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Theoretical approach to study the light particles induced production routes of ^{22}Na

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ABSTRACT

To create a roadmap for the industrial-scale production of sodium-22, various production routes of this radioisotope involving light charged-particle-induced reactions at the bombarding energy range of threshold to a maximum of 100 MeV have been calculated. The excitation functions are calculated by using various nuclear models. Reaction pre-equilibrium process calculations have been made in the framework of the hybrid and geometry dependent hybrid models using ALICE/ASH code, and in the framework of the exciton model using TALYS-1.4 code. To calculate the compound nucleus evaporation process, both Weisskopf–Ewing and Hauser–Feshbach theories have been employed. The cross sections have also separately been estimated with five different level density models at the whole projectile energies. A comparison with calculations based on the codes, on one hand, and experimental data, on the other hand, is arranged and discussed.

1. Introduction

Cross section data for charged-particle-induced nuclear reactions are required in many practical applications such as both medical and industrial radioisotope production, monitoring of light charged particle beams at cyclotron and accelerators, and surface analysis in industrial application. Knowledge of the cross sections for charged-particle-induced reactions on different target material leading to the isotopes of interest (and possible contaminants) is needed if optimization of production routes has to be performed (Király et al., 2008). Also, integral excitation functions to produce the residual nuclides through light charged-particle activation constitute basic data for different applications (Ditrói et al., 2013). In the present work, a comprehensive study of charged-particle-(p, d, ^{3}He- and α-particle) induced nuclear reactions on F, Ne, Na, Mg and Al stable isotopes to the formation of ^{22}Na has been accomplished.

A typical radioisotope can be classified as a medical or an industrial radionuclide, depending on its half-life and decay properties. The ^{22}Na is potentially an attractive radionuclide for the nuclear industry, especially as a standard source for calibration of PET cameras (Gonzales-Lepera, 1994) due to its radiophysical properties. This radionuclide with a long half-life of 2.6 y which decays by β^+ (90.3%) and electron capture (9.6%) mainly to the 1275 keV level of ^{22}Ne (Table de Radionucléides, 2009), is an important positron emitter for production of slow β^+ beams (Saam et al., 1989) and is often used in radionuclide metrology. It can be considered as an available industrial radioisotope by its interesting characteristics such as above mentioned as well as those may be identified during its production process, for instance, if irradiated production target is a gas (Ne or F), the ^{22}Na can be remained in solid phase among co-produced gaseous contaminations, resulting in an easy radiochemical separation (Eslami et al., 2015). In the radioisotope production procedure, the nuclear reaction data are mainly needed to optimize the production rates. This process implicates a selection of the projectile energy range that will maximize the yield of the product and minimize that of the isotopic and non-isotopic contaminations (Qaim, 2004; Eslami and Kakavand, 2014). There are several routes to produce ^{22}Na which take into account the available accelerator, the production yield and contamination level. These production routes along with corresponding details have been summarized in Table 1. This work aims to provide a representation of the nuclear reactions induced by charged particle with incident energies up to 100 MeV. Nuclear reaction models can be helpful to provide estimates of the excitation functions, especially if the experimental data are missing or not satisfactory. Also, data obtained from various techniques are necessary to develop additional nuclear theoretical calculation models to

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Table 1
A comprehensive list of production routes of ^{22}Na via proton, deuteron, ^{3}He- and α-particles-induced reactions on isotopes of F, Ne, Na, Mg and Al along with related literature. The ejectile *x* stands for variety decay channels through which the ^{22}Na may be produced, subsequently, asterisk E_{th} and *Q*-values belong to the first possible decay channel.

Reaction	*Q*-value (MeV)	E_{th} (MeV)	Experimental cross section references
^{20}Ne(^{3}He,p)	5.78	0	–
^{21}Ne(^{3}He,d)	1.24	0	–
^{22}Ne(^{3}He,t)	−2.86	3.25	–
^{nat}Ne(^{3}He,*x*)	5.78*	0*	Fenyvesi et al. (1997)
^{23}Na(^{3}He,α)	8.15	0	–
^{27}Al(^{3}He,*x*)	−1.93*	2.14*	Cochran and Knight (1962), Condratyev et al. (1997)
^{19}F(α,n)	−1.95	2.36	Norman et al. (1984), Ismail (1993), Wrean and Kavanagh (2000)
^{20}Ne(α,d)	−12.57	15.08	–
^{21}Ne(α,t)	−13.07	15.56	–
^{22}Ne(α,*x*)	−23.43*	27.70*	–
^{nat}Ne(α,*x*)	−12.57*	15.08*	Fenyvesi et al. (1997)
^{24}Mg(α,*x*)	−21.88*	25.54*	–
^{25}Mg(α,*x*)	−22.96*	26.63*	–
^{26}Mg(α,*x*)	−34.05*	39.30*	–
^{nat}Mg(α,*x*)	−21.88*	−25.54*	Lindsay and Carr (1960), Lange et al. (1995), Paul et al. (1995)
^{27}Al(α,*x*)	−22.51*	25.85*	Bouchard and Fairhall (1959), Porile (1962), Karpeles (1969b), Bowman and Blann (1969), Martens and Schweimer (1970), Probst et al. (1976), Rattan et al. (1985, 1986, 1990), Ismail (1989, 1990, 1993), Lange et al. (1995)
^{20}Ne(d,γ)	11.18	0	–
^{21}Ne(d,n)	4.51	0	–
^{22}Ne(d,2n)	−5.85	6.38	–
^{23}Na(d,*x*)	−6.16*	6.70*	Lange et al. (1969)
^{24}Mg(d,*x*)	1.95*	0*	Röhm et al. (1969)
^{25}Mg(d,*x*)	−5.37*	5.80*	–
^{26}Mg(d,*x*)	−16.46*	17.74*	–
^{nat}Mg(d,*x*)	1.95*	0*	Hermanne et al. (