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Light Water Reactor Sustainability Program

IMAC Database v.0.1. – Minerals

Yann Le Pape



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Light Water Reactor Sustainability Program
Fusion and Materials for Nuclear Systems Division

IMAC Database v.0.1. – Minerals

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ACRONYMS

ASR	alkali-silica reaction
BASH	Bourne-again shell
CBS	concrete biological shield
hcp	hardened cement paste
HLW	high-level waste
IMAC	Irradiated Minerals, Aggregates and Concrete
KJMA	Kolmogorov-Johnson-Mehl-Avrami
LMA	Levenberg-Marquardt algorithm
LWR	light water reactor
LWRS	Light Water Reactor Sustainability
MD	molecular dynamics
mXRF	micro X-ray fluorescence
ORNL	Oak Ridge National Laboratory
QA	quality assurance
RIVE	radiation-induced volumetric expansion
TEM	Transmission Electron Microscopy
VCS	version control system
XML	Extensible Markup Language

1. CONTEXT

Light water reactors (LWRs) concrete biological shields (CBSs) are exposed to high neutrons and gamma irradiations [Fukuya et al., 2002, Esselman and Bruck, 2013, Remec et al., 2016] potentially reaching levels for which degradation has been reported in the literature, i.e., $5 \times 10^{18} \text{ n.cm}^{-2}$ at $E > 0.1 \text{ MeV}$ [Hilsdorf et al., 1978, Seeberger and Hilsdorf, 1982]. Reviews of current knowledge on irradiated concrete can be found in [Willam et al., 2013, Rosseel et al., 2016]. At ~ 80 years of operation, it is estimated that the bounding fluence approaches $6 \times 10^{19} \text{ n}^{E>0.1 \text{ MeV}}.\text{cm}^{-2}$, i.e., about 12 times, the potentially critical dose for irradiation-induced damage onset (As countries other than the U.S. may consider different operation extension periods, the bounding fluence can be estimated proportionally). Susceptibility of concrete to neutron irradiation greatly varies as a function of its constituents, i.e., coarse aggregates, sand, and hardened cement paste (hcp). In particular, higher irradiation-susceptibility was found as a direct function of aggregates RIVE [Elleuch et al., 1972, Field et al., 2015, Le Pape et al., 2015], i.e., the propensity of swelling as a function of their minerals contents, structures and textures. Irradiation-induced amorphization, also referred to as *metamictization* when occurring naturally by α -decay in rocks bearing U, Th . . . , also induces significant density change, especially in silicates. For example, the maximum volumetric expansion of quartz and feldspars – a group of rock-forming tectosilicate minerals that make up as much as 60% of the Earth’s crust [Clarke and Washington, 1924, Wedepohl, 1971] – has been shown to be as large as $\approx 18\%$ [Primak, 1958, Zubov and Ivanov, 1966] and $\approx 8\%$ [Krivokoneva, 1976], respectively, while the change of density in calcite remains rather low ($\approx 0.3\%$ according to [Wong, 1974]) Depending on the mineralogical content, considerable variations in aggregate RIVE [Dubrovskii et al., 1967, Kelly et al., 1969, Dubrovskii et al., 1970, Seeberger and Hilsdorf, 1982] have been observed as described in the comprehensive review by Field et al. [2015]. Moreover, some observed post-irradiation expansions exceed what is considered as detrimental by alkali-silica reaction (ASR) researchers (e.g., [Fournier and Bérubé, 2000, Rajabipour et al., 2015]). Because the CBS structural concrete is made of $\approx 70\%$ of aggregates by volume, RIVE imposes severe stresses on the surrounding hcp leading to micro-cracking, or even fracturing [Le Pape et al., 2015, Giorla et al., 2016]. Because, for obvious economical reasons, the concrete used for the construction of any nuclear power plants structures is made with local materials, large variations of mineralogical composition of aggregate are expected causing major differences in terms of susceptibility against irradiation. Hence, the significance of irradiated structure depends directly on its constituents, and in particular on the aggregate-forming minerals composition, texture and volume fraction.

