# ACCELERATORS USE TO ENGINEER NANO-MATERIALS FOR ENERGY

L. POPA-SIMIL
LAVM llc
Los Alamos, USA
Email: lps@lavmllc.com

**Abstract**

Starting from 1980 we looked for improvements in nuclear materials and the related energy devices with emphasis on materials. The novel nuclear materials for fission were developed in 5 families; each of them is intended to bring in harmony the structure with a nuclear agent active inside that material as:

- Micro-hetero structures, generally called "cer-Liq-Mesh" that self-separates the fission products from the nuclear fuel and minimizes their fuel damage, allowing breed &burn to near perfect burning; the fission products behave like medium mass accelerated ions, where the use of accelerators will help test the novel material structure and optimize it.
- Nano-hetero structures generically called "CIci", that form a super-capacitor, charged by nuclear energy and directly discharged as electricity; This structure has broad use for almost all moving nuclear particles except neutrons and gamma, and for each type of particle, the use of a similar accelerated one bring a valuable contribution to material selection and optimization as well to the entire structure test and characterization.
- Nano-clustered structure that enhances self-separation of transmutation products; where the initial idea was generated by UTLA method development, where the recoil energy is used for implantation, but because this energy inside neutron zones is small, nano-cluster enhanced selective diffusion properties are also used. Using low energy accelerators/implanters we may test various nano-clustered structures.
- Fractal immiscible materials with radiation damage self-repairing capabilities eliminating the need for re-cladding in near perfect burning structures. The dimensions of these structures may be optimized using ion-beams simulating the radiation damage inside nuclear reactors.
- Nano-structures with active NEMS used as fast control of nuclear reactivity by guiding neutrons in desired directions or ultralight shielding for mobile reactors. The guiding is similar to radiation channeling being possible to use ion-beams to test the NEMS operation.

## 1. INTRODUCTION

Civil nuclear power is in free fall due to the production cost competition with methane gas and renewables, safety and security issues and other drawbacks specific to the technology. It is not yet extinct but the guild is talking about its renaissance, ignoring that it is not about fictitious Phoenix bird, but a very real thing and its rejuvenation may be achieved only by solving its problems. The actual nuclear technology is 70 years old; it is mature, and any little progress becomes harder to achieve, therefore the nuclear power has to reinvent itself, and this is not hopeless. We know for about 2500 years, when first nano-material 'Damascus steel", has been unconsciously invented and used to make "Damascus swords" with exceptional properties, that materials determine the ultimate properties of the objects made from, and in this modern endeavour in nuclear materials accelerators plays a tremendous role, in inventing and perfecting novel micro-nano-hetero structures from idea to application, and they already did. Starting from 1980s we developed novel ideas for the betterment of nuclear power applications, which followed a spiral of evolution, as Fig. 1 shows, up to present when achieved TRL=3 (Technology Readiness Level), and prototypes should be built. The basic concept being the development were transferred from accelerator practice, and helped the development of 6 families of materials, each used to solve a nuclear reactor problem. The actual nuclear energy has lower CO2 emission, but because it is in its infancy, it is based on homogeneous "hot-rod" technology, it is complex, expensive and raises security and proliferation issues, has the potential for large scale accidents, and generates difficulties in dealing with waste fuel dispositioning.

The novel developed families of engineered nano-materials eliminate almost all the drawbacks of the actual nuclear power, rendering it among the most efficient and environmental friendly energy source. Developing and optimizing these novel energy materials require intensive accelerator use in fundamental knowledge development and structural optimization experiments. The use of these advanced materials in future nuclear energy related application will render a high efficiency, minimal nuclear waste, and optimal nuclear fuel cycle, isotope, fission and fusion "batteries", delivering the needed planetary clean energy at will for the next 10,000 years, and even more.

