig. 4. This matching will be achieved via compatibility of action space and reaction time of the engineered structure with agents' features. Continuous red dot-dash-double line shows the actual state of the art, that has to advance up to the thick blue double-dotted line using micro-nanoengineered nuclear materials developed using common accelerator culture, and experimental equipment and infrastructure.

A holistic approach of the nuclear technology starting with materials basics up to nuclear reactor design, construction and testing is now required.

#### 3. Fission products as accelerated particles

As known from 1950s and 1960s measurements <sup>235</sup>U thermal neutron fission releases over time about 203 MeV, from which 167

MeV are in the form of kinetic energy of the fission products.

Fig. 5 shows that after absorbing a neutron, the compound <sup>236</sup>U is breaking into two symmetrical products relative to <sup>118</sup>Pd, process marked by the pink dashed line, and double blue arrow. Instantly, due to very high instability of the primordial fission products, few neutrons during the first fs after fission, split-off taking away about 8 MeV in kinetic energy, cooling down the fission product and forming what is called prompt neutron. After this, FPs follow sequences of betta decays, see the blue arrows, crawling towards stability region, marked by black dots, as isotopes stability map; data offered by http://www.nndc.bnl.gov/chart/ website. On the bottom-right is a chart, showing probability of occurrence distribution as function of atomic mass number "A", that is a 2D integral of the 3D isotope occurrence probability performed at some moment in time usually being placed between orange double line and stable isotope location. On the right is presented the case of



decay of a FP pair, starting with <sup>89</sup>Kr and <sup>144</sup>Ba, elements belonging to group 8 and respectively to group 2 of Mendeleev table, which after the chain of beta decays end up in stable elements <sup>89</sup>Y, group 3B and <sup>144</sup>Nd, a 4<sup>th</sup> Lanthanide, changing their chemical properties, atomic structure due to beta decay. Some time, in about 0.3% of the cases, the neutron does not promptly evaporate from the fission product but a little bit later, creating the delayed neutrons, so useful for nuclear reactor controllability.

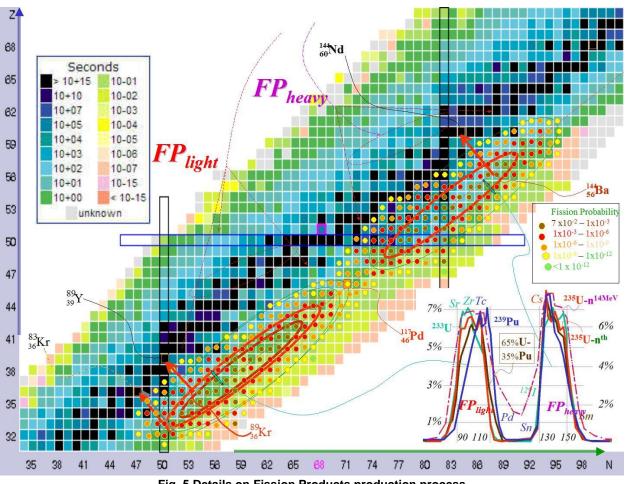


Fig. 5 Details on Fission Products production process

#### Fission products effects in Nuclear fuel

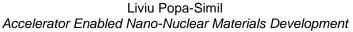
As one may see in Fig. 5 FP represent a very complex problem for nuclear reactor welfare, being the main cause of fuel's premature damage, power limitations and LOCA accident consequences, ending up in nuclear accidents as shown in Fig. 1 many ending in meltdown and FP release.

As previously shown, FPs take away about 8 MeV per fission in beta decay, makes nuclear reactor require intensive cooling after shut down,

as Fig. 6a shows. This is associated with about another 8 MeV for the antineutrino release, which is basically lost, from energy point of view, but may become useful in the future neutrino strategic communication and detection.

Low thermal conductivity Fig.6b,c and elasticity of ceramic fuel, corroborated with specific power deposition pattern, makes nuclear fuel crack at every power cycle, creating paths for FPs to reach





cladding and escape in the cooling agent, is briefly shown in Fig. 6d,e.