2. MOTIVATIONS AND OBJECTIVES

The DOE LWRs Program Materials and Aging Degradation Pathway has developed a holistic approach, based on materials characterization and modeling, to assess the susceptibility of concrete against irradiation effects and the structural significance of irradiated concrete biological shield in light water reactors (LWRs). – Fig. Figure 1. This approach aims at using experimental data collected in test reactors, and possibly after harvesting from in-service reactor, to help the development and the validation of irradiated concrete models to be utilized for the structural assessment of any specific LWR CBS. The development of a materials database is central in order to:

1. Connect materials characterization and modeling tools with reliable irradiated properties;
2. Facilitate data searching for correlation analysis;
3. Validate irradiated concrete models, in particular, upscaling models (micromechanics or meso/micro-scale numerical models), i.e, minerals → aggregate → concrete; and,
4. Assess the susceptibility of a specific aggregate or concrete against irradiation.

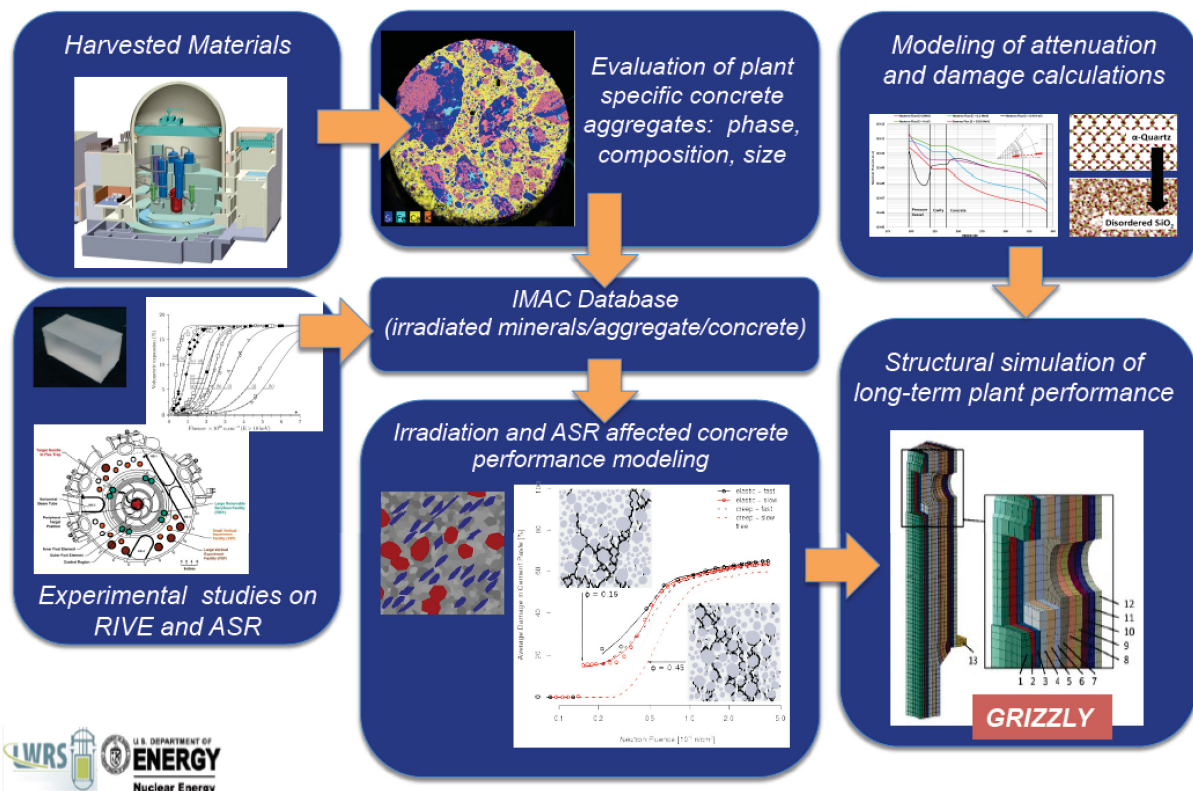


Figure 1. Risk-assessment of the irradiation effects on concrete and their structural significance. DOE LWRs Strategy.

A number of irradiated concrete and aggregate properties (compressive and tensile strength, Young modulus, loss of mass and radiation-induced expansion) have been previously collected [Field et al., 2015]. Although likely-silicate-bearing aggregates were found to be more RIVE-prone than likely-carbonate-bearing aggregates, it appears that the ASTM classification [ASTM C294-12] of aggregates for concrete fails to define

the resistance of aggregates against neutron irradiation. Typical examples can be found in Gray [1971] where different aggregates categorized as *limestone*, i.e. primarily carbonated rocks, exhibit very low expansions, as expected for carbonates, to high linear expansions >1%. The lack of information on the detailed mineralogical contents result in inherent limitations when interpreting the data, in particular, with regard to the large observed scatter. Moreover, the representativity of irradiated aggregate or concrete data against the actual concrete composition used for CBS is more difficult to assess.

