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FLUKA MONTE CARLO SIMULATIONS ON NEUTRON INTERACTIONS WITH FeCrP AND FeTiP

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Abstract: Andreyivanovite was found in the Kaidun meteorite as individual grains and linear arrays of grains with a maximum dimension of 8 μm within two accumulations of Fe-rich serpentine present in the meteorite. Florenskyite was found as four dispersed grains with a maximum dimension of 14 μm within a single particle of Fe-rich serpentine within the Kaidun meteorite. Their general chemical formulas are FeCrP and FeTiP while stochiometric formulas are $Fe^{0+}Cr_{0.58}Fe^{0+}{}_{0.15}V^{0+}{}_{0.1}Ti_{0.08}Ni_{0.06}Co_{0.002}P$ and $Fe^{0+}{}_{0.98}Ni_{0.13}Ti_{0.85}P$, respectively. We simulated interactions between these two substances and neutron particles (fusion neutrons by reactors, ^{241}Am-Be and ^{252}Cf neutrons used in many scientific investigations and industrial applications). The FLUKA code was used to calculate such interaction parameters as macroscopic cross sections, neutron fluencies and isotope production. Macroscopic cross sections of andreyivanovite and florenskyite are better than concrete (widely used neutron shielding processes). Also radioactive isotopes produced after neutron interactions with these materials are stable. This information may be useful in space and chemistry investigations.

Keywords: *Kaidun meteorite, andreyivanovite, florenskyite, Monte Carlo simulations*

Introduction

The Kaidun meteorite fell on Earth on 3 December 1980 in Yemen (15° 0' N, 48° 18' E). Out of the nearly 60 minerals found within the meteorite, several have not been found in nature, including florenskyite (FeTiP). The meteorite has 842 g of mass and it contains carbonaceous chondrite material. Two phospide based minerals were discovered in the meteorite (Ivanov et al., 2000; Zolensky et al., 2008). They were named andreyivanovite for Andrey Ivanov (Russian geochemist and mineralogist) and florenskyite for Cyrill P. Florensky (Russian geochemist).

Basically, the structure of andreyivanovite consists of Fe, Cr and P elements (Zolensky et al., 2008). Its luster is metallic, transparency is opaque and it has a creamy white color. Crystal system of andreyivanovite is orthorhombic and it belongs

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to the dipyramidal class. The density of andreyivanovite is calculated as 6.65 g/cm^3. The empirical formula of andreyivanovite found in the Kaidun meteorite is $Fe^{0+}Cr_{0.58}Fe^{0+}{}_{0.15}V^{0+}{}_{0.1}Ti_{0.08}Ni_{0.06}Co_{0.002}P$. Since andreyivanovite is a newly discovered mineral, studies on its properties are limited.

Elements that form the structure of are iron, nickel, titanium and phosphorus. It is a Fe-rich serpentine like andreyivanovite (Ivanov et al., 2000). The empirical formula of florenskyite found in the Kaidun meteorite is $Fe^{0+}{}_{0.98}Ni_{0.13}Ti_{0.85}P$.

There are many studies on the Kaidun meteorite. The studies generally are focused on chronology (Petitat et al., 2011), geochemistry (Ivanov et al., 2010) and space research (Ivanov et al., 2004). Interactions between different Kaidun's minerals and cosmic rays were studied to determine the history of Kaidun meteorite (Kashkarov et al., 1995). It appears that the studies about Kaidun meteorites are inadequate. In this paper we investigated neutron and gamma interactions with andreyivanovite ($Fe^{0+}Cr_{0.58}Fe^{0+}{}_{0.15}V^{0+}{}_{0.1}Ti_{0.08}Ni_{0.06}Co_{0.002}P$) or generally FeCrP and florenskyite ($Fe^{0+}{}_{0.98}Ni_{0.13}Ti_{0.85}P$) or generally (Fe, Ni)TiP.

