

(n, α) TRANSMUTATION OF AlN NANOPARTICLES UNDER THE NEUTRON FLUX

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Abstract. (n, α) transmutation in the AlN nanoarticles has been studied by computer modeling at the different neutrons energies. Neutron transformation have been investigated separately for Al and N atoms in the AlNnanoparticles. Due to the dissimilar probability of (n, α) transformation cross-section for various stable isotope of Al and N atoms, modeling have been carried out separately for individual isotopes. The energy for (n, α) transmutation in both N and Al isotopes were defined.

Keywords: nano AlN, (n, α) transmutation, effective cross-section.

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1. Introduction

Recently silicon and nitrogen based compounds are one of the important materials to application in the nuclear science due to the perfect physical properties (Huseynov *et al.*, 2020; Huseynov *et al.*, 2019a, 2019b; Huseynov & Jazbec, 2019; Huseynov, 2018a; Franco & Shanafield, 2004; Guinan, 1989; Kinoshita, 1992; Berzina *et al.*, 2007; Feneberg *et al.*, 2010). High thermal conductivity and good mechanical and chemical stability are the specific properties of these type of ceramic materials. These properties confirm that such type of materials are good candidate in the nuclear environments are under consideration for a wide range of application. On the other hand, above-mentioned materials are semiconductor ceramics with having good optical properties and very large application areas due to the wide bandgap and high concentration doping capabilities. Note that, the physical properties can be controlled depneding on the doping type and methods.

Spectral properties of AlN ceramics have been intensively investigated during last years (Franco & Shanafield, 2004; Guinan, 1989; Kinoshita, 1992) and it's known that AlN have a good photoluminescence propertiesin the UV – visible light spectral region (Franco & Shanafield, 2004; Guinan, 1989). Simultaneously, we have to note that this compound can be doped with rare-earth elements using different methods and the optical properties can be controlled depending on the rare-earth ions due to the different valence and optical centers (Berzina *et al.*, 2007; Feneberg *et al.*, 2010). Thus, the

application area of the AlN is not only cover in the visible range of the wavelength also cover from UV to IR range of the light [11]. Moreover, AlN properties of high thermal conductivity for about 170–220 W/m·K at room temperature and low thermal expansion coefficient of $4.3\text{--}4.6 \cdot 10^{-6} \text{ K}^{-1}$ in the range of about 300 ÷ 670 K temperature are approximately comparable to silicon carbide (SiC) which is widely used in nuclear applications (Franco & Shanafield, 2004).

The neutron irradiation method is one of the best ways to study nuclear application possibilities of the materials. Also, here should note that the neutron irradiation method is the most accurate method in doping. The physical properties of materials can be controlled and improved by this method (Huseynov, 2016). This high energy neutron causes changes in structure of the materials, produces a host is displacement cascades. In general, modification in micro- and nanostructure of irradiated materials can be occurred by many factors: namely temperature, primary knock-on atom energy, displacement dose, damage rate, crystal structure, solute additions, and transmutant elements such as Si and P (Kinoshita, 1992; Zinkle & Snead, 2014; Zinkle & Busby, 2009; Zinkle & Ghoniem, 2000; Zinkle & Kinoshita, 1997; Yano & Iseki, 1991; Huseynov, 2018b; 2018c; 2017a; 2017b).

Since bulk AlN compound have been widely investigated by world scientist (Parks & Tittmann, 2014; Brian *et al.*, 2015; Bernard, 2013; Boris *et al.*, 2002; Parks *et al.*, 2012). But, a very limited study of nano AlN particles has been reported. Thus, in this study, we are investigated (n, α) transmutation and its probable effective cross-section formed under the influence of the neutron flux in AlN nanoparticles using computer modelling.

2. Result and discussions

(n, α) transmutation and its probable effective cross-section formed under the influence of the neutron flux in AlN nanoparticles have been studied in wide range of energy by computer modelling using various sources. (n, α) transmutation in nanomaterial formed by neutron flux has been separately studied for each Al and N atoms of AlN nanoparticles. The modelling was separately carried out for two possible stable isotopes of Al and N atoms. The modelling carried out separately in different types of isotopes of the Al and N atoms, because (n, α) transmutations possibilities are different. Since the effective energy of up to approximately 30 MeV is active for the Al atoms, modeling was carried out only up to the corresponding energy (Figure 1). As can be seen from the figure, aluminum can be transmuted into two isotopes (n, α). There are formed appropriate Na atoms as a result of the (n, α) transmutations in both Al isotopes.