Hence, to develop a more rational classification of irradiation-sensitive aggregate, the Light Water Reactor Sustainability (LWRS) Program approach is to adopt a “bottom-to-top” methodology aiming at characterizing irradiated mineral analogues, as a first step, before studying irradiated aggregates. i.e., understanding and modeling the interactions between rock-forming minerals, in a second step, and finally, address irradiated concrete using tools previously developed [Le Pape et al., 2015, Giorla et al., 2015, 2017]. Numerous neutron-irradiated minerals RIVE are scattered in the public ‘Western’ literature, e.g., [Wittels, 1957, Primak, 1958, Wong, 1974, Seeberger and Hilsdorf, 1982]. . . along with on-going irradiated minerals analogues study at Oak Ridge National Laboratory (ORNL) [Rosseel, 2016]. In addition, more recently, Russian literature was made available to the LWRS Program researchers. These data are extremely valuable as varied minerals, aggregates formed with similar minerals, and concrete made with the same aggregate were tested in similar irradiation conditions. It must also be noted that past research programs related to high-level waste (HLW) storage resulted in the publication of data on the resistance of minerals against ion-irradiation [Eby et al., 1992, Dran et al., 1992]. More recently, electron-irradiation amorphization of minerals was also studied [Muto and Maruyama, 2016]).

However, limited data on irradiated elastic properties are still available: all elastic tensor constants, c_{ij}^* , [Mayer and Gigon, 1956, Mayer and Lecomte, 1960, Zubov and Ivanov, 1967] are available for irradiated quartz only. On-going experiments of mineral analogues aims at providing elastic properties for other minerals. It must also be said that molecular dynamics (MD) can help estimate RIVE amplitude and the c_{ij}^* constants of irradiated minerals (in particular, where data is missing), although, some uncertainties about the energy potential in complex crystalline system limit the use of these results.

Finally, the experimental characterization of rock-forming minerals in concrete aggregate using, for example micro X-ray fluorescence (mXRF) and petrographic analysis, requires elements and oxides compositions data.

The Irradiated Minerals, Aggregates and Concrete (IMAC) database aims a collecting all the aforementioned scattered information and data using a systematic approach, including the use of publicly available standard format to export the database and the documentation of the original sources. The database development tools and schedule are provided in sections 3. and 6., respectively.

3. DEVELOPMENT TOOLS

The IMAC database is currently hosted on an internal server at ORNL: https://code-int.ornl.gov/y1b/IMAC_database. Access is currently limited to a small number of developers. However, a public release is envisioned for Summer 2017. For the sake of increased quality assurance (QA), the database is being developed and managed by GitLab <https://about.gitlab.com/>, a web-based version control system (VCS) Git <https://git-scm.com/> repository manager with wiki and issue tracking features, using an open source licence. Any committed change, i.e., addition/modification of new/existing data and features, is tracked and recorded. The database uses primarily Scilab <http://www.scilab.org/>, a free open source software for numerical computation, similar to MathLab, to:

1. Input and structure data in the database,
2. Export the database in Extensible Markup Language (XML) files to allow the use of the third-parties software such as finite element code, and,
3. Export the database in L^AT_EX-format automatically-generated documentation.

The data structures generated in Scilab can advantageously be utilized by upscaling micromechanics-type analysis, e.g, [Le Pape et al., 2015]: minerals → aggregate → concrete.

The IMAC repository currently includes the following folders:

bib contains the bibliographic database `IMAC.bib`, using BiB_TE_X reference management software (<http://www.bibtex.org/> – For the sake of convenience, the installation of a graphical application for managing BiB_TE_X files is recommended: e.g., JabRef, <http://www.jabref.org/>, an open software using Java). Whenever accessible, copies of the original data sources, i.e., journal articles, proceedings, and sometimes books, are stored in `bib/pdf`. This feature allows future verification of anomalous or suspicious data. Note that BiB_TE_X citations entries correspond strictly to the cross-reference entries in the database `.sci` files to exchange information between the bibliographic database and the *materials* database

doc/pub contains the L^AT_EX file `IMAC_database.tex` necessary to compile the database in `.pdf` format. Note that `IMAC_database.pdf` being automatically generated, some information can be redundant. For example, each of the < 21 elastic constants data of the minerals includes the information on the experimental technique used (In most cases, the same technique was used to derive all elastic constants of the same mineral). That information is repeated in the exported file. The main reason for these duplications in the `.sci` data files is to ensure that each data point is correctly and thoroughly informed in its data structure to permit efficient data search.