Monte Carlo simulations

The Monte Carlo method is based on random numbers and mathematical algorithms (Ramírez-López et al., 2011). It can be applied for physical systems, especially in nuclear science. In this study we used FLUKA (Ferrari et al., 2005; Battistoni et al., 2006) as a Monte Carlo simulator. FLUKA is a Monte Carlo package used in interactions between all subatomic particles and matter. It has many advantages in terms of wide energy range. For example, it can simulate neutrons from thermal level to 20 TeV. Also it is useful in many scientific areas (high energy experimental physics and engineering, shielding, detector and telescope design, cosmic ray studies, dosimetry, medical physics and radio-biology). We used the FLUKA Monte Carlo code to simulate neutron and gamma radiation with different materials in our latest studies (Korkut et al., 2010; Korkut et al., 2011; Korkut et al., 2012). In some of these studies we compared FLUKA results with experiments. The FLUKA Monte Carlo Simulation code was used to calculate neutron attenuation coefficients, neutron fluencies and radioisotope productions. These two Monte Carlo packages are open codes and their usage is very simple. Firstly, an input file was created in accordance with experimental conditions. This file includes several parameters as primary beam type and energy, material definitions, geometrical setups, some physical sets (if required), desired outputs (transmission, radioisotope production etc…) and finally total number of particles. And then simulation is run and results are read from the output files.

Simulation setups

We used the 2011.2.8 version of FLUKA. For reactor neutrons 14.1 MeV, for ^{241}Am-Be source a neutron spectrum from 100 keV to 12 MeV and for gamma beam 59.54

keV primary energies were used in the simulations. Number of primary particles was entered as 10^6 in simulations. Andreyivanovite consists of 2.79% Ti, 4% V, 21.99% Cr, 46.27% Fe, 0.08% Co, 2.54% Ni and 22.32% P while florenskyite includes 30.36% Ti, 40.83% Fe, 5.69% Ni and 23.11% P. We used these numbers in our simulations. The shape of sample is cylindrical. Thickness of mineral samples is entered in simulations as 5 cm. Detector area and volume values were taken as defaults of the code. We wanted to get particle transmissions, neutron fluencies and radioisotope production after neutron interactions with mineral samples.

Results and discussions

We have simulated neutron interactions with two meteoritic minerals by the FLUKA Monte Carlo simulation code. Also the FLAIR (Vlachoudis, 2009) tool was used to perform data analysis, simulation geometry and create plots. Simulation results obtained for these two minerals are given below into two sections.

Simulation results for andreyivanovite

Microscopic cross section (σ) is related to probability of interaction of neutrons with the target material. The sum of the microscopic cross sections of the individual nuclei in the target material per unit volume is called the Macroscopic Cross Section (Σ)

$$\Sigma = N\sigma \tag{1}$$

where N is the atomic density of the target. To obtain neutron transmissions by simulations, we used USRBDX score card. Neutron transmission values were used from

$$\Sigma = \frac{\ln T}{x} \tag{2}$$

where x is sample thickness. Neutron transmissions and total neutron macroscopic cross sections for three different three neutron energies are shown in Table 1.

Isotope products after neutron irradiations on mineral samples were calculated by using RESNUCLEI score options in FLUKA. As shown in Tables 2 and 3 different isotopes are formed as a result of interactions. As a result of interactions ^{56}Fe was formed in high amounts for the three neutron energies.

Table 1. Neutron transmissions and total macroscopic cross sections for andreyivanovite

Source	Energy (MeV)	Transmission	Total Macroscopic Cross Section (cm^{-1})
^{241}Am-241	4.5	0.26	0.27
^{252}Cf	2.16	0.32	0.23
Reactor	14.1	0.39	0.19

Table 2. Isotope yields after neutron irradiations as a function of mass numbers for andreyivanovite

