



Granta EduPack White Paper

Materials for Nuclear Power Systems

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Abstract

This Paper describes a resource designed to support introductory and higher level courses on nuclear power systems, focusing on the choice of materials. It centers on a pair of databases for materials of fission and fusion-based Nuclear Engineering - fuels, materials for fuel cladding, moderators and control rods, first-wall materials, materials for pressure vessels and heat exchangers, providing data for their properties. Where relevant the records contain data for both nuclear and engineering properties. The databases are accessed through the Granta EduPack software, allowing its full data-retrieval and selection functionality to be exploited.

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1. Introduction and synopsis

Electricity generation, at present largely from fossil fuels, accounts for 33% of the carbon entering the atmosphere annually; transport accounts for another 28%. Fossil fuels are non-renewable and their use releases carbon into the atmosphere with consequences that are causing concern. Renewable energy sources (wind, wave, tidal, solar, hydro, geothermal) can, realistically, provide only a fraction of the energy we use today, and a smaller fraction of the much larger demand for energy that is predicted for 20 years from now. All have a very small *power-to-land-area* ratio. An option that is receiving increasing attention is to replace carbon-based fuels by nuclear power (using it for transport via electric or hydrogen-powered vehicles) at the same time reducing an uncomfortable dependence on imported hydrocarbons and an unacceptably extensive use of land area.

Currently there are some 436 operational nuclear reactors world-wide. They are predominantly pressurized water reactors, PWRs, (60% of total) and boiling water reactors, BWRs (21%). The rest are gas cooled reactors, AGRs, deuterium-moderated reactors, CANDU and D₂O-PWRs, light water graphite moderated reactors, RBMKs, and fast breeder reactors, FBRs.

Examples of the number of operational reactors and projections for new build.

Country	Operating reactors, 2009	Estimates of needed new reactors	Source of information
US	86	Not known	
Russia	35	Not known	
Europe: France	59	Not known	
Europe: Germany	12	Not known	
Europe: UK	10	15	The Times, 4 Oct 2009
Japan	60	Not known	
China	11	300	The Times, Sept 2009
India	18	450	The Times, Sept 2009

There has been a virtual moratorium on building nuclear power plants for the last 20 years. One consequence has been the loss of expertise required to construct and maintain them. The renewed interest in nuclear power creates a need for engineers with appropriate training. With hundreds of new reactors planned worldwide, such training will be required on a significant scale. Universities are seeking to respond by developing and expanding courses on Nuclear Engineering.

A second consequence of the moratorium is the paucity of texts for teaching about materials in nuclear reactors – most date from 1980 or before. There are, however, good web sites. Two, particularly, provide current information about the field. They are listed in *Further Reading*, at the end of this White Paper under International Nuclear Safety Center (2009) and European Nuclear Society (2009).

This White Paper describes a resource designed to support introductory and higher level courses on nuclear power systems, focusing on the choice of materials. It centers on a pair of databases for materials of fission and fusion-based Nuclear Engineering – fuels, materials for fuel cladding, moderators and control rods, first-wall materials, materials for pressure vessels and heat exchangers, providing data for their properties. Where relevant the records contain data for both nuclear and engineering properties. The databases are accessed through the Granta EduPack software, allowing its full data-retrieval and selection functionality to be exploited.

The following sections describe and illustrate the use of the two databases. The content is summarized below:

- Reactor systems are introduced in Section 2, each with a figure identifying the principal structural and functional materials. Records for the reactor systems are linked to records for the engineering properties of the materials in them in a new database called “Nuclear power systems”. Its structure, content, and uses are described in Section 3.
- Fundamental nuclear properties of the elements are stored in an expanded version of the “Elements” database, the subject of Section 4. Charts for nuclear properties, created with this database, illustrate how it is used to select materials with nuclear properties that best meet the needs for moderators, control rods and fuel cladding.
- Two Appendices list definitions of nuclear properties and tabulate the materials used in each reactor system.

2. Reactor types

A number of reactor types have been developed for commercial service. The British Magnox reactors and the Canadian Candu reactors are now reaching the end of their lives. Most current commercial reactors are based on boiling water (BWR) or pressurized water (PWR) heat-transfer systems. Interest now focuses on Generation IV designs: fast breeder, gas-cooled and high-temperature reactors. Early versions of some, like the Liquid-metal Cooled Fast Breeder Reactor (LMFBR) and the Advanced Gas Cooled Reactor (AGR), already exist. Others, such as the Pebble Bed Reactor (PBR) are under study. Research on Fusion Reactors has been underway for 30 years, but a commercial system is still far away. One example, the ITER reactor, is described here.

Reactor systems and the principle materials of which they are made are introduced in this section.

2.1 Boiling Water Reactor (BWR)

See *Figure 1*. Coolant: light water; outlet temperature 560 K.

The direct cycle BWR system generates steam that is fed to the same sort of steam turbine used in coal or gas-fired power systems. The nuclear core assembly consists of an array of Zircaloy 2 tubes encasing enriched UO_2 ceramic fuel pellets. Some of the fuel rods contain gadolinium oxide (Gd_2O_3), which acts as a burnable “poison” absorbing neutrons when the fuel is fresh but burning up as the fuel decays, buffering the neutron flux. The power is controlled by control rods inserted from the bottom of the core and by adjusting the rate of flow of water. The control rods are made of boron carbide (B_4C) clad in stainless steel 304 or 304L. Water is circulated through the reactor core where it boils, producing saturated steam.

The water acts as both a coolant and a moderator, slowing down high energy neutrons. The steam is dried and passed to the turbine-generator through a stainless steel steam line. On exiting the turbine the steam is condensed, demineralized, and returned as water to the reactor. The schematic in *Figure 1* shows the most important materials of the system.

The BWR operates at constant steam pressure (7 MPa), like conventional steam boilers and with a steam temperature of about 560K.

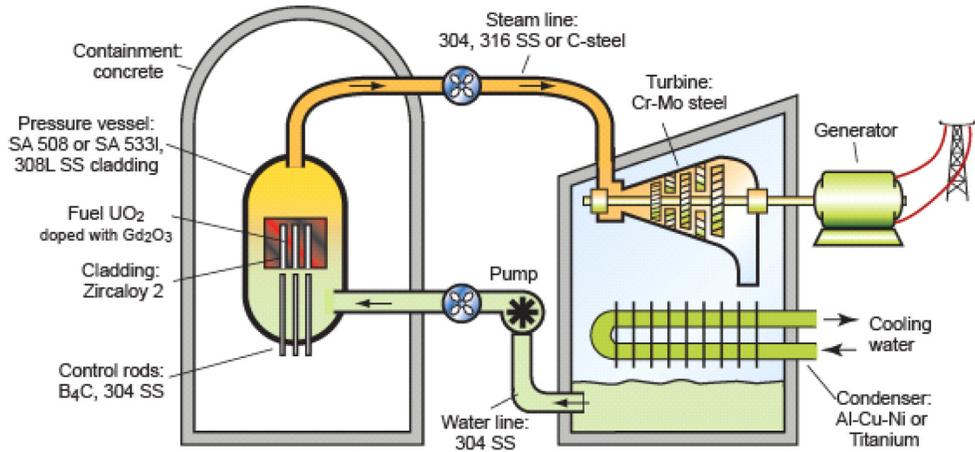


Figure 1. The Boiling Water Reactor

2.2 Pressurize Water Reactor (PWR)

See *Figure 2* (overleaf). Coolant: light water; outlet temperature 600 K.