minerals contains the minerals database *per se*. Each mineral corresponds to a specific folder name, e.g., `minerals/albite`, containing multiples data files (generally `.sci` files, although some information can also be stored in `.txt` (plain text) files when appropriate, e.g., long tables or figure captions. or `.png` image files, for scanned figure before digitization). For each mineral, a master Scilab file loads all information/data. The name of the master file corresponds to the folder name, i.e., the mineral names, e.g., `minerals/albite/albite.sci`. XML exports also use the mineral names, e.g., `minerals/albite/albite.xml`. L^AT_EX exports use the extension `_pub.tex`, e.g., `minerals/albite/albite_pub.xml`.

scilab contains Scilab executable files need to run the database. In particular, loading the database library and exporting the minerals database are performed by launching

`quick-screen-minerals.sce` in a Scilab console, after configuring and launching `environment_variable.sci` (See config).

`config` contains only one configuration file, `environment_variable.sci`, to be edited by each user to provide information about the path to the IMAC database end export options.

`lib` contains all Scilab functions library files necessary for description of the data structures, e.g., `mineral_template.sci`, exports, e.g., `xml_export.sci`. It also contains Bourne-again shell (BASH) scripts to extract some general information from publicly-accessible minerals web-database, e.g., `mineral_classification.sh`.

`reactors` contains currently one file only: `list_reactors.sci` linking test reactor names and channels to codes used in the database. Future developments envision to add information on the neutron fluence spectrums.

4. CURRENT DEVELOPMENT STATUS

The December 2016 release includes *minerals* data only. **Currently, the IMAC database contains only 42 minerals which corresponds to about 120 Mb of source code files, pdf documentation, and 72,000 lines of XML output data.** The number of imported mineral may seem poor compared to the >4,500 different known minerals. However, it must be noted that this database is oriented toward concrete aggregate. In that regards, more than 90% on the crust is composed of silicate minerals. Most abundant silicates are feldspars – plagioclase (*approx*40%) and alkali feldspar (\approx 10%). Other common silicate minerals are quartz (\approx 10%) pyroxenes (\approx 10%), amphiboles (\approx 5%), micas (\approx 5%), and clay minerals (\approx 5%) [Wedepohl, 1971]. The rest of the silicate family comprises 3% of the crust. Only 8% of the crust is composed of non-silicates, i.e., carbonates, oxides, sulfides. . . Although the IMAC database is subject to expansion in the future, the current list of minerals covers, to a large extent, concrete aggregate-forming minerals. Minerals currently available in IMAC are albite, analcime, andesine, ankerite, anorthite, anorthoclase, augite, biotite, bromellite, bronzite, bytownite, calcite, cassiterite, chamosite, clinocllore, cordierite, corundum, diopside, dolomite, enstatite, fluorapatite, forsterite, hematite, hornblende, hydroxylapatite, labradorite, lizardite, magnesite, magnetite, microcline, muscovite, nepheline, oligoclase, orthoclase, periclase, phlogopite, pyrope, quartz, rutile, sanidine, siderite, silica (amorphous), and, spinel.

5. PRELIMINARY INTERPRETATION OF THE RIVE DATA

On-going studies aims to analyze the minerals RIVE data by series or groups (e.g., Dana's [Dana, 1892] new classification) and provide best-fit parameters assuming two different isothermal RIVE models (S-shaped curve – details of the equations not given here): (1) (**Z**) Zubov and Ivanov's model [Zubov and Ivanov, 1966], or, (2) (**N**) Kolmogorov-Johnson-Mehl-Avrami (KJMA) nucleation-growth model [Kolmogorov, 1937, Johnson and Mehl, 1939, Avrami, 1939, 1940, 1941]., in conjunction with different three temperature-dependent RIVE models: (1) (**L**) linear [Le Pape et al., 2016], or, (2) (**A**) activation energy, or, (3) (**D**) Denisov's tabulated values. . The RIVE data from the IMAC database are fitted with combined models (ZL), (ZA), (NA) and (ZD) neutrons and all fluence are normalized [Denisov et al., 2012] at $E > 10$ keV. Because of the uncertainties related to the *average irradiation temperature*, temperature is analyzed as a probabilistic variable.