Am-Be		Cf-252		Reactor	
A	Isotope yield (nuclei/cm3/pr)	A	Isotope yield (nuclei/cm3/pr)	A	Isotope yield (nuclei/cm3/pr)
65	8.38E–08	65	4.94E–08	65	5.31E–09
64	7.18E–06	64	3.36E–06	64	2.42E–06
63	7.82E–09	63	9.96E–08	63	4.17E–06
62	2.09E–05	62	1.11E–05	62	1.33E–05
61	7.78E–06	61	8.82E–06	61	1.50E–05
60	1.62E–04	60	7.90E–05	60	1.11E–04
59	3.06E–04	59	2.25E–04	59	1.53E–04
58	1.43E–03	58	8.40E–04	58	8.16E–04
57	8.77E–03	57	8.22E–03	57	3.79E–03
56	3.13E–01	56	2.25E–01	56	2.43E–01
55	2.83E–05	55	2.77E–05	55	1.08E–01
54	2.10E–02	54	1.03E–02	54	1.23E–02
53	1.22E–03	53	9.73E–04	53	1.94E–02
52	9.25E–03	52	5.08E–03	52	8.88E–03
51	1.35E–04	51	1.06E–04	51	3.55E–03
50	7.84E–04	50	5.34E–04	50	6.38E–04
49	4.36E–04	49	2.09E–04	49	7.48E–04
48	5.77E–03	48	3.83E–03	48	4.21E–03
47	6.21E–04	47	4.75E–04	47	2.05E–03
46	6.71E–04	46	4.47E–04	46	6.48E–04
44	5.62E–06	44	2.33E–07	45	2.71E–04
32	6.21E–07	32	1.46E–06	44	2.89E–05
31	1.02E–03	31	6.62E–04	43	4.26E–05
28	2.47E–06	4	1.41E–06	42	2.33E–06
4	1.16E–04	1	5.80E–04	32	2.30E–07
1	5.24E–03			31	2.64E–04
				30	5.44E–04
				28	1.72E–04
				27	1.91E–05

Fluence is specified as the number of particles traversing a unit surface in a particular point in void per unit time. Neutron fluence means the number of neutrons per unit area (cm^2). We show the neutron fluencies as three different lines plotted in Figs 1-3 for ^{241}Am-Be, ^{252}Cf and reactor neutrons, respectively. As can be seen in these figures, andreyivanovite mineral does not produce thermal or epithermal neutrons.

Table 3. Isotope yields after neutron irradiations as a function of atomic numbers for andreyivanovite

Am-Be		Cf-252		Reactor	
Z	Isotope yield (nuclei/cm^3/pr)	Z	Isotope yield (nuclei/cm^3/pr)	Z	Isotope yield (nuclei/cm^3/pr)
28	5.01E–04	28	2.87E–04	28	2.80E–004
27	4.15E–04	27	2.41E–04	27	5.54E–004
26	3.38E–01	26	2.44E–01	26	3.21E–001
25	4.87E–03	25	5.31E–04	25	5.42E–002
24	1.11E–02	24	6.60E–03	24	2.32E–002
23	2.16E–04	23	1.05E–04	23	1.41E–003
22	7.76E–03	22	5.14E–03	22	7.26E–003
21	5.40E–05	21	7.66E–06	21	6.17E–004
20	5.70E–06	20	2.33E–07	20	2.18E–004
15	8.85E–04	15	6.33E–04	15	1.54E–004
14	1.34E–04	14	3.04E–05	14	6.54E–004
13	2.47E–06	2	1.41E–06	13	1.91E–004
2	1.11E–04	1	5.80E–04	2	1.32E–002
1	5.24E–03			1	5.70E–002