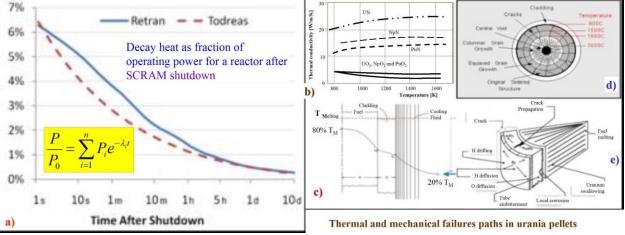


Fig. 6 – Actual fuel induced issues for thermal nuclear reactor safety a) –Decay heat after SCRUM; b) Thermal conductivity of nuclear fuels; c) temperature radial distribution in fuel cell; d) nuclear fuel failing mechanisms; e) pellet slice falling issues

In order to solve this problem is needed to better understand this nuclear fuel damage in its smallest detail and here the accelerator knowledge provided a boost.

#### <u>Accelerator knowledge use in FPs' behavior</u> understanding

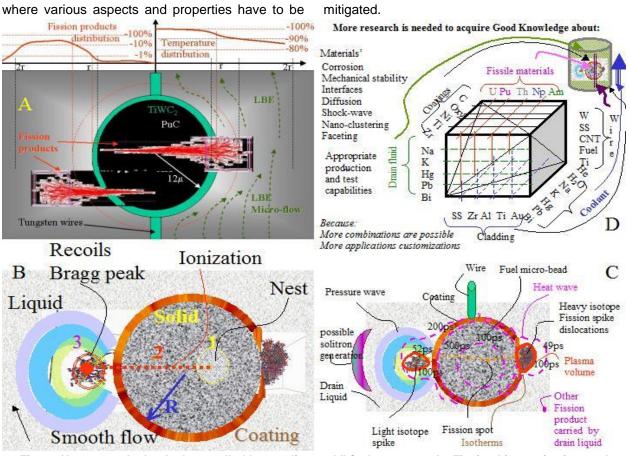
The analogy between FP and medium mass accelerated charged particles is outstanding.

after Immediatelv leaving the "close neighborhood" of the fissioned nucleus, that is of few lattice constants in radius, usually smaller than 1 nm, FP s behave like accelerated ion beams, hitting a material surface that is made of the fuel constituents, and Bethe-Bloch formula may be successfully used, in its modern form of SRIM MC code. This characterizes the interaction between charged particles and matter, respectively FPs and fuel, because much less than 1% of FPs have the opportunity to directly interact with fuel's cladding. Using SRIM it was possible to simulate and understand various aspects of the stopping of the FPs in the fuel and cladding, as shown in Fig. 7 and to develop new material structures able to avoid structural damage, and even more to be able to self separate the fission products from the fuel.

The novel design of micro-hetero structure exhibits exceptional other collateral properties that have driven towards a novel nuclear fuel structure generically called "cer-liq-mesh".

Fig. 7A shows the new design of metallic uranium 10 microns in diameter bead supported on a tungsten micro-wire immersed in a liquid metal. Inside the bead there are presented the trajectories of FPs stopping in that area. Stopping range is longer than bead's dimensions therefore FPs are stopping inside the liquid metal. Fig. 7B shows the main zones of the fission process, where "1" is the near-by zone, "2" is the ionization stopping range, and "3" is the recoil nuclei end of range, also known as Bragg peak. Fig. 7C shows the results of a molecular dynamics (MD) simulation, showing that the FPs' stopping process takes about 50 ps, there are about 100, 000 dpa for each FP. Because most of dpa take place in liquid metal, a cavitation-like explosion-implosion takes place and no remnant dislocation survives, only FP is immersed and bound to liquid, which is a great progress compared to solid structure where more than 10,000 dpa are left over each fission act. In Fig. 7A was given a constructive example, but Fig. 7D shows the real complexity of the problem,





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Fig 7 – Heterogeneity by design applied in "cer-liq-mesh" fuel structure; A –Fission kinematics in novel micro-bead structure; B - Processes in micro-hetero fuel bead; C - MD details on fision products effects; D -Material diversity to fabricate a fuel pellet.

The new fuel material produced using accelerator knowledge allows the construction of nuclear reactors with exceptional properties, where power density may be increased by a factor of 4, construction may be simplified, the fuel self separates the FPs that are easy to extract without using the actual chemistry, but simple thermomechanical procedures. Due to this easy FP extraction, separation and partitioning, followed by fuel usage, fuel cycle is drastically modified.

More, accelerators may be use to effectively measure the parameters of the new fuel, its reactivity and capability to self separate FPs based on fission reaction's kinematics.

#### 4. Nuclear Energy conversion in Electricity

During this analysis on heating mechanisms in nuclear fuel using SRIM and e-Casino MC codes showed that is possible to engineer a metamaterial that resembles a heterogeneous supercapacitor, that loads from the kinetic energy of the nuclear particle crossing it and discharges as electricity as shown in Fig. 8e.