For the sake of illustration, the analysis made on irradiated plagioclases (feldspars) is presented. Feldspars (KAlSi_3O_8 - $\text{NaAlSi}_3\text{O}_8$ - $\text{CaAl}_2\text{Si}_2\text{O}_8$) are a group of rock-forming tectosilicate minerals that make up as much as 60% of the Earth's crust [Clarke and Washington, 1924, Wedepohl, 1971] Feldspars crystallize in both intrusive and extrusive igneous rocks, are also present in many types of metamorphic rock, and are also found in many types of sedimentary rocks. Feldspars are generally separated in two groups: plagioclase (Pl, sodium-calcium bearing minerals, triclinic) and alkali feldspar, also known as potash feldspars, or K-feldspar (Kfs, sodium-potassium bearing minerals, triclinic or monoclinic). The two groups meet at the high-sodium end-members, i.e., albite (Ab), oligoclase (Olg) and anorthoclase (Ano) – Figure 2. The regression model

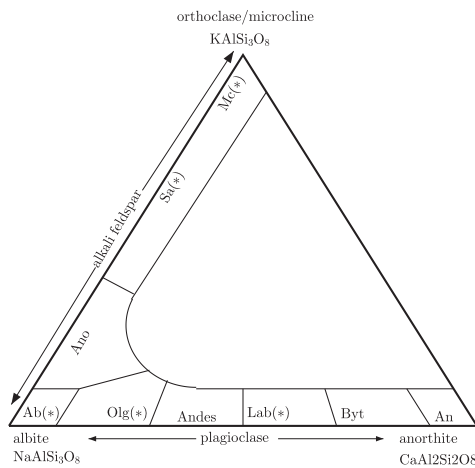


Figure 2. Feldspar ternary diagram (sodium-calcium-potassium). (*) indicates minerals for which RIVE data are available. Ab: albite, An: anorthite, Andes: andesine, Ano: anorthoclase, Byt: bytownite, Lab: labradorite, Mc: microcline, Sa: sanidine

results for plagioclases expansions are presented in the scatter plots Figure 3 and in Table 1. The most *reliable* expansion model was found to be model (ZA) with $r^2 = 0.96$ and a 90% confidence interval error of 0.76%. Similar on-going analysis are being performed on other silicates and carbonated groups. These minerals-RIVE models will be used in subsequent analysis/modeling of the irradiated aggregates to be implemented in phase 2 (v0.2) of the IMAC database.