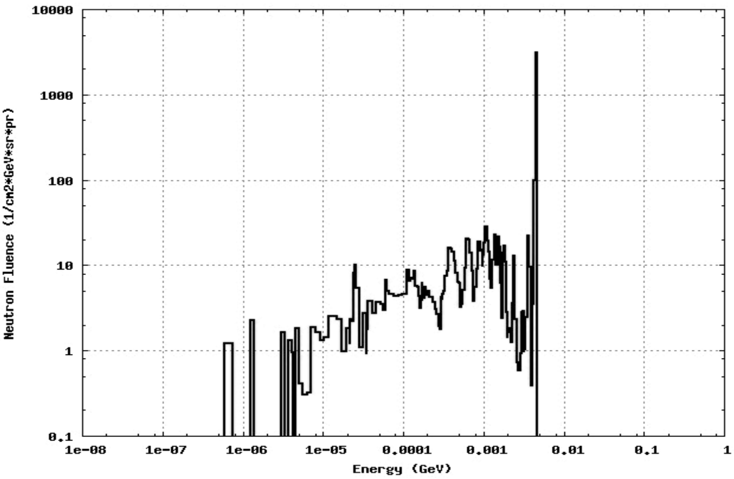

Fig. 1. Andreyivanovite neutron fluence for ^{241}Am-Be

Simulation results for florenskyite

The same FLUKA Monte Carlo simulations shown above were performed for florenskyite. Neutron transmissions and total macroscopic cross sections are given in Table 4. Radioisotope fragments after neutron irradiation as a function of A and Z are shown in Table 5 and Table 6. Neutron fluencies as a function of energy are illustrated in Figs 4-6 for ^{241}Am-Be, ^{252}Cf and reactor energies, respectively.

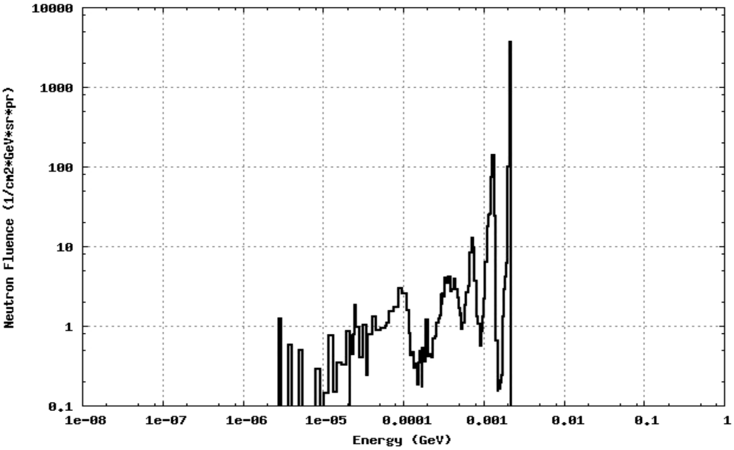

Fig. 2. Andreyivanovite neutron fluence for ^{252}Cf source

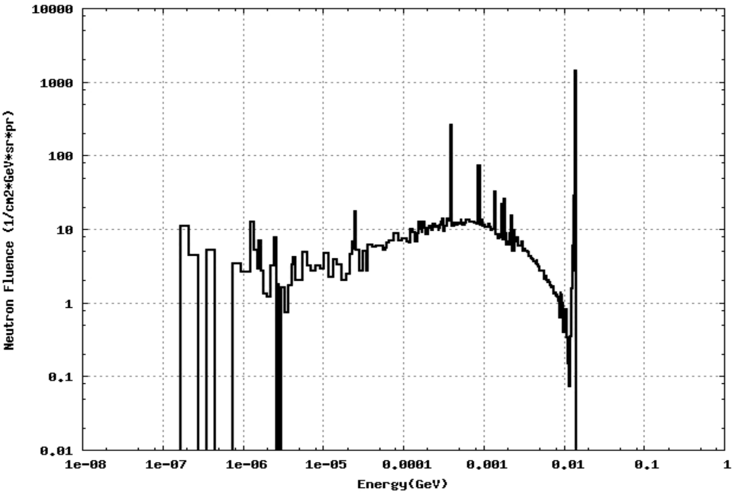

Fig. 3. Andreyivanovite neutron fluence for reactor

Table 4. Neutron transmissions and total macroscopic cross sections for florenskyite

Source	Energy (MeV)	Transmission	Total macroscopic cross section (cm^{-1})
^{241}Am-241	4,5	0.27	0.27
^{252}Cf	2.16	0.28	0.26
Reactor	14.1	0.41	0.18

Table 5. Isotope yields after neutron irradiations as a function of mass numbers for florenskyite