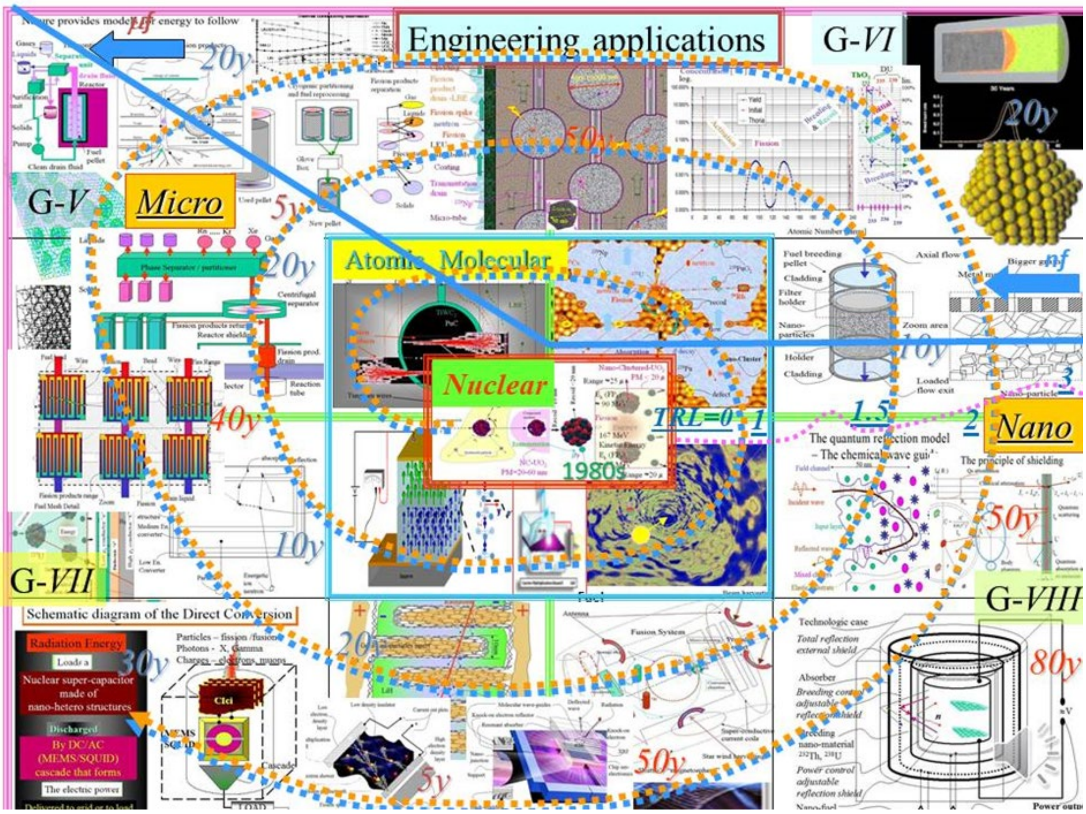


*FIG. 1 Engineered, nano-nuclear materials knowledge evolution from concept to application*

During the entire research period showed in Fig. 1 with a spiral of evolution accelerators had a primordial role in conceiving, developing the concepts and further providing means to build and optimize the structure, from the early stage of understanding the nuclear reaction kinematics to the interaction of fission products with matter inside the active reactor core.

### 1.1. Fission Products as Accelerated Particles

During fission of $^{235}U$ triggered by absorption of a thermal neutron, fission releases over time about 203 MeV, from which 167 MeV as kinetic energy of the fission products, shared according conservation rules.

As seen on isotopic map, in Fig. 2, it shows that after absorbing a neutron, the compound $^{236}U$ is breaking into two symmetrical products relative to median mass ($^{118}Pd$, marked by the pink line), having n in excess as one may see the reddish ellipses, with elements marked after the probability of occurrence. Instantly, due to very high instability of the primordial fission products, few neutrons during the first fs (femyo-second) 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, resulted from excess n disintegration, see the red arrows, crawling towards stability region, marked by black dots, forming isotopes stability region, in the mapped data offered by Brookhaven natl. Lab. nndc.bnl website [1]. 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 $^{89}Kr$ and $^{144}Ba$, 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 $^{89}Y$, group 3B and $^{144}Nd$, a 4th 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 [1,2]. It is known that the shape of fission products depends on the type of actinide and neutron energy and possible on some local quantum states.