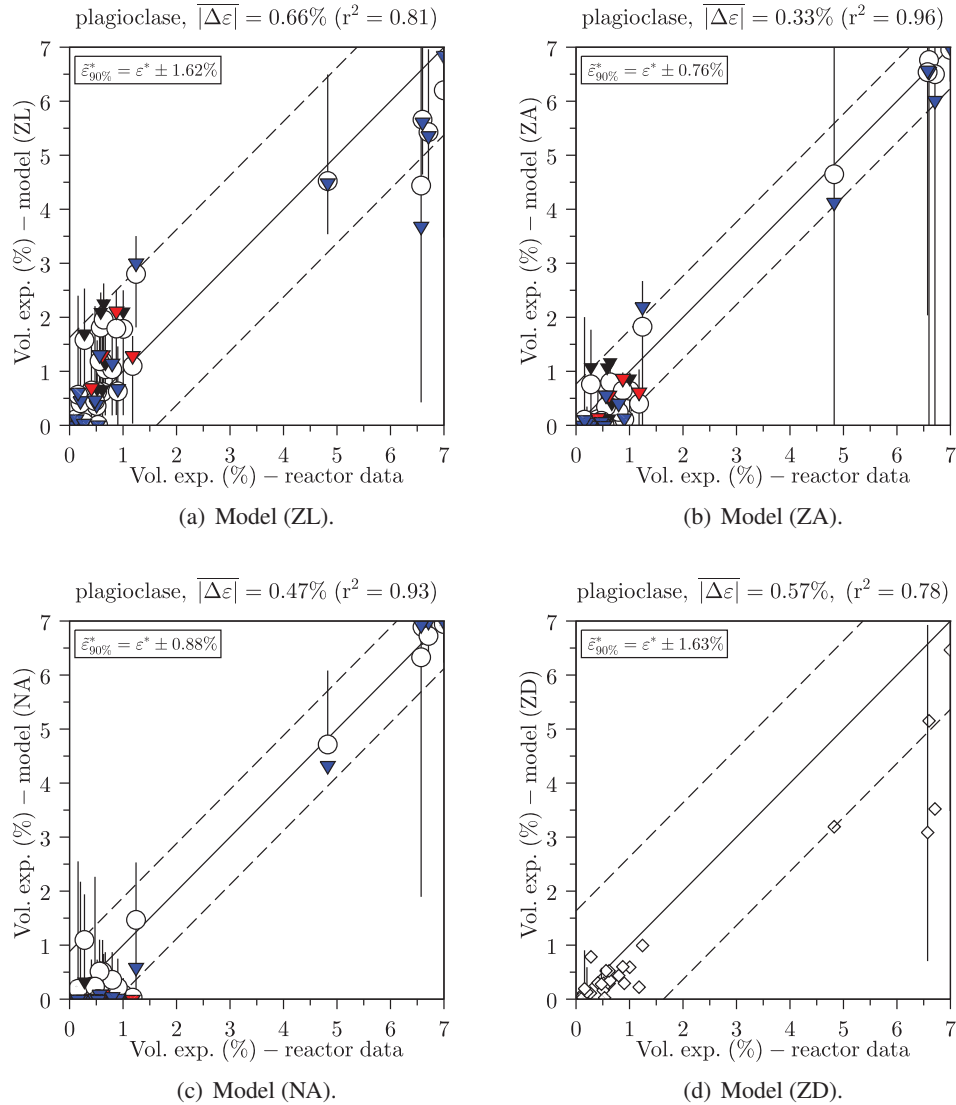


Figure 3. Scatter plot (plagioclase). (○): Mean calculated expansions, i.e., $\bar{\varepsilon}^*$. (▼): albite; (▼): labradorite; (▼): oligoclase: Calculated expansions assuming the mean values of the best-fit parameters. (◇): expansion at mean temperature (model ZD only). Vertical bar: min./max. calculated expansions (temperature uncertainties). Dashed lines: model error at a 90% interval confidence (See equation provided in upper-left corner of the plot).

Table 1. Plagioclases: Best-fit parameters, regression coefficients and errors. (†): $n^{E>10 \text{ keV}} \cdot \text{pm}^{-2} \text{C}^{-1}$, (‡): $n^{E>10 \text{ keV}} \cdot \text{pm}^{-2}$, (*): $K \cdot \tilde{\varepsilon}_{90\%}^* = \varepsilon^* \pm \text{err}$

model	parameters				err	$ \overline{\Delta\varepsilon} $	r^2
	$a_c^{(\dagger)}$	$b_c^{(\ddagger)}$	$a_L^{(\dagger)}$	$b_L^{(\ddagger)}$			
(ZL)	0.0173 (39%)	-0.7672 (51%)	0.0330 (20%)	-0.1765 (386%)	1.62%	0.67%	0.82
	$\Phi_c^{(\ddagger)}$	$E_{a,c}/R^{(*)}$	$\Phi_L^{(\ddagger)}$	$E_{a,L}/R^{(*)}$			
(ZA)	0.1451 (66%)	3728 (44%)	1.6110 (16%)	2118 (18%)	0.76%	0.34%	0.96
	$\Phi_c^{(\ddagger)}$	$d^{(\#)}$	$E_{a,c}/R^{(*)}$				
(NA)	1.7034 (20%)	9.3311 (164%)	2172 (17%)		0.88%	0.47%	0.94
	Tabulated values in Denisov's et al.						
(ZD)					1.64%	0.47%	0.79

The interpretation of highly-valuable data from the Russian literature provide new perspectives on irradiated minerals and guidance on the susceptibility of aggregates against irradiation:

- The susceptibility (ε_{max}^*) of silicates against neutron-irradiation can be ranked as follows: quartz ($\approx 18\%$) > feldspar ($\approx 8\%$) > pyroxene ($\approx 3\%$). Due their nearly perfect basal cleavage, micas RIVE data are subject to large uncertainties.
- The susceptibility (ε_{max}^*) of carbonates against neutron-irradiation, much lower than for silicates, seems to vary slightly with the substitution of calcium by magnesium: dolomite/siderite ($\approx 0.7\%$) > calcite/magnesite ($\approx 0.4\%$).

6. FY2017 DEVELOPMENT SCHEDULE

IMAC v.0.1 – Minerals (December 2016): This document.