The core of a pressurized water reactor (PWR) is not unlike that of a BWR. It has some 200 tube assemblies containing ceramic pellets consisting of either enriched uranium dioxide (UO_2) or a mixture of both uranium and plutonium oxides known as MOX (mixed oxide fuel). These are encased in Zircaloy 4 cladding. Either $\text{B}_4\text{C}-\text{Al}_2\text{O}_3$ pellets or borosilicate glass rods are used as burnable poisons. Water, pumped through the core at a pressure sufficient to prevent boiling, acts as both a coolant and a moderator, slowing down high energy neutrons. The water, at about 600 K, passes to an intermediate heat exchanger. The power is controlled by the insertion of control rods from the top of the core and by dissolving boric acid into the reactor water. As the reactivity of the fuel decreases, the concentration of dissolved boron ions is reduced by passing the water through an ion-exchanger. Control rods made of boron carbide (B_4C) or an Ag-In-Cd alloy are clad in Inconel 627 or stainless steel (304) tubes.

The primary pressurized water loop of a PWR carries heat from the reactor core to a steam generator. The loop is under a working pressure of about 15 MPa - sufficient to allow the water in it to be heated to near 600 K without boiling. The heat is transferred to a secondary loop generating steam at 560 K and about 7 MPa, which generates heat that drives the turbine.

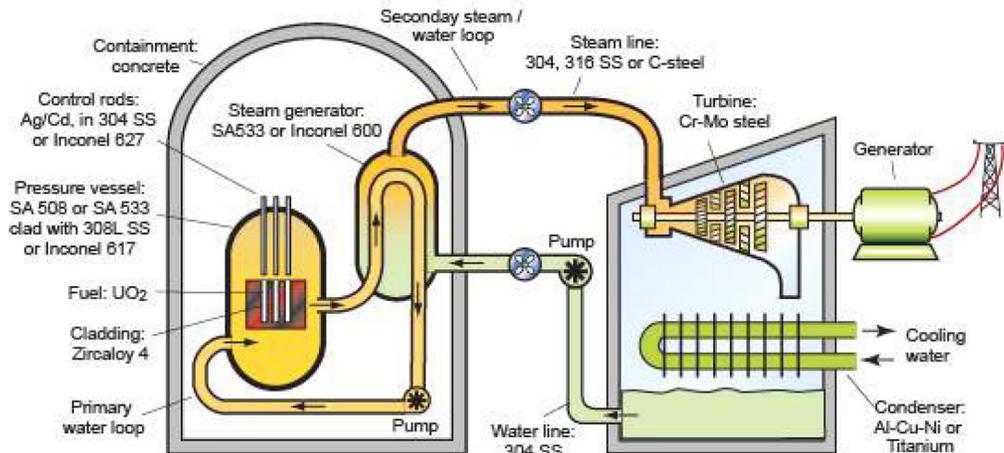


Figure 2. The Pressurized Water Reactor

2.3 Liquid Metal Fast Breeder Reactor (LMFBR)

See Figure 3. Coolant: sodium; outlet temperature 800K.

A LMFBR is a liquid sodium cooled reactor that makes use of a fast neutron spectrum and a closed fuel cycle. The liquid sodium coolant transfers heat from the reactor core and is pumped through the primary loop at about 800K. This sodium in this loop becomes radioactive, requiring an intermediate sodium filled heat-exchange loop to prevent possible leakage of radioactive material outside the containment structure. The sodium in this secondary sodium loop, made of type 324 and 316 stainless steel, alloy 800 or Cr-Mo steels, passes to a steam generator where it heats water to generate steam at 750 K. The turbine and generator are essentially the same as those of a BWR or PWR.

A variety of fuel materials have been proposed. These include mixed uranium and plutonium oxides (~25% PuO₂), metal alloys such as U-Pu-Zr, and mixed uranium or thorium carbides and nitrides. The usual choice is a fuel assembly made up of mixed uranium dioxide (UO₂) and plutonium dioxide (PuO₂) fuel rods clad in type 316 stainless steel. This is surrounded by the "breeding blanket" containing depleted UO₂ pellets. The control rods, like those of a BWR, are boron carbide (B₄C) clad in type 316 stainless steel and enter from the top of the core.

An LMFBR can have either pool or loop designs. A pool design has the intermediate heat exchangers and primary sodium pumps immersed in the reactor vessel whilst a loop design has these elements external to it. The schematic shows a loop design. One of the selected generation IV systems, the sodium-cooled fast reactor (SFR) utilizes a similar design to the LMFBR described above. The next generation lead-cooled fast reactor (LFR) uses liquid lead as a coolant and utilizes a somewhat different reactor design.

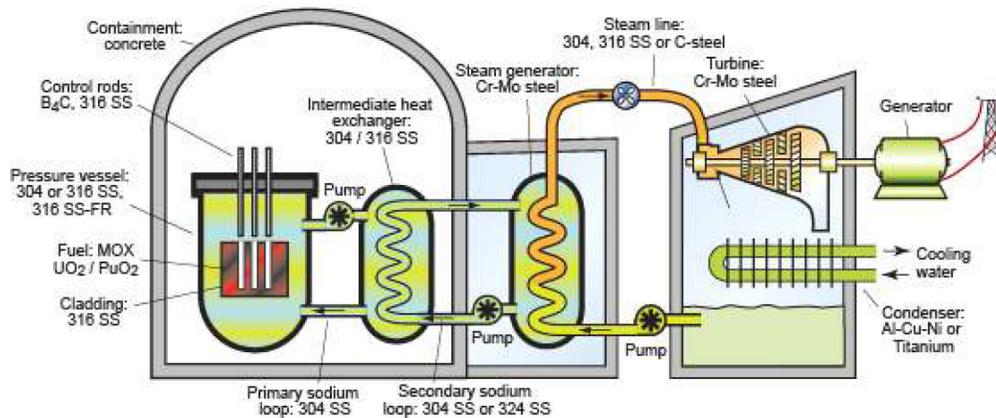


Figure 3. The Liquid Metal Cooled Fast Breeder Reactor.

2.4 Advanced gas-cooled reactor (AGR)

See Figure 4 – typical power 660 MW. Coolant: CO₂ ; outlet temperature 943 K.

The advanced gas-cooled reactor (AGR) is graphite moderated and cooled with carbon dioxide (CO₂). The core consists of high strength graphite bricks mounted on a steel grid. Fuel rods of enriched UO₂ clad in stainless steel (20-Ni 25-Cr) are placed in graphite sleeves and inserted into vertical channels in the bricks. Gas circulators blow CO₂ up through the core and down into steam generators. Holes in the graphite allow access to the gas. The outlet temperature of the CO₂ is about 943K at a pressure of 4MPa. The graphite in the core is kept at temperatures below 723K to avoid thermal damage.

The reactor core, gas circulators, and steam generators are encased in a pressure vessel made of pre-stressed concrete lined with a mild steel to make it gas tight. Mild steel is used in areas of the pressure vessel that are exposed to temperatures less than 623K. In regions at temperatures between 623K and 793K, annealed 9Cr-1Mo steel is used whilst austenitic steel (316 H) is used for regions hotter than this. Power is primarily controlled through the insertion of control rods made of boron-steel, with back-up by insertion of nitrogen into the cooling gas or by releasing fine boron-rich balls into the gas stream.