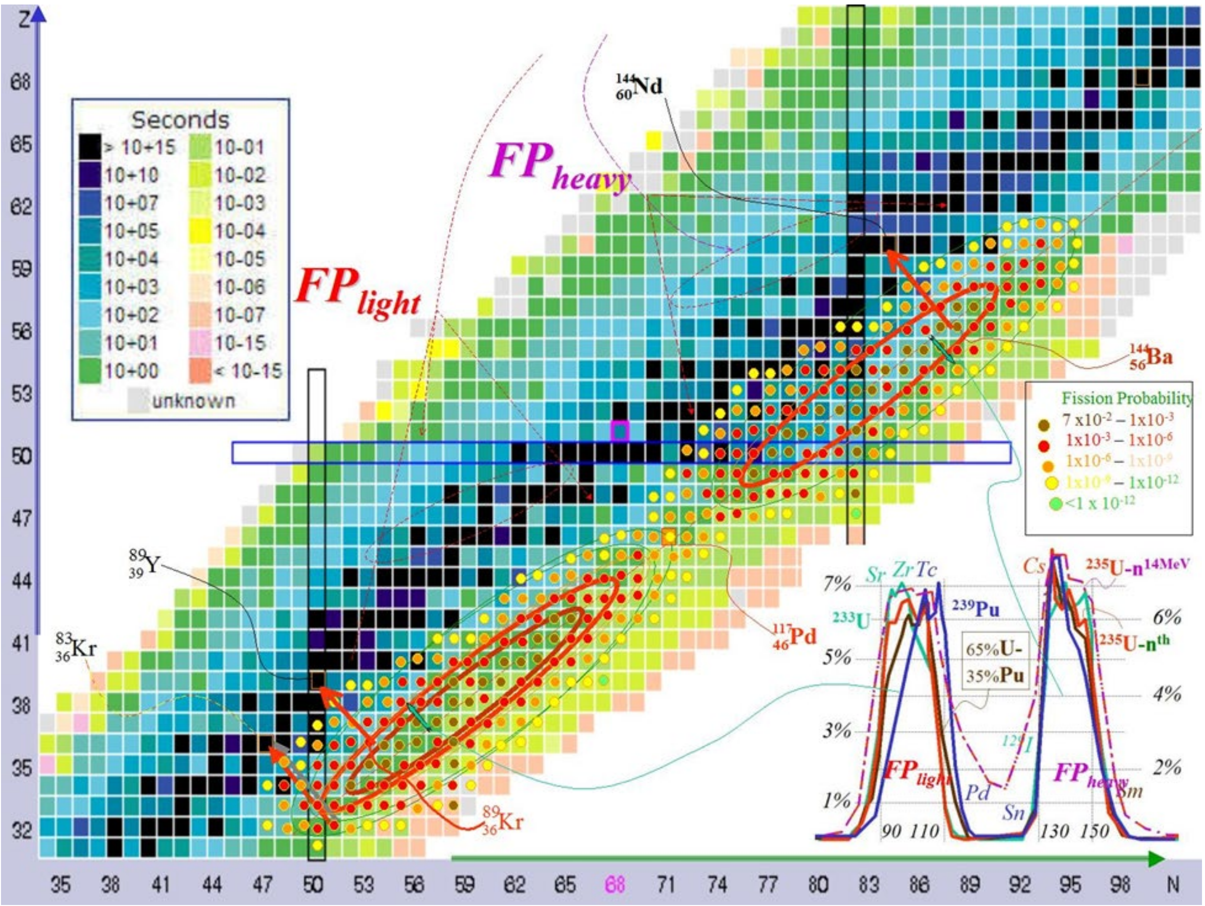


*FIG. 2: Details on Fission Products production process*

## 1.2. Fission products effects in nuclear fuel

As one may see in Fig. 2 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.

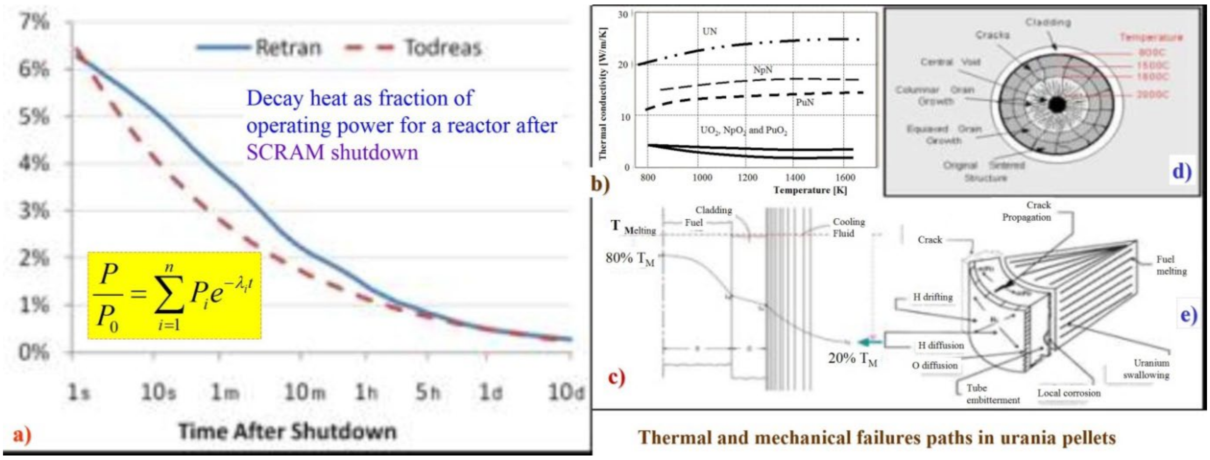


*FIG. 3: Actual fuel induced issues for thermal nuclear reactor safety a) –Decay heat after SCRUM; b) Thermal conductivity of nuclear fuels; c) temperature radial distribution in fuel cell; d) nuclear fuel failing mechanisms; e) pellet slice falling issues*

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

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 [2].

### 1.3. Accelerator knowledge use in FPs' behavior understanding

The analogy between FP and medium mass accelerated charged particles is outstanding. Immediately after 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. 4 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".