IMAC v.0.2 – Aggregate (April 2017): A first database of irradiated concrete properties has been created at ORNL [Field et al., 2015]. The development task will consist in (1) creating a more advanced data structure to include additional properties and metadata, (2) transferring the previously acquired data in IMAC, and, (3) including addition data from the Russian and German literature.

IMAC v.0.3 – Concrete (August 2017): A first database of irradiated concrete properties has been created at ORNL [Field et al., 2015]. The development task will consist in (1) creating a more advanced data structure to include additional properties and metadata, (2) transferring the previously acquired data in IMAC, and, (3) including addition data from the Russian literature.

IMAC v.1.0 – public release (September 2017): This version of the database will be put on a publicly-accessible server.

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A APPENDIX A: AGGREGATES AND MINERALS HIERACHICAL CLASSIFICATION

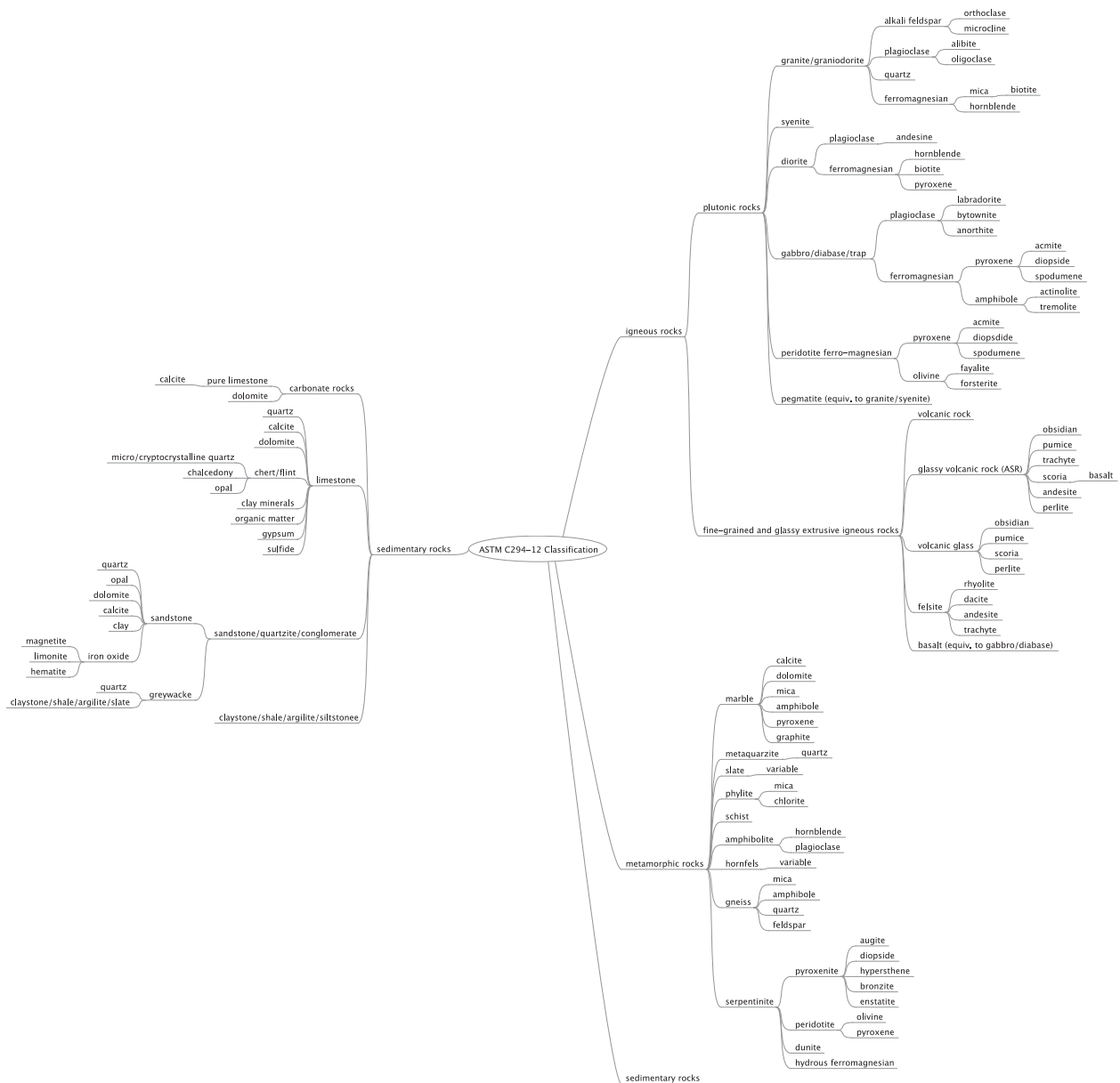


Figure 4. ASTM C294 hierarchical classification of aggregate used in concrete. The ramification extremities show the possible minerals constitutive of the rocks.