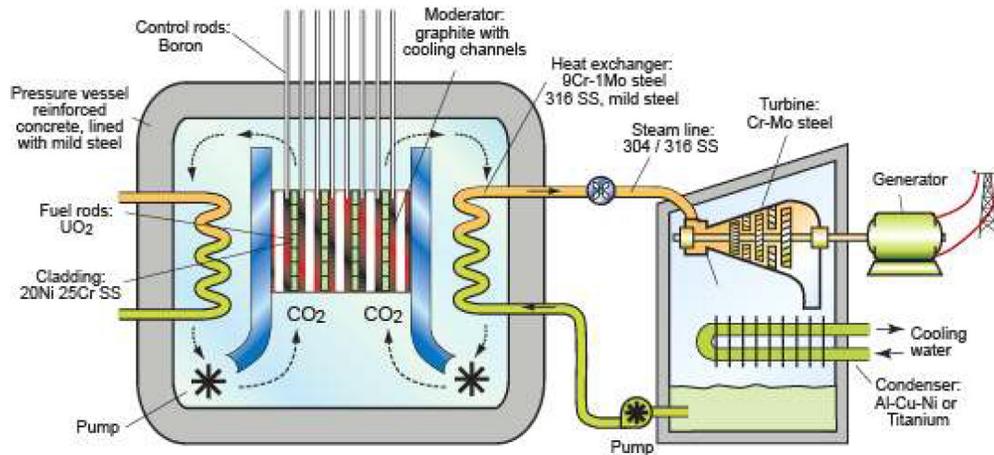


Figure 4. The Advanced Gas-cooled Reactor (AGR).

2.5 Very High Temperature Reactors (VHTR).

E.g., the Pebble Bed Reactor (PBR). See *Figure 5* (overleaf). Coolant: He; outlet temp. 1123–1223 K.

The very high temperature reactor (VHTR) is a proposed IV generation design, moderated with graphite and cooled with helium gas. The development of new materials able to tolerate the higher operating temperatures presents a major engineering challenge. The outlet temperature of the coolant is about 1123-1223K at a pressure of 7MPa. Internal reactor temperatures may reach up to 1470K. Candidate materials for regions at temperatures between about 1030K and 1270K are alloys 617, X, XR, 230, 602CA or variants of alloy 800H. For regions with higher temperatures than this, the leading material candidates are composites with a carbon fiber reinforced carbon matrix (Cf/C) or carbon fiber reinforced silicon carbide (SiCf/SiC). The most promising pressure vessel material is modified 9 Cr-1 Mo steel. Some designs maintain the vessel at lower temperatures, in which case current pressure vessel materials could be used such as SA 508 steels.

The helium coolant is heated in the reactor vessel and flows to the intermediate heat exchanger (IHX). Heat is transferred to a secondary loop with either helium, nitrogen and helium, molten salt, or pressurized water. The materials of the IHX depend on the operating temperatures and the nature of the secondary coolant; Alloy 617 is a primary candidate. The heated fluids can either be used to drive a turbine or to produce hydrogen.

All VHTR designs make use of tri-structural isotropic (TRISO) coated fuel particles. The particles are 750-830 μm in diameter and consist of a kernel of fuel material coated with two layers of pyrolytic carbon with a layer of silicon carbide in between. These particles can be utilized in either prismatic or pebble bed reactors. In a prismatic reactor the kernel consists of enriched uranium oxycarbide (UCO) and the particles are packed into cylindrical compacts which are placed into graphite fuel elements. However a

pebble bed reactor uses particles with an enriched uranium dioxide (UO_2) kernel and these are formed into 60 mm diameter spheres (the “pebbles”). The fuel pebbles are fed into the core mixed with non-fuel graphite pebbles that act as reflectors to even the heat generation.

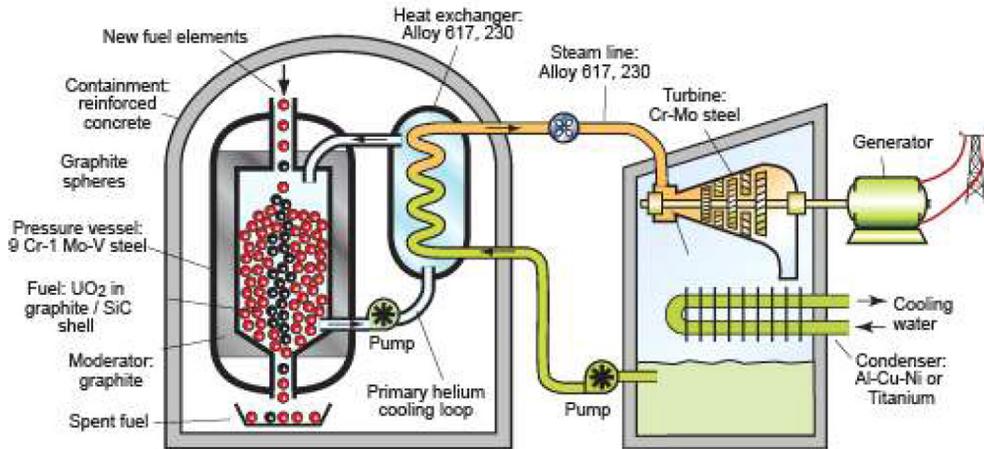


Figure 5. A pebble bed advanced nuclear reactor. In some designs the helium heat-transfer medium drives turbines to compress the gas and generate power; in others it is fed to a heat exchanger where it passes its heat to a secondary helium loop or to steam loop, as pictured here.

2.6 Fusion Reactors: the International Thermonuclear Experimental Reactor (ITER)

See Figure 6.

The International Thermonuclear Experimental Reactor (ITER) is an experimental fusion reactor designed to produce 500MW of power from an input of 50MW. It is a step towards the use of the fusion energy for electricity production and other commercial applications.

In all proposed fusion reactors, energy is released from the fusion of deuterium and tritium nuclei. This requires a temperature of about 100MK at which the gases forms a plasma. No materials operate at such temperatures, so the ITER uses magnetic confinement to contain the plasma, allowing fusion without contact between the plasma and the containing walls. The ITER uses a tokamak design. The plasma is contained in a torus shape using strong magnetic fields produced by circumferential superconducting coils and a large central solenoid. The coils are made of a superconducting niobium-tin alloy (Nb_3Sn) or niobium-titanium ($NbTi$) alloy cooled to 4K with supercritical helium.

The plasma is enclosed in a sealed torus vacuum vessel made up of two steel walls with water coolant circulating between them. The main structural materials are 316L(N)-IG,304 and 660 stainless steels. The inside of the vacuum vessel is covered with the blanket that shields the vessel and magnets from heat and neutron radiation. This consists of shield modules attached to the vacuum vessel inner wall. Each module has a 316L(N)-IG stainless steel shield block carrying a first wall panel of beryllium facing the plasma. These are joined to a heat sink made of a copper alloy ($CuCrZr$) with 316L(N)-IG stainless steel tubes with a coolant flowing through them. It is the energy transferred to this coolant that would be used in electricity production in future plants.

At the bottom of the vacuum vessel is the diverter which removes heat, helium ash and plasma impurities. Materials of the diverter facing the plasma must withstand temperatures of up to 3300K. The current choice of materials are a carbon fiber composite (CFC SEP NB31) and tungsten (99.94wt% W). The entire structure, including the magnets, is enclosed in a stainless steel vacuum cryostat.

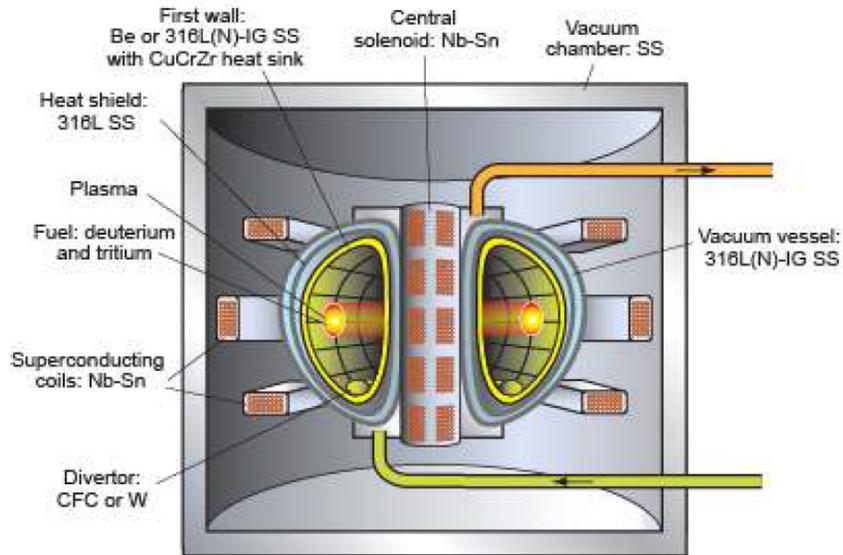


Figure 6. The International Thermonuclear Experimental Reactor (ITER)

3. The Materials for Nuclear Power Systems database

The database has three linked data-tables (*Figure 7*). The first contains records for the power systems themselves, each with an image indicating the principle structural materials as described in Section 2. Each reactor-system record is linked to records for the materials of which it is made, contained in the second data table, basically that of Granta EduPack’s Level 3, enlarged to contain records for fuels, control-rod materials and special reactor-grade steels and graphites, listed below.