Am-Be		Cf-252		Reactor	
A	Isotope yield (nuclei/cm^3/pr)	A	Isotope yield (nuclei/cm^3/pr)	A	Isotope yield (nuclei/cm3/pr)
65	1.29E–07	65	3.98E–07	65	7.85E–08
64	1.85E–04	64	7.66E–05	64	7.23E–05
63	1.19E–06	63	2.25E–06	63	1.24E–04
62	7.06E–04	62	3.42E–04	62	3.98E–04
61	2.52E–04	61	2.35E–04	61	4.81E–04
60	5.10E–03	60	2.34E–03	60	3.49E–03
59	1.57E–05	59	3.66E–05	59	1.59E–03
58	1.31E–02	58	6.43E–03	58	7.16E–03
57	3.41E–03	57	3.11E–03	57	7.12E–03
56	1.21E–01	56	8.48E–02	56	9.37E–02
55	3.62E–04	55	2.25E–05	55	4.32E–02
54	8.08E–03	54	3.80E–03	54	4.72E–03
53	1.85E–05	53	2.36E–07	53	7.34E–03
51	5.00E–06	51	1.27E–06	52	1.22E–04
50	4.63E–03	50	2.56E–03	51	5.11E–04
49	6.27E–03	49	2.97E–03	50	3.03E–03
48	8.31E–02	48	5.33E–02	49	5.57E–03
47	8.89E–03	47	6.77E–03	48	6.01E–02
46	9.70E–03	46	6.21E–03	47	2.92E–02
44	8.38E–05	44	2.61E–06	46	9.28E–03
43	5.87E–07	32	1.09E–04	45	3.88E–03
32	5.37E–05	31	4.83E–02	44	4.48E–04
31	7.62E–02	4	1.42E–05	43	6.02E–04
28	1.66E–04	1	3.14E–03	42	3.33E–05
4	6.34E–04			32	1.29E–05
1	1.65E–02			31	1.94E–02
				30	4.07E–02
				28	1.28E–02
				27	1.51E–03
				4	2.37E–02
				3	4.22E–07
				2	9.03E–04
				1	8.82E–02

Table 6. Isotope yields after neutron irradiations as a function of atomic numbers for florenskyite

Am-Be		Cf-252		Reactor	
Z	Isotope yield (nuclei/cm^3/pr)	Z	Isotope yield (nuclei/cm^3/pr)	Z	Isotope yield (nuclei/cm^3/pr)
28	1.54E–02	28	8.67E–03	28	8.67E–03
27	3.55E–03	27	5.46E–04	27	1.01E–02
26	1.32E–01	26	9.18E–02	26	1.25E–01
25	1.88E–03	25	2.00E–04	25	2.11E–02
24	3.14E–05	24	4.13E–07	24	4.92E–03
22	1.12E–01	22	7.17E–02	22	1.00E–01
21	7.66E–04	21	1.06E–04	21	8.72E–03
20	8.59E–05	20	2.61E–06	20	3.16E–03
15	6.59E–02	15	4.62E–02	15	1.10E–02
14	1.04E–02	14	2.29E–03	14	4.92E–02
13	1.66E–04	2	1.42E–05	13	1.43E–02
2	6.34E–04	1	3.14E–03	2	2.37E–02
1	1.65E–02			1	8.91E–02