The probability of (n, α) transmutations in ^{26}Al isotopes is intensive up to 30 MeV of energy. On the other hand, the probability of (n, α) transmutations in ^{27}Al isotopes is approximately intensive in the range of 7-10 MeV of energy (Figure 1). In general approach, $^{26}\text{Al}(n, \alpha)^{23}\text{Na}$ and $^{27}\text{Al}(n, \alpha)^{24}\text{Na}$ transmutation is possible starting from 7 MeV of energy. Analogical modelling also carried out for N isotopes in the AlN nanoparticles. Naturally, the nitrogen has two isotopes and (n, α) transmutations is possible at both isotopes. Initially, let's consider effective cross-section of (n, α) transmutations at ^{14}N isotope (Figure 2). The results show that the (n, α) transmutations at ^{14}N isotope are most probable in the range of about 2-20 MeV. The maximum of the effective cross-section of the process corresponds to about 4 MeV of energy.

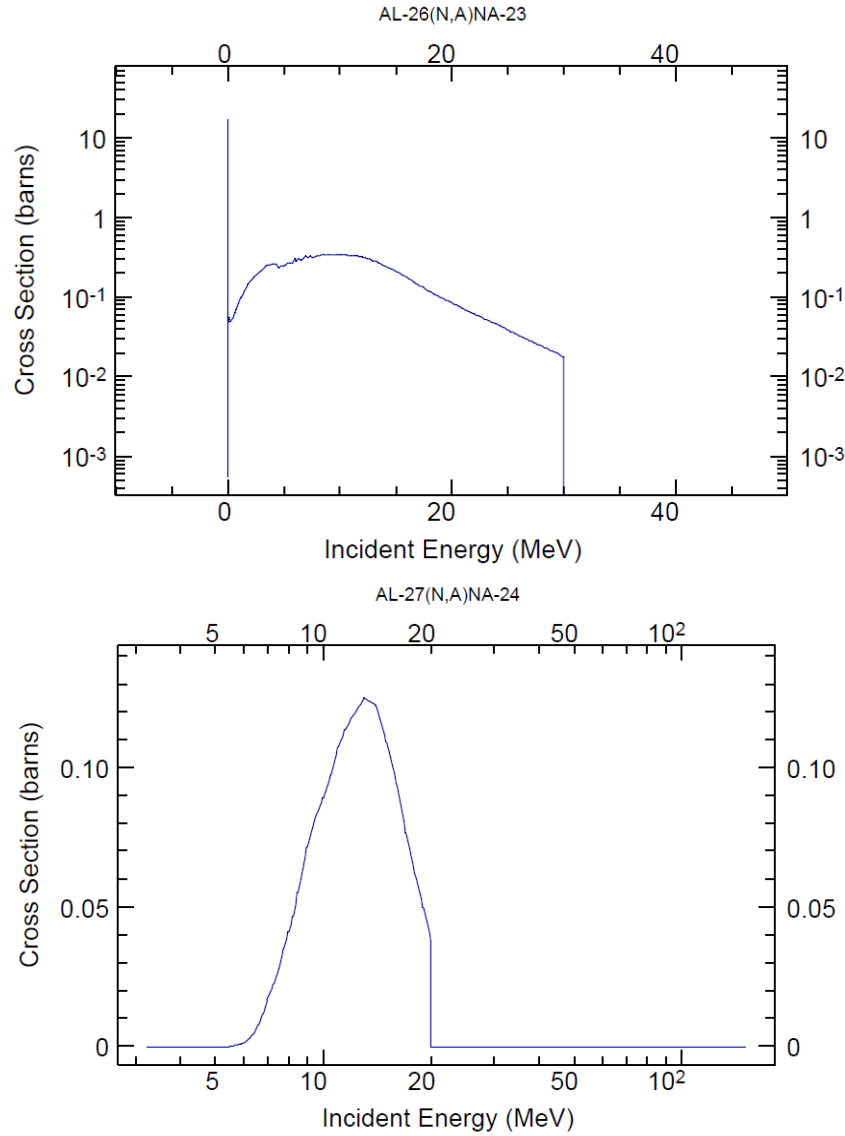


Figure 1. Effective cross-section spectra of (n, α) transmutations formed by neutron flux in different Al isotopes

On the other hand, slightly different cases are observed when considering (n, α) transmutations at ^{15}N isotope. Thus, (n, α) transmutation at ^{15}N isotope more probable in the range of 7-20 MeV of energy. If we consider that, ^{14}N isotopes are dominated in naturally, then it's clear that existing transmutations at ^{15}N isotopes haven't a practical significance. Note that, the nitrogen atoms are substituted with corresponding boron atoms during the (n, α) transmutations at both nitrogen atoms. The minimum energy is 2 MeV in both $^{14}\text{N}(\text{n}, \alpha)^{11}\text{B}$ and $^{15}\text{N}(\text{n}, \alpha)^{12}\text{B}$ transformations. In general approach, these calculated values for Al and N isotopes must be considered in other investigation with AlN nanoparticles.