- Graphite (isotropic, HTR grade IG-110)
- Graphite (semi-isotropic AGR Gilsoncarbon)
- Uranium dioxide (UO₂)
- Uranium carbide (UC)
- Mixed oxide (U,Pu)O₂ (MOX) 20% PuO₂
- Uranium nitride
- Zirconium-1.5%tin alloy, reactor grade, "Zircaloy 4"
- 9Cr-1Mo steel
- Modified 9Cr-1Mo-V steel (Grade 91)
- SA-508 Gr.3 Cl 1 and 2
- SA-533 Gr B

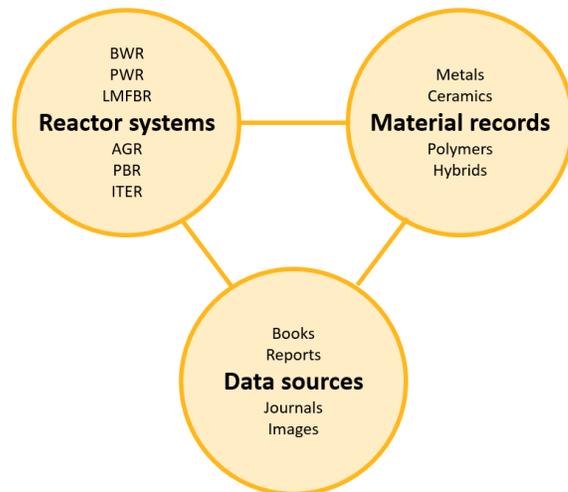


Figure 7. The data structure of the Nuclear Power Systems database.

Records in both these data-tables are linked to listings of relevant data sources stored in the third table.

The records for the principal structural materials include the temperature dependence of Young’s modulus, yield strength, ultimate strength and thermal conductivity, stored as functions. This allows the dependence to be plotted as in *Figures 8 and 9*, and the property values to be displayed for a given operating temperature.

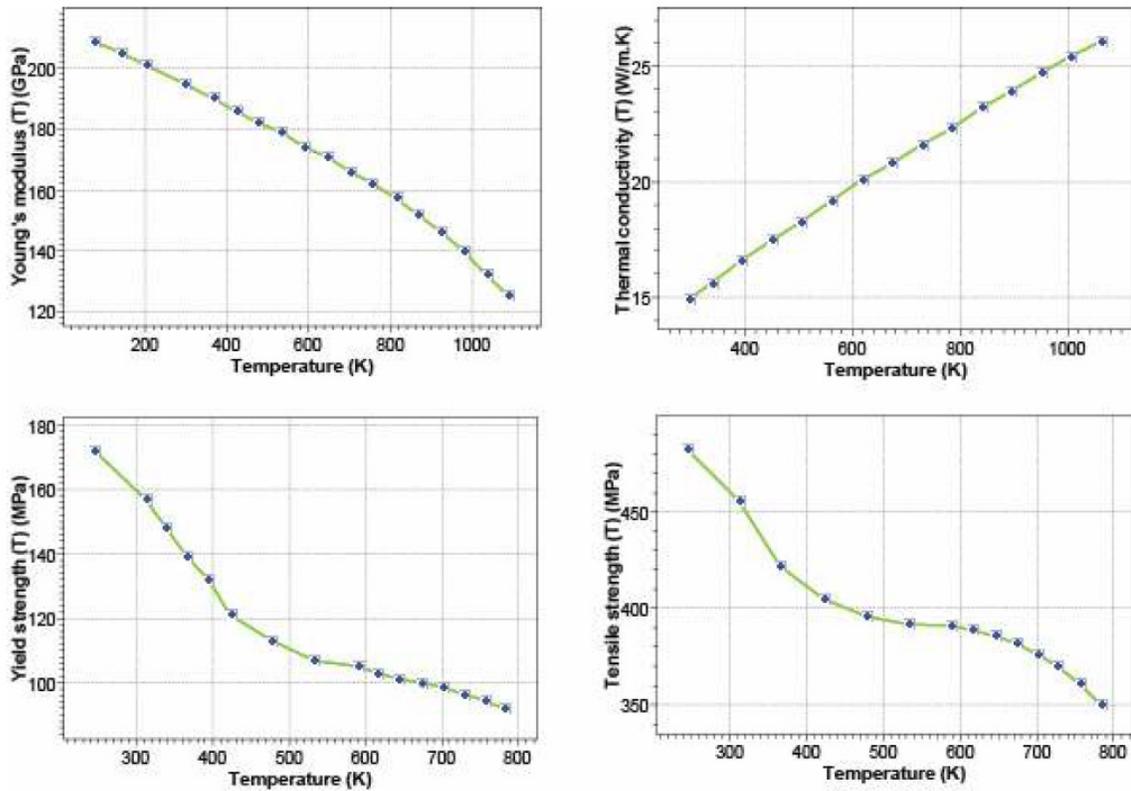


Figure 8. The thermal conductivity, Young's modulus, ultimate tensile strength and yield strength of 304L stainless steel.

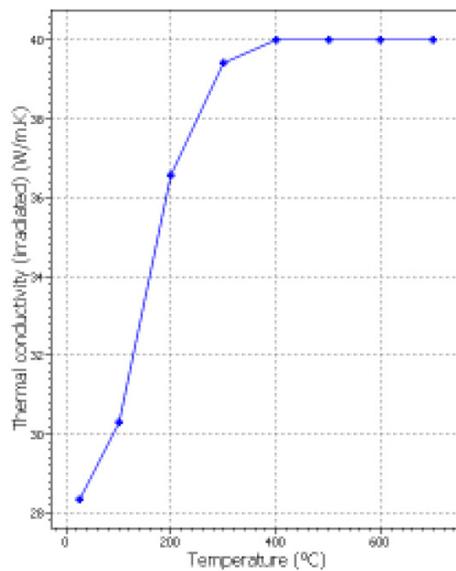


Figure 9. The temperature dependence of the thermal conductivity of irradiated AGR graphite.

The values of the thermal conductivity of the irradiated graphite are considerably lower than the room temperature value for the material (129-133 W/m.K). This emphasizes that the change in properties under neutron irradiation can be considerable and therefore the inclusion of the properties of irradiated materials where possible is important.

Using the database

The features of the database are best illustrated by examples.

Example 1. Browsing and searching the Reactor Systems data-table. The records for the reactor systems, identified by both long and short name (e.g. Pressurized water reactor, PWR) can be found by browsing the record list, or by a text-search for the name. Each record contains a descriptive image and text that are essentially identical with those in subsections of Section 2 of this White Paper. They can be copied and pasted into Word.

Example 2. Browsing and searching the Materials data-table. The Granta EduPack software allows the user to explore nuclear power systems by *Browsing* through the hierarchically structured Materials tree, or by *Searching* by name. The record on the next page shows the result of a search on Zircaloy 2.