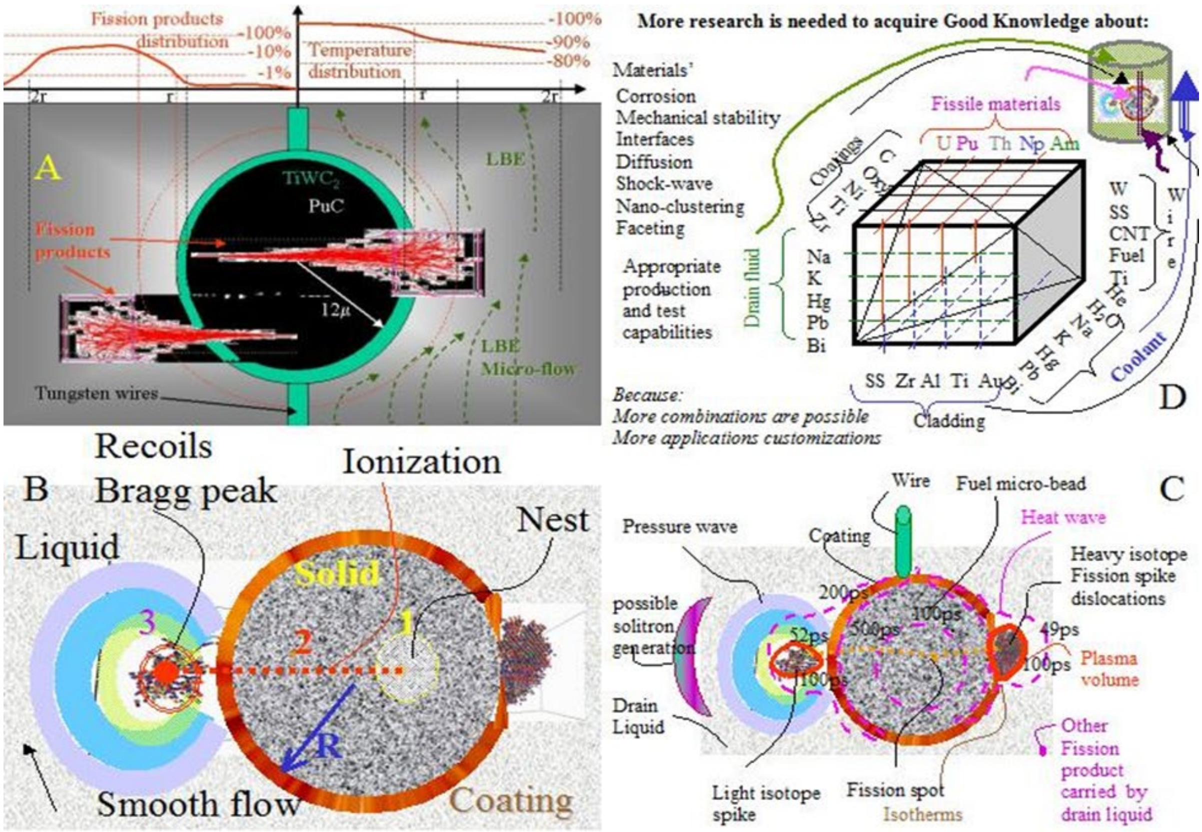


*FIG. 4: Heterogeneity by design applied in "cer-liq-mesh" fuel structure; A –Fission kinematics in novel micro-bead structure; B - Processes in micro-hetero fuel bead; C - MD details on fission products effects; D - Material diversity to fabricate a fuel pellet.*

Fig. 4 D shows that there are several combinations that may be used and work well to create a fuel pellet with identical properties of the actual fuel, that to offer the advantages of micro-hetero-fuel without major changes in the nuclear reactor structure. The critical feature is at the boundary between the fuel bead and drain liquid, when Bragg peak is in coating that has to recover in izo-morphism, protecting bead, is simulated using accelerators.

## 2. TYPES OF ENGINEERED NANO-NUCLEAR STRUCTURES

### 2.1. Micro-hetero structures, generally called "cer-Liq-Mesh"

FIG. 4A 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. 4B 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. 4C 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. 4A was given a constructive example, but FIG. 4D shows the real complexity of the problem, where various aspects and properties have to be mitigated.

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 thermo-mechanical 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.

### 2.2. 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 meta-material that resembles a heterogeneous super-capacitor, that loads from the kinetic energy of the nuclear particle crossing it and discharges as electricity as shown in FIG. 5e.