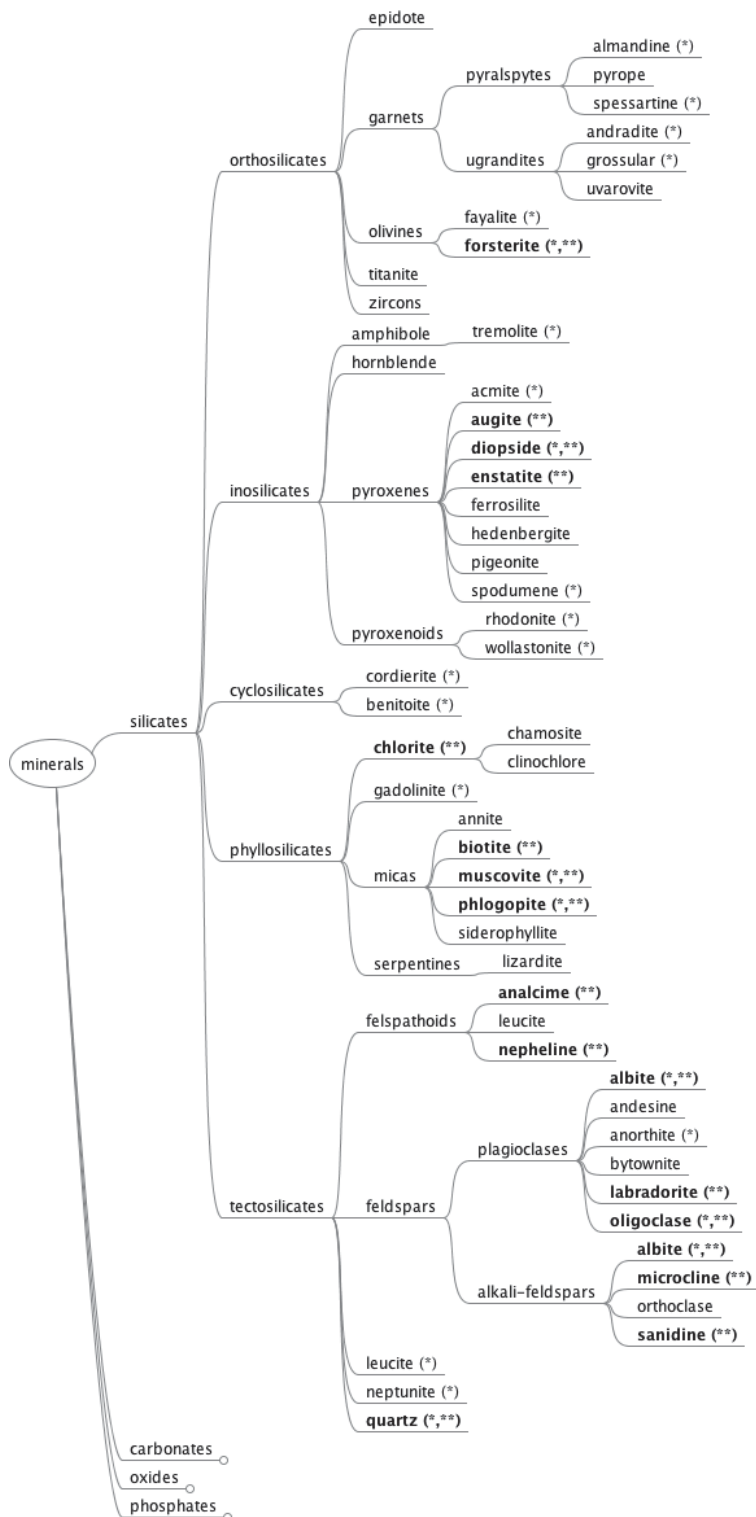


Figure 5. Hierarchical classification of silicates (non exhaustive list). (*) indicates available data obtained by ion-beam irradiation, i.e., critical amorphization dose; (**) corresponds to available data obtained by neutron irradiation.