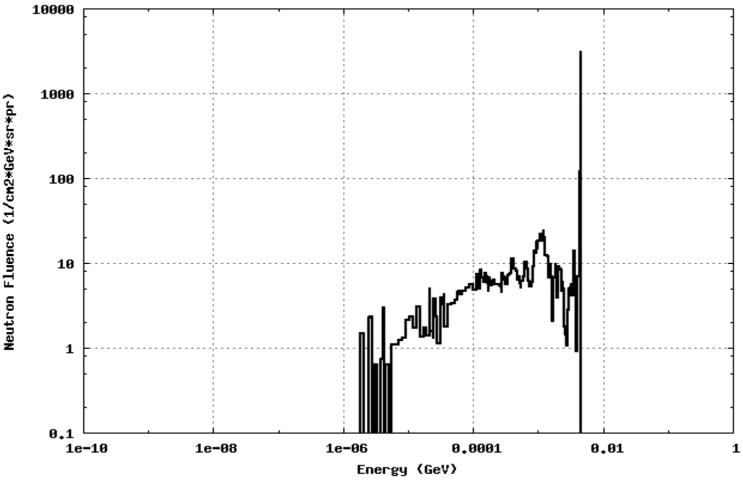

Fig. 4. Florenskyite neutron fluence for ^{241}Am-Be source

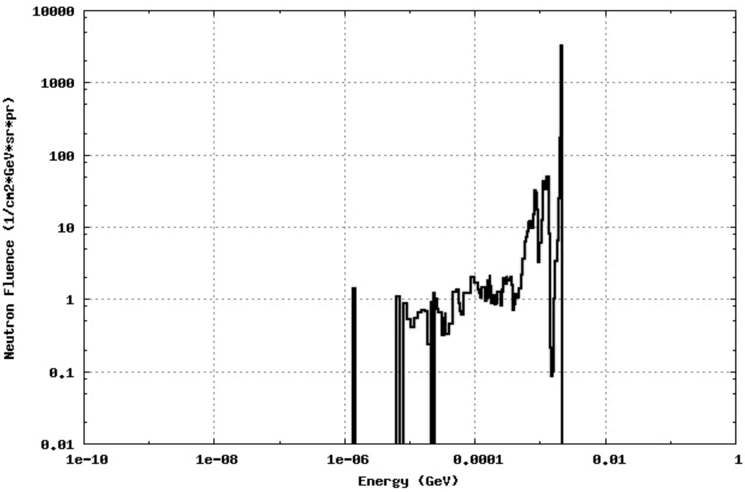

Fig. 5. Florenskyite neutron fluence for ^{252}Cf source

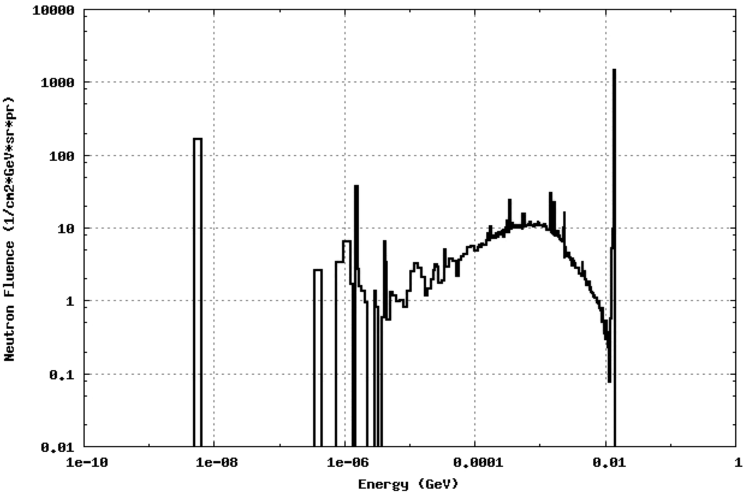

Fig. 6. Florenskyite neutron fluence for reactor

Conclusions

In this paper we calculated several parameters regarding interactions between three different energy neutrons and andreyivanovite and florenskyite, minerals found in the Kaidun meteorite. Kaidun is a meteorite which fallen in the Yemen region in 1980. After this event two new minerals were identified by Ivanov et al., 2000 and Zolensky et al., 2008. It was reported by Ivanov (2004) that Kaidun might originate from Phobos (Martian moon). Therefore, information on interactions between radiation and these compounds may be useful in terms of space research and radiation physics. Also we calculated neutron total macroscopic cross section values for these materials. If these values are compared with the results by FLUKA ($\Sigma_{\mathbf{Cf\text{-}252}}$= 0.149 cm^{-1}, $\Sigma_{\mathbf{Am\text{-}241/Be}}$= 0.148 cm^{-1} and $\Sigma_{\mathbf{Reactor}}$= 0.120 cm^{-1}), the neutron shielding capacity values for the investigated minerals are satisfactory.

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