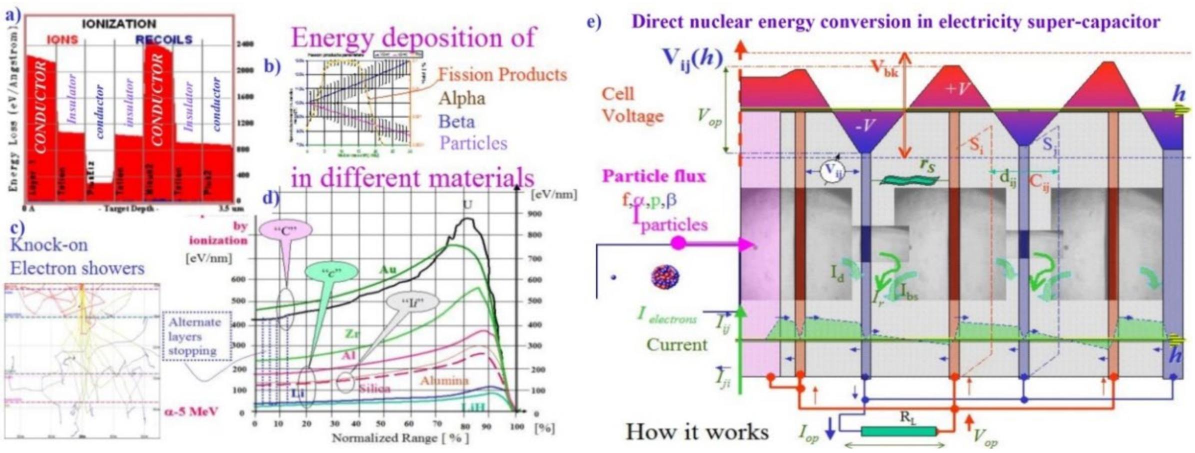


*FIG. 5 Development of meta-materials for direct nuclear energy conversion in electricity a) SRIM Ionization simulation; b) FPs as accelerated ions; c) Primary knock-on electron trajectories; d) Ionization stopping power deposition in various materials; e) principle of direct nuclear energy conversion [3].*

FIG. 5a 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. 5e. Knock-on electrons interact with other electrons forming showers and are tunnelling through the insulator layer and stop in the next conductive layer, polarizing the layers, as the e-Casino electron path simulation in FIG. 5c shows. There are many materials that exhibit these properties, as the plot in FIG. 5d for few materials of interest showing ionization versus the relative stopping range. In the FIG. 5b 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/mm3, 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. A single layer alpha battery made of this meta-material using $^{238}Pu$ will look like a paper sheet being about 50 micron thick.

The research and development of this material intensively uses particle accelerators for material parameters optimization, energy conversion efficiency measurement, and construction, and the structure itself was discovered during a failed accelerator experiment by 1980s which aimed to measure beam's temperatures.