Example 3. Listing the principal materials of a given reactor system. The *Tree Selection* tool in Granta EduPack allows names of all the records linked to a given reactor system to be listed. The table shows the result of tree selection for materials for pressurized water reactors. Clicking on any member of the list opens the record.

Materials in PWRs	
Alumina, pressed and sintered	Stainless steel, austenitic, AISI 304, wrought, annealed
Boron carbide (hot pressed)	Stainless steel, austenitic, AISI 308, wrought, annealed
Borosilicate - 2405	Stainless steel, austenitic, AISI 308L, wrought, annealed
Carbon steel, AISI 1020, normalized	Stainless steel, austenitic, AISI 316, wrought, annealed
Mixed oxide (U,Pu)O ₂ (MOX) 20% PuO ₂	Stainless steel, austenitic, AISI 347, wrought
Nickel-Cr-Co-Mo alloy, INCONEL 617, wrought	Stainless steel, ferritic, AISI 403, wrought, annealed
Nickel-Fe-Cr alloy, INCOLOY 800, annealed	Thoria, ThO ₂
Nickel-chromium alloy, INCONEL 600, wrought, annealed	Titanium, alpha-beta alloy Th-6Al-4V
SA-508 Gr.3 Cl 1 and 2	Uranium dioxide , UO ₂
SA-533 Gr B	Zirconium-tin alloy, Zircaloy- 4, 1.5%Sn (reactor grade)

Example 4. Materials and reactor sub-systems. One material listed above is AISI 347 austenitic stainless steel. In which subsystem is this used? Opening the record for AISI 347 and scrolling to Reactor Subsystem reveals the answer – the primary cooling system.

Example 5. Materials proposed for use in fusion reactors. A tree stage to isolate materials linked to the ITER fusion reactor design results in the list below.

Materials proposed for use in fusion reactors	
Beryllium, grade 0-50, hot isostatically pressed	Beryllium, grade I-250, hot isostatically pressed
Beryllium, grade S-200FH, hot isostatically pressed	Carbon fiber reinforced carbon matrix composite (Vf:40%)
Carbon fiber reinforced carbon matrix composite (Vf:50%)	Epoxy SMC (glass fiber)
Epoxy/E-glass fiber, woven fabric composite, ql laminate	Nickel iron aluminum bronze, (wrought) (UNS C63020)
Hi conductivity Cu-Cr-Zr (wp) (UNS C18100)	Nickel-chromium alloy, INCONEL 718, wrought
Nickel iron aluminum bronze, (wrought) (UNS C63020)	OFHC copper, 1/2 hard (wrought) (UNS C10200)
Nickel-chromium alloy, INCONEL 718	Silver, commercial purity, fine, cold worked, hard
PTFE (unfilled)	Stainless steel, austenitic, AISI 304, wrought, annealed
Stainless steel, austenitic, 316L(N)-IG	Stainless steel, austenitic, AISI 316, wrought, annealed
Stainless steel, austenitic, AISI 304L, wrought	Nitronic 50, XM-19, wrought, (nitrogen strengthened)
Stainless steel, austenitic, AISI 316L, wrought	Stainless steel, ferritic, AISI 430, wrought, annealed
Stainless steel, ferritic, AISI 430F, wrought, annealed	Stainless steel, ferritic, AISI 430FR, wrought, annealed
Titanium, alpha-beta alloy, Ti-6Al-4V, annealed, generic	Tungsten, commercial purity, R07004, annealed

Zircaloy-2 (reactor grade)

Designation

ASTM Standard B350-80: Zirconium-Tin Alloy, UNS R60802

Tradenames

ZIRCALLOY 2; SANDVIK ZIRCALLOY 2, Sandvik Steel Co. (USA); ZIRCALLOY-2, Sandvik/Coromant (USA); ZIRCALLOY-2, Westinghouse Electric Corp. (USA);

Composition (summary)

Zr/1.2-1.7Sn/.07-.2Fe/.05-.15Cr/.03-.08Ni+ various lesser impurities

Composition detail

	Zr (Zirconium)			
Base				
Cr (chromium)	0.05	-	0.15	%
Fe (iron)	0.07	-	0.2	%
Ni (nickel)	0.03	-	0.08	%
Sn (tin)	1.2	-	1.7	%
Zr (zirconium)	97.9	-	98.7	%
Density	6450	-	6650	kg/m ³
Price	* 24.7	-	27.2	USD/kg

Mechanical properties

Young's modulus	* 90	-	105	GPa
Shear modulus	* 30	-	40	GPa
Bulk modulus	* 100	-	150	GPa
Poisson's ratio	* 0.35	-	0.38	
Yield strength (elastic limit)	240	-	490	MPa
Tensile strength	410	-	520	MPa
Compressive strength	* 240	-	490	MPa
Flexural strength (modulus of rupture)	* 240	-	490	MPa
Elongation	14	-	32	%
Hardness - Vickers	200	-	240	HV
Fatigue strength at 10 ⁷ cycles	* 160	-	260	MPa
Fracture toughness	* 115	-	150	MPa.m ^{1/2}
Mechanical loss coefficient (tan delta)	* 3e-4	-	9e-4	

Thermal properties

Melting point	2100	-	2130	K
Maximum service temperature	* 643	-	783	K
Thermal conductivity	11	-	14	W/m.K
Specific heat capacity	274	-	286	J/kg.K
Thermal expansion coefficient	5.5	-	5.9	µstrain/°C

Typical uses

Fuel rod cladding in boiling water reactors (BWR).

Warning

May become radioactively contaminated during use. Small pieces of zirconium, e.g. machine chips and turnings, can be a fire hazard. Non-radioactive Zirconium is toxic, but only if ingested in large quantities.

Other notes

The mechanical properties of Zr alloys vary strongly with oxygen impurity levels. Zirconium ore naturally contains a few per cent Hafnium, which has v. similar properties to Zr. For nuclear applications, this has to be removed, as Hf absorbs neutrons.

Figure 10. The record for the cladding material Zircaloy 2. Nuclear properties for zirconium (the base of Zircaloy) are contained in the extended Elements database, described in Section 4.

Example 6. Using the links between material and reactor system. Which reactor systems use Graphite Grade IG-110 as a moderator? Opening the record for this Graphite (found by *Browsing* or by *Searching*) and activating the link to Reactor Systems gives the result shown below.

Nuclear power systems
Very high temperature reactor (VHTR)

Example 7. Using the links between material and reactor system. Which reactor system can use uranium carbide as a fuel? Opening the record for Uranium Carbide (found by *Browsing* or by *Searching*) and activating the link to Reactor Systems gives the result shown below.

Liquid metal fast breeder reactors

Example 8. Listing properties at temperature. What is the thermal conductivity and the yield strength of wrought 316L stainless steel at 350°C? Entering 350°C (or 623 K) as the temperature parameter value for the Tdependent properties of 316L (found by *Browsing* or by *Searching*) gives

Thermal conductivity	19 W/m/C
Yield strength	104 MPa

4. Nuclear properties in the Elements database

The existing Elements database has been expanded to include relevant nuclear properties for reactor engineering: the binding energy per nucleon, thermal neutron absorption cross section, thermal neutron scattering cross section, and, for fuels, the half life. These properties are defined more fully in Appendix 1. Additional records have been added for particular isotopes of interest: deuterium (2), tritium (3), the four isotopes of plutonium (239, 240, 241, 242), the three isotopes of uranium (233, 235, 238), the two of thorium (232, 233) and one each of protactinium (233), samarium (149), xenon (135) and boron (10).