Fig. 8a shows the case of an alpha battery meta-material, comprising of alternating layers, few nm thick, of high electron density conductors "**C**", separated by insulators "**I**" and "**I**" and low density electron conductors "**C**", repeated to cover the entire moving particles' stopping range. The idea is that during charged particle stopping process, the "C" layers will emit a large shower of knock-on



electrons than the "c" layers as the chart in top-left of Fig. 8a shows, in a SRIM simulation, that led to the meta-material capacitor like construction shown in Fig. 8e. Knock-on electrons interact with other electrons forming showers and are tunneling through the insulator layer and stop in the next conductive layer, polarizing the layers, as the e-Casino electron path simulation in Fog 8c shows. There are many materials that exhibit these properties, as the plot in Fig. 8d for few materials of interest showing ionization versus the relative stopping range. In the Fig. 8b there are shown main particles of interest, which exhibit stopping ranges in mm or less range, in order to harvest their energy. The chart shows the fission product energy distribution as function of abatement from the central mass, and shows that the lighter FP usually has higher energy and speed than its heavier partner.

This type of meta-materials may handle impressive power density in the range of kW/mm<sup>3</sup>, bout 1000 times higher than the actual nuclear fuel, based on heat flow power transport, based on phonons and electrons, because it may be interpreted as being dominant electron-based cooling. The amount of energy that was not removed by electric conduction has to be removed by heat flow, and that is a limiting factor in the acceptable power density.

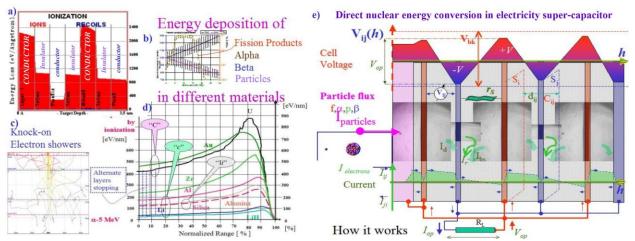


Fig. 8 Development of meta-materials for direct nuclear energy conversion in electricity a) SRIM Ionization simulation; b) FPs as accelerated ions; c) Primary knock-on electron trajectories; d) Ionization stopping power deposition in various materials; e) principle of direct nuclear energy conversion.

A single layer alpha battery made of this metamaterial using <sup>238</sup>Pu will look like a paper sheet being about 50microns thick.

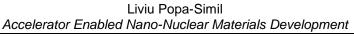
The research and development of this material intensively uses particle accelerators for material parameters optimization, energy conversion efficiency measurement, and construction, and was discovered during a failed accelerator experiment in 1980s.

## 5. Nuclear Transmutation Products Extraction and Fuel Cycle

A concurrent process in nuclear reactors is transmutation that is used in nuclear fuel breeding, or isotope production, process that currently involves intensive hazardous chemistry.

An alternative to this is the usage of nanobeaded hetero-structures, where nuclear reaction's kinematics as shown in Fig. 9-1, and nano-cluster enhanced diffusion properties are used to create a material with self-separation capabilities.





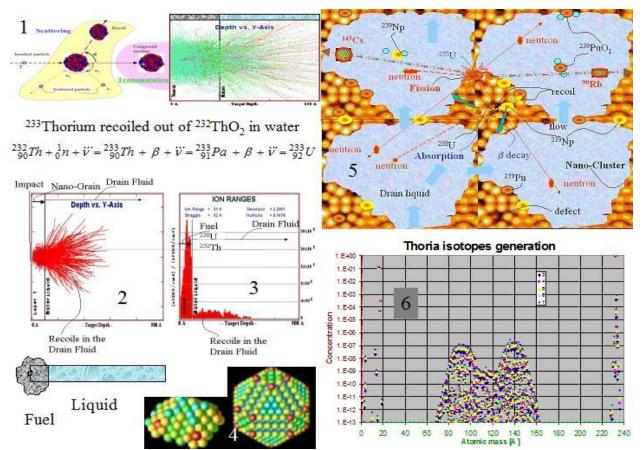


Fig. 9 – Mechanisms of separation in nano-beaded hetero materials: 1 – Nuclear reaction schematics; 2 – Recoils paths by SRIM; 3 – Ion ranges; 4 – Nano-cluster with impurities on interface; 5 – processes in a hetero naon-clustered structure; 6 – Th breeding inventory.