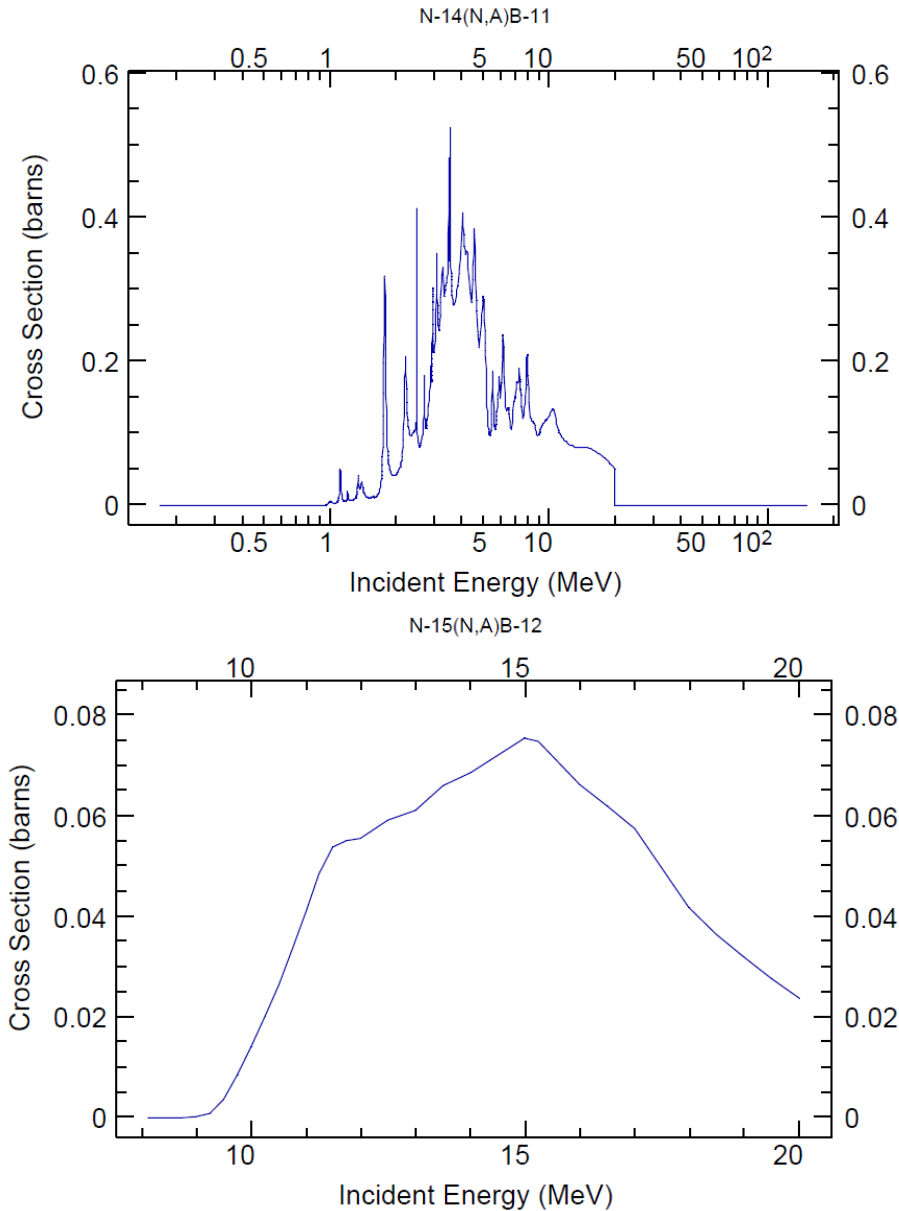


Figure 2. Effective cross-section spectra of (n, α) transmutations formed by neutron flux in different N isotopes.

3. Conclusions

Computer modelling of the (n, α) transmutations of various isotopes in the AlN nanoparticles reveals that the transmutation processes for each stable isotope starts at different energies. It was revealed that $^{26}\text{Al}(n, \alpha)^{23}\text{Na}$ and $^{27}\text{Al}(n, \alpha)^{24}\text{Na}$ transmutations are possible starting from about 7 MeV of energy. Unlike the Al isotopes the minimum energy is 2 MeV at $^{14}\text{N}(n, \alpha)^{11}\text{B}$ and $^{15}\text{N}(n, \alpha)^{12}\text{B}$ transmutations. Same modelling also conducted for N isotopes in the AlN nanoparticles and the results show that the (n, α) transmutations at ^{14}N isotope are most probable in the range of about 2-20 MeV. The

maximum of the effective cross-section of the process corresponds to about 4MeV of energy.

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