Data for the binding energy per nucleon data were largely drawn from the tabulation of Audi et al (2003,a). Binding energy per nucleon is isotope-specific, so unless the isotope was specified, the value for the most abundant isotope was used. The half lives of isotopes, from Audi et al (2003,b) are listed only for records that are isotope-specific. Values of the absorption and scattering cross-sections are from Glasstone and Sesonske (1994), which also contained the cross sections of some isotopes not found elsewhere. The remaining cross sections for the isotopes are from the compilation of nuclear data of the IAEA (2008).

Granta EduPack allows the data to be presented in ways that bring out features of interest – *Figures 11 to 14*.

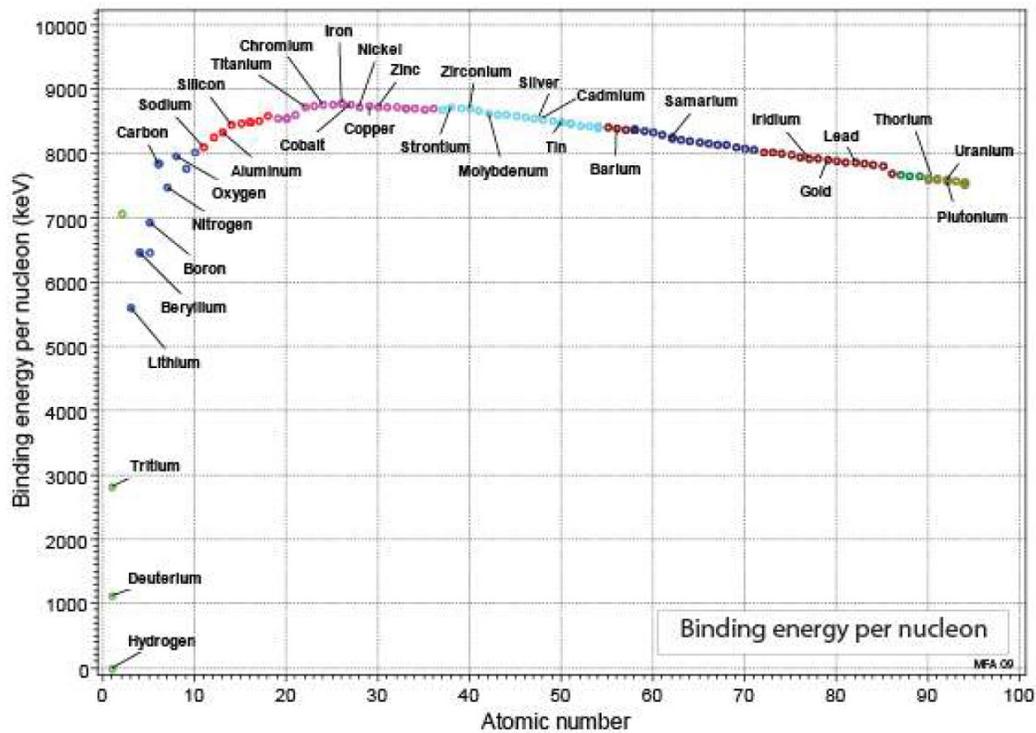


Figure 11. The binding energy per nucleon, a measure of nuclear stability, for the elements of the periodic table. The most stable nucleus is that of iron, though many others lie close.

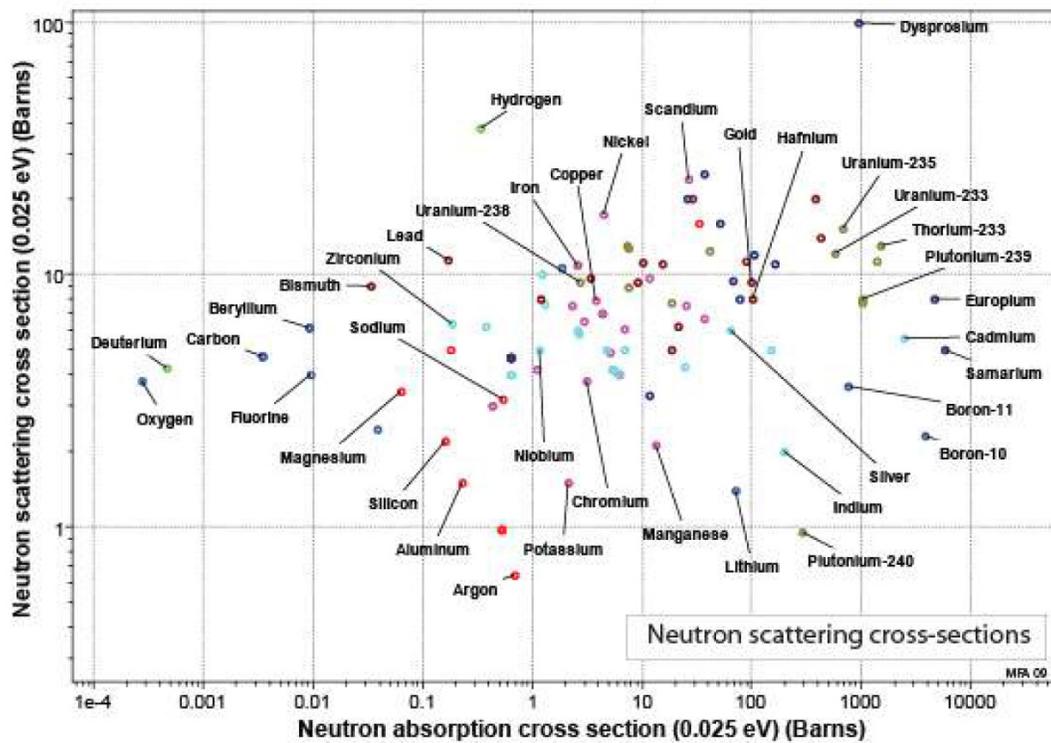


Figure 12. The neutron capture cross-section for scattering and for absorption for the elements of the periodic table. Diagonal contours show the ratio of the two.

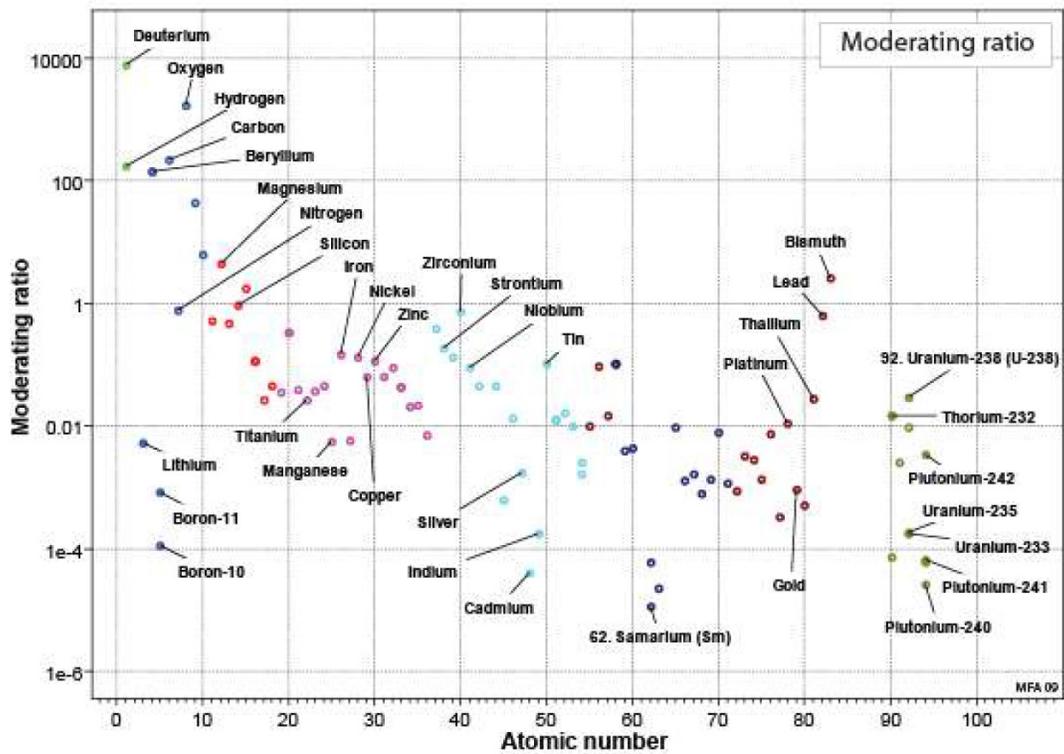


Figure 13. The combination of scattering cross sections and atomic weight that characterizes the effectiveness of an element as a neutron moderator. Hydrogen, oxygen (water) and graphite are all effective moderators.