Fig. 9-1, is the first part of the process in Fig. 2, where after a neutron absorption, a compound nucleus is formed, that recoils a little bit from its initial position in the lattice, shown in SRIM simulation near by, where 5 nm thin foil of thoria covered by water have been considered, in order to mimic a nano-cluster. The chart "2" show trajectories of recoils in the structure shown under it, formed of a 10 nm diameter, nano-bead immersed in water while the chart "3", shows the distribution of recoiled particle density along the radius. In picture"4" it is shown a nano-cluster structure with some impurity atoms, in red, on surface. Picture "5" shows a section through a thoria hetero-structure, showing trajectories of main particles resulted in that reaction. Chart "6"

shows isotopic production calculated with ORIGEN code for thorium fuel.

In accelerator technology recoil implantation is a well known radioactive labeling process that works together with nano cluster mechanisms to produce direct separation of TPs.

#### **Nuclear Reactor Control**

The actual nuclear reactor control is based on electro-mechanical systems, that are slow and mainly uses delayed neutrons to control the process that makes reactor maneuverability low.

It is anticipated that using channeling process, discovered using accelerators by 1970s, where neutrons to be trapped and guided in nanostructures with capability to switch their trajectory using electronic controlled NEMS devices, to



produce more efficient nuclear reactor control reaction time by 1,000 times faster [6]. systems able to use prompt neutrons, making the

# Fundamentals

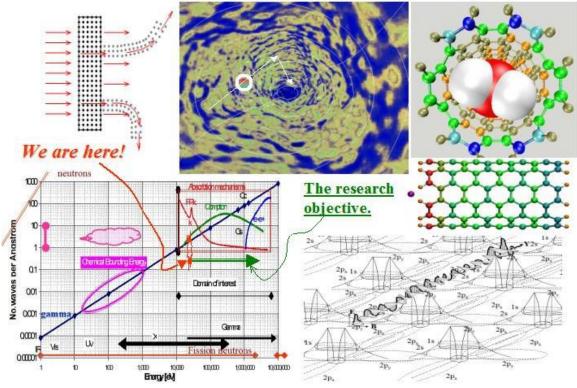


Fig. 10 - Principles of neutron channeling in nano-structures

Inside a nuclear reactor this control blanket made of guiding nano-structures may turn out coming neutrons into core to increase reactivity or direct them into an absorbent material for radioisotope production. Fig. 10 shows a layer of the blanket in upper-left side, and underneath a chart showing the number of wavelength per angstrom, showing overlapped the energy domain for nuclear applications. In top center is an ideographic view of the magnetic fields a neutron may encounter traveling inside a nano-tube. On the right side is shown a water molecule traveling inside a CNT, obtained by MD simulation. On the bottom-right is depicted a neutron associated wavelet traveling inside an atomic structure, and bouncing on electron orbitals magnetic moments.

Accelerators are further used to test this material, during construction, generating neutrons and gamma rays and using IBA technologies.

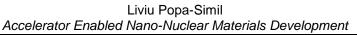
### Nuclear Reactor Structural Materials Degradation And Safety

Cladding material is seldom exposed to FP induced damage, but it is exposed to neutron and gamma rat damage that renders it unsafe after a burnup of less than 100MWDay/kg, that is not compatible with near perfect burning requirements, and recladding is needed.

A novel composite material made of immiscible fractions may be used instead.

This new material "NSICM" shown in Fig. 11 may not have the performances of stainless steel





but will assure the same performances over a large radiation dose, which will allow fabrication of a thicker cladding to offer same mechanical properties.

#### 6. Conclusions

Novel nano-micro engineered materials developed using knowledge gained in accelerator

applications will provide the necessary support for the development of new generations of nuclear reactors and advanced nuclear applications.

Accelerators will be further used during the research, production and test of the novel nanonuclear materials, and may be integrated in nuclear power structures.

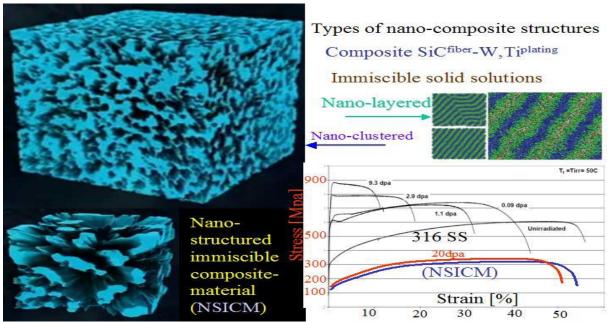


Fig. 11 Novel multi-phase material structure and anticipated properties

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