### 2.3. Nuclear Transmutation Products Extraction and Fuel Cycle

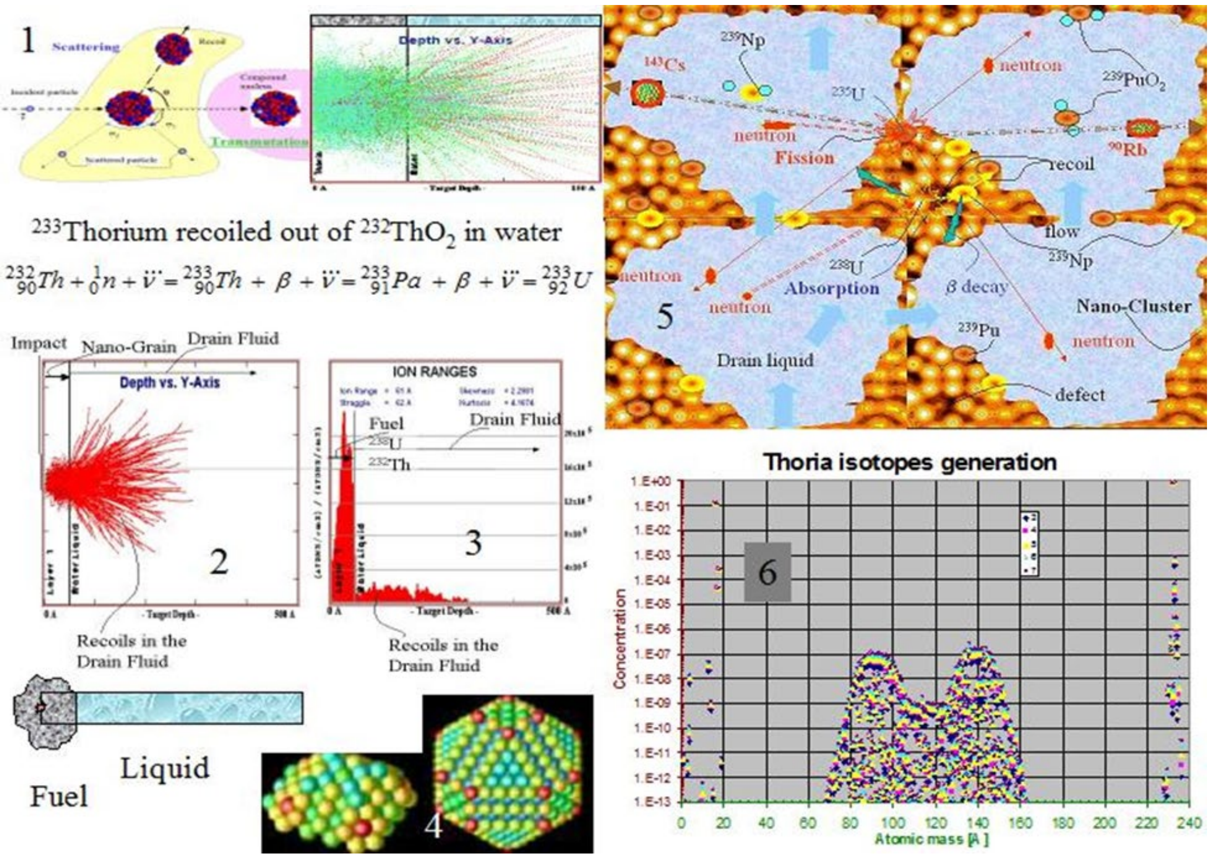


*FIG. 6: Mechanisms of separation in nano-beaded hetero materials: 1 – Nuclear reaction schematics; 2 – Recoils paths by SRIM; 3 – Ion ranges; 4 – Nano-cluster with impurities on interface; 5 – processes in a hetero nano-clustered structure; 6 – Th breeding inventory.*

FIG. 6-1, 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 nearby, 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 [4]. From the radioactivity point of view, in a 1 $cm^3$

sealed fuel pellet it may reach hundreds of Sv/h, having a thermal power of less than 10W, while after 1 month it decays by 3 om (orders of magnitude) being easy to reprocess in a specialize glovebox.

In accelerator technology recoil implantation is a well-known radioactive labelling process that works together with nano cluster mechanisms to produce direct separation of TPs. And in this case it may be used to simulate the behaviour of nano-cluster fluid interfaces as function of radioactivity, temperature, etc.

### 2.4. Nuclear Reactor Control using guiding nano-structures

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 manoeuvrability low.

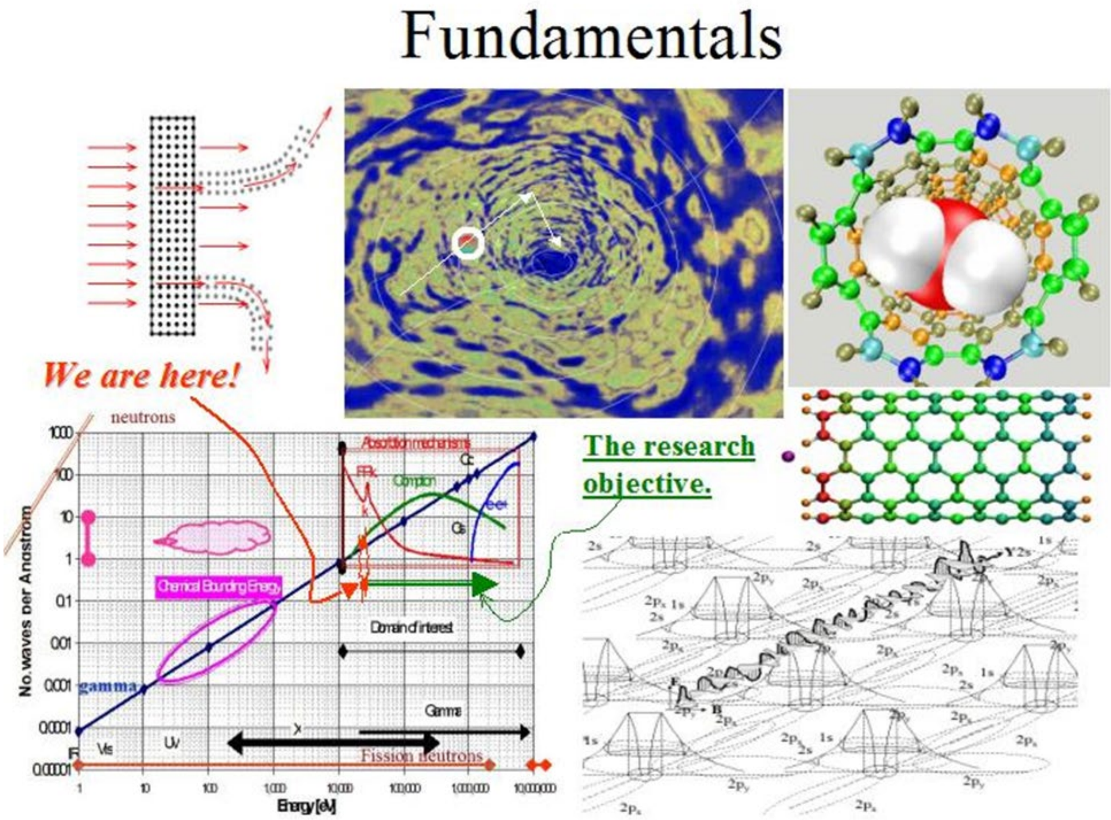


*FIG. 7 – Principles of neutron guiding or channelling in nano-structures*

It is anticipated that using channelling process, discovered using accelerators by 1970s, where neutrons to be trapped and guided in nano-structures with capability to switch their trajectory using electronic controlled NEMS devices, to produce more efficient nuclear reactor control systems able to use prompt neutrons, making the reaction time by 1,000 times faster [5].

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 centre 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. The channelling properties of nanostructures are well known for charged particles, what it remains to do is to engineer such nanostructures able to trap neutrons inside with larger angle than the actual grazing angle and to attach the trajectory switch on it controlled by electric field, generically calling it a NEMS. This feature will make the guiding material suitable for being used for reactor criticality control, and applications in modulating radiation, criticality and even reactor’s neutrino emission.

## 2.5. 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.

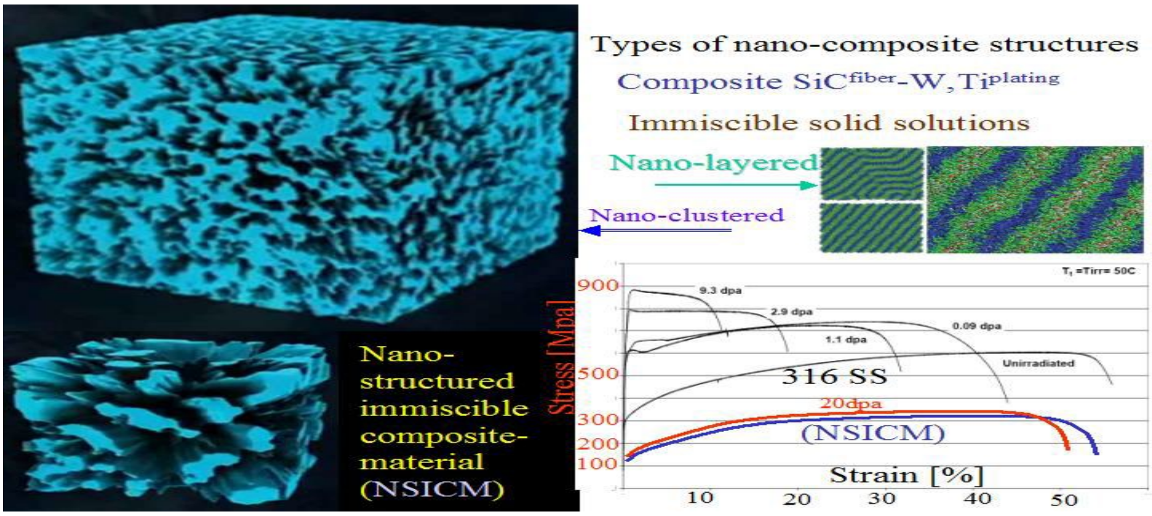


*FIG. 8 Novel multi-phase material structure and anticipated properties*

This new material "NSICM" shown in FIG. 8 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.

## 3. THE USE OF ACCELERATORS IN DEVELOPING NANO-HETERO-NUCLEAR MATERIALS

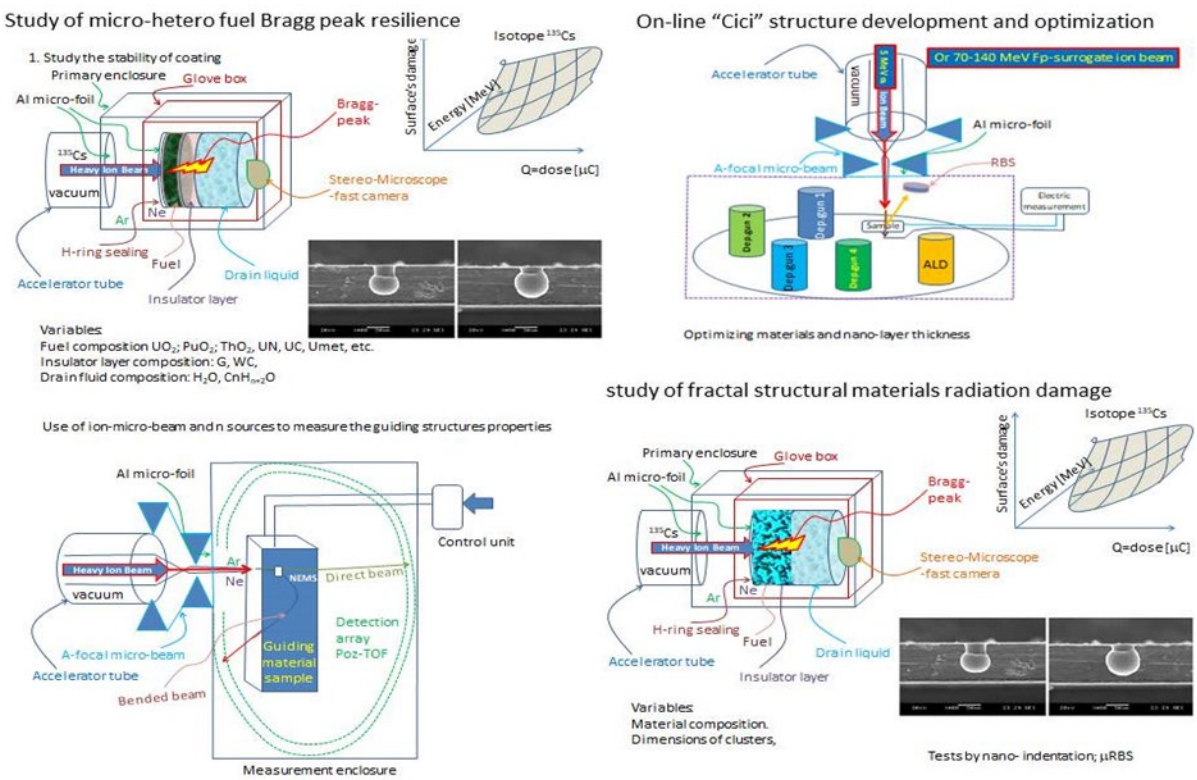


*FIG. 9 – accelerator use to develop micro-nano engineered nuclear hetero-structures*

As one may see, accelerators are indispensable tools in the development of novel micro-nano nuclear materials, able to speed up the R&D process by an order of magnitude. It will start with micro-hetero structures as FIG. 9 shows in upper left side, implanting surrogates of fission products to generate Bragg peak in the interfaces. The use of a 5 MeV □ beam or 60 MeV to 150 MeV FPs surrogate to optimize the layers of a direct nuclear energy conversion structure may be done by measuring the beam current before and after entering the structure, and using RBS to profile the thickness and interpenetration of different nano-layers. In lower-left side is shown how a micro-beam may be used to characterize a nano-guiding structure used for nuclear reactor control, switching the neutron direction from leaving the active zone, to returning into ha being switched by means a NEMS device acting on each track. Similar measurement but this time using accelerator to simulate and measure radiation damage into fractal materials is presented on lower-right side. The big advantage using accelerators instead direct exposure in nuclear reactor, resides in its analytical capabilities, possibility of using various size of beams, from micron to cm size, various incidence angles, particle beams and energies distinctly covering the entire palette of functional circumstances the future products may encounter in normal running.

Active quantum environments is a frontier domain in nuclear physics, that may be explored using accelerators in various modes, from producing the environment to triggering the quantum exchange and to visualize different aspects of collective quantum interactions helping us to understand the relationship between material quantum assemblies and quantum fields, in the attempt to master the processes and control them to our advantage [6].

## 4. 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 nano-nuclear materials, and may be integrated in nuclear power structures, because they allow small scale simulations with full access for observations of the effects obtained inside a nuclear reactor core critical structure with little and difficult access for real time observations on the tested structure.

## ACKNOWLEDGEMENTS

I am grateful to all of those with whom I have had the pleasure to work during this and other related projects. Each of the team members have provided me extensive personal and professional guidance and taught me a great deal about both scientific research and life in general. I would especially like to thank Prof. Ionel Purica, Acad. Ioan-Iovitz Popescu, Dr. Geavidt Musa, Dr. Michael Nastasi the team leader as my coordinator and mentor, he has taught me more than I could ever give him credit for here. They have shown me, by example, what a good scientist and person should be. Deep gratitude to our friends, Dr. Gordon Jarvinen and Dr. David Poston, from LANL, for advices and life model, and to all our collaborators who supported the research and co-authored various papers over time.

## REFERENCES

[1] BNL, NNDC "Interactive Chart of Nuclides" - NNDC https://www.nndc.bnl.gov/nudat3/, (2022)

[2] POPA-SIMIL L.,"Applied Nano-technologies Improves Nuclear Power Safety and Performances" (Nano-technologies in Nuclear Power, Book 1), Kindle Edition (2012).

[3] POPA-SIMIL L., "Strategic space applications of nano-engineered nuclear-materials", Apple Books, (2015).

[4] POPA-SIMIL, L., Nuclear Power Renaissance Based on Engineered Micro-Nano-Nuclear Materials. Energy and Power Engineering, 13, 65-74, (2021).

[5] POPA-SIMIL L., Nano-structured nuclear radiation shielding. US20110001065, (2011)

[6] POPA-SIMIL L., The Fusion Battery, A Novel Type of Nuclear Battery and Potential Outcomes and Applications (Nuclear Power - Fusion Book 1), Kindle Edition (2012)