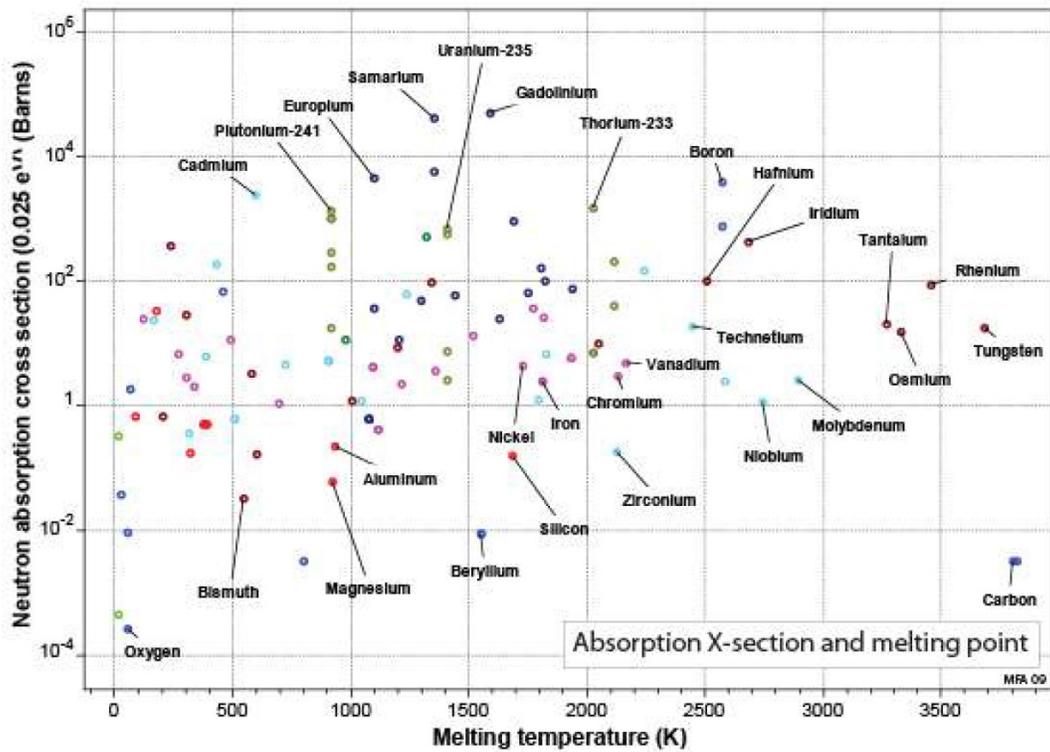


Figure 14. Materials for cladding: adequate melting point, resist corrosion in the cooling medium and have minimal cross-section for absorption.

The first is a plot of binding energy per nucleon against atomic number. The most stable nuclei (those with the greatest binding energy) cluster around iron. It is clear from this plot that elements with a higher atomic number than iron will generally favor fission whilst those lower than iron will generally favor fusion, and that fission releases, at most, a few hundred keV per event, whereas fusion can release many thousands.

Moderator materials. *Figure 12* shows the scattering cross-section σ_s against the absorption cross-section σ_a . Neutron moderators slow neutrons by elastic collisions that ultimately reduce their energy from keV to a few kT (about 0.1 eV) by elastic collisions, without absorbing them (absorption results in transmutation and unwanted fission products). Thus good moderator materials have high σ_s and low σ_a . They are the materials at the upper left of *Figure 12*. The effectiveness of a moderator also depends on the mass of the nucleus, since this determines the momentum transfer in a collision with a neutron. A more meaningful measure of effectiveness as a moderator takes this into account. It is the *moderating ratio* M :

$$M = \xi\sigma_s/\sigma_a,$$

where ξ is the fraction of neutron energy lost per scattering event and is given by

$$\xi = 6/(3A+1)$$

where A is the atomic mass number. *Figure 13* is a plot of the moderating ratio against atomic number. A high ratio indicates a good moderating behavior. The most used moderators are light water H_2O , heavy water, D_2O , carbon (graphite) and beryllium, exactly as the figure suggests.

Control-rod materials. Control rods absorb neutrons, controlling the rate of fission of the fuel by quenching the chain reaction that generates them. The best materials for such control have high absorption cross-sections, but do not themselves transmute to fissionable material. These are the material on the extreme right of *Figure 12*, excluding the fuels uranium, plutonium and thorium. Thus control rods are generally made of cadmium, indium, silver, boron, cobalt, hafnium, europium, samarium or dysprosium, often in the form of alloys such as Ag-In-Cd or compounds such as boron carbide, hafnium diboride or dysprosium titanate. The absorption capture cross-sections of these elements depends on neutron energy so the compositions of the control rods is chosen for the neutron spectrum of the reactor that it controls. Light water reactors (BWR, PWR) operate with thermal neutrons, fast reactors with high-energy “fast” neutrons.

Cladding materials. Nuclear fuel rods are made up of fuel pellets contained in tubular cladding, which separates the fuel from the coolant. Cladding materials must be corrosion resistant, they must conduct heat well, and have low absorption cross-section so that neutrons pass through them easily; and of course they must have a melting point well above the operating temperature of the fuel rods. *Figure 14* shows absorption cross-section and melting temperature of potential cladding materials. Those most commonly used are based on zirconium or beryllium (bottom row of elements) or on stainless steel, the ingredients of which (iron, nickel, chromium) appear in the second row up. Advanced reactors, now under consideration, may require cladding with a higher melting point.

5. Summary and conclusions

As outlined above, the Granta EduPack software provides a useful means of exploring nuclear power systems and the materials associated with them. The ability to find out about reactor systems and immediately access details of the associated materials is something offered by the data structure of the Nuclear Power Systems database. The fact that it is possible to view the materials in the context of the reactor system and then access the relevant properties is of educational benefit and allows a greater understanding of materials selection for nuclear power systems. The inclusion of temperature dependent properties of materials and the effect of neutron irradiation represents some of the most important factors in materials selection for reactor design. This is an example of how the existing Granta EduPack database has been adapted in the most appropriate manner for the topic as well as considering what is useful in an educational context. The absence of functional data for some materials is mainly a result of the lack of publicly available data. The fact that the Granta EduPack selection tools can also be applied to temperature dependent data shows benefits of accessing it through the software.

The modifications to the Elements database bring out the influence of fundamental physics on material selection considerations. As shown in the previous section, the production of a small number of graphs using the Granta EduPack software are able to largely justify the materials selected for reactor systems as well as demonstrating fundamental principles behind the fission process. Energy dependent cross section data for certain isotopes has been included. These have been selected on the basis of educational considerations. However the Elements database is not a comprehensive database of neutron reactions. The Granta EduPack software is not designed to accommodate the volume of data associated with such a database and access to comprehensive reaction data is readily accessible through the internet. Therefore the focus of the Granta EduPack database has been to be selective about the data stored such that it is useful in bringing out the issues discussed above.

Overall, it is now possible to view nuclear power systems at different levels through the Granta EduPack system. From largest scale of reactor systems to smallest scale of nuclear properties it is possible to gain an understanding of materials selection issues of nuclear reactor systems. With the inclusion of details on certain next generation reactors including a prototype fusion reactor the software allows the exploration of material considerations of future technologies. This is during a time in which the process of materials selection for next generation technologies is still underway. An understanding of the relevant considerations at all levels is therefore vital.

Appendix 1: Definition of nuclear properties

Binding energy per nucleon (Usual units: keV)¹

The binding energy B is the energy required to break apart a nucleus into its constituent nucleons. The difference between the mass of the isolated nucleons and the mass of a bound nucleus is the mass defect Δm . The total binding energy of the nucleus, B is given by

$$B = \Delta m c^2$$

where c is the speed of light in a vacuum. The binding energy per nucleon is B/A where A is the number of nucleons in the nucleus. It varies between isotopes so that some are more stable than others. The value listed in the database is that for the most abundant isotope unless otherwise stated.

Half life (Usual units: years)

The time after which the number of a given radioactive nuclides in a sample halve by radioactive decay. If there are N_0 radioactive nuclides at a time $t = 0$, the number of radioactive nuclides N at a time t is given by

$$N = N_0 \exp - \lambda t$$

where λ is the decay rate. The half life $t_{1/2}$ is the time at which $N = N_0/2$, giving

$$t_{1/2} = (\ln 2)/\lambda$$

Cross sections (Usual units: barns)²

The cross section for a process is the measure of a probability of the process occurring. For a neutron induced process it is the effective area presented by a target nuclei to a beam of neutrons, and thus has the dimensions of area. For a thin sheet of nuclei with number density n and an incident neutron beam of flux Φ , the rate of the process occurring per unit volume R is given by

$$R = \Phi n \sigma$$

σ is the cross section (also called the microscopic cross section).

- **Absorption cross section, σ_a** . The microscopic cross section for the absorption of a neutron by an atom. This is the sum of the fission and capture cross sections.
- **Scattering cross section, σ_s** . The microscopic cross section for the scattering of a neutron by an atom.
- **Fission cross section, σ_f** . The microscopic cross section for the absorption of a neutron by an atom and the subsequent splitting of the target atom.

Different isotopes have different values of σ . Unless otherwise stated the value is given for a natural mixture of isotopes. The value of σ is strongly dependent on neutron energy; the values in the database are for thermal neutrons of energy 0.025eV.

¹ 1 keV = 1.6×10^{-16} Joule = 3.38×10^{-17} calories

² 1 barn = 10^{-24} cm² = 10^{-28} m²

Appendix 2: Materials in nuclear power systems, listed by subsystem

Materials in fission reactors

PWR*

Fuel and cladding	Coolant / Moderator	Control	Pressure vessel	Piping/ Internals	IHX/Steam generator
Enriched UO ₂ /MOX Zircaloy 4	Light Water	Ag-In-Cd B ₄ C 304 SS Inconel 627 Boric Acid Borosilicate glass Al ₂ O ₃	SA508 Gr.3 Class 1,2 SA533 Gr.B 308SS, Inconel 617 (Clad)	304SS 316SS ASTM 516 Gr.70 308L	SA533 Gr.B Inconel 600 Incoloy 800 SA515 Gr.60

* Andrews and Jelley (2007); Glasstone and Sesonske (1994); Roberts (1981)

BWR*

Fuel and cladding	Coolant / Moderator	Control	Pressure vessel	Piping/ Internals	IHX/Steam generator
Enriched UO ₂ Gd ₂ O ₃ Zircaloy 2	Light Water	B ₄ C 304 SS	SA508 Gr.3 Class 1,2 SA533 Gr.B 308L SS (Clad)	304 SS 316, 316L 304L 347Inconel SA106 Gr.B SA333 Gr.6	SA533 Gr.B Inconel 600 Incoloy 800 SA515 Gr.60

* Andrews and Jelley (2007); Glasstone and Sesonske (1994); Roberts (1981)

AGR*

Fuel and cladding	Coolant / Moderator	Control	Pressure vessel	Piping/ Internals	IHX/Steam generator
Enriched UO ₂ 25Cr-20Ni SS Graphite*	CO ₂ Graphite	Boron Steel Cd Nitrogen Boronated glass	Pre-stressed concrete Mild steel	Mild Steel Annealed 9Cr- 1Mo steel 18Cr-12Ni SS	Mild Steel Annealed 9Cr- 1Mo steel 18Cr-12Ni SS

*Frost B.R.T. (1994); Nuclear_Graphite_Course; Marshall W. (1983)

LMFBR*

Fuel and cladding	Coolant / Moderator	Control	Pressure vessel	Piping/ Internals	IHX/Steam generator
MOX U-Pu-Zr MC MN 316 SS Depleted UO ₂	Liquid Sodium	B ₄ C 316SS Eu ₂ O ₃ EuB ₆	304SS 316SS 316-FR	304SS 316SS 316-FR Alloy 718	2¼ Cr 1 Mo Steel (SA336) 9Cr-1Mo steels (Modified) Incoloy 800 304SS 316SS

* Andrews and Jelley (2007); Roberts (1981) ; Generation IV Nuclear Energy Systems (2007) Appendix 5.0

VHTR*

Fuel and cladding	Coolant / Moderator	Control	Pressure vessel	Piping/ Internals	IHX/Steam generator
UCO UO ₂ Pyrolytic Carbon* Silicon carbide*	Helium Graphite Nitrogen Molten Salt	Cf/C,SiCf/SiC (Clad)	Modified 9Cr- 1Mo-V Steel P91 SA508 Gr.3 Class 1,2 SA533 Gr.B	Alloys 617 X, XR, 230, 602CA, 800H Carbon fiber reinforced carbon Cf / C SiCf / SiC	Alloy 617 Alloy 230

*Petti et al (2009); Riou et al (2004); Natesan et al (2006); Generation IV Nuclear Energy Systems (2007) Appendix 1.0

Materials in fusion reactors: ITER*

Material	Forms
<p>Thermal shield</p> Stainless steel AISI 304L Ti-6Al-4V Steel grade 660 INCONEL 718 Al ₂ O ₃ coatings Glass epoxy G10 Ag coating	Plates, tubes Plates Fasteners Bolts Plasma sprayed insulation Insulation Coating, 5µm (emissivity)
<p>Vacuum vessel and ports</p> Stainless steel 316L(N)-IG Stainless steel AISI 304 Steel 660 Ferritic stainless steel 430 Borated steels 304B7 and 304B4 INCONEL 718 Stainless steel 316L (B8M) Austenitic steel XM-19 (B8R) Pure Cu	Plates, forgings, pipes Plates Fasteners, forgings Plates Plates Bolts Bolts Bolts Clad

VV support Stainless steel AISI 304 Steel 660 INCONEL 718 NiAl bronze PTFE	Plates, rods Fasteners Bolts Rods Plates
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First wall Beryllium (S-65C or equivalent) CuCrZr Stainless steel 316L(N)-IG	Armor tiles Plates/cast/powder heat sink Plates, pipes
--	--

Blanket and support 316L(N)-IG Ti-6Al-4V CuCrZr INCONEL 718 NiAl bronze Plates Al ₂ O ₃ coatings CuNiBe or DS Cu	Plates, forgings, pipes Cast, powder HIP Flexible support Sheets Bolts Plates Plasma sprayed insulation Collar
--	--

Diverter Cf / C (NB31 or equivalent) Tungsten CuCrZr Stainless steel 316L(N)-IG Steel 660 Austenitic steel XM-19 INCONEL 718 NiAl bronze	Armor tiles Armor tiles Tubes, plates Plates, forgings, tubes Plates, bolts Plates, forgings Plates Plates, rods
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*Barabash et al, (2007); Ioki K. et al (1998); Nishi, H. et al (2008); Tokamak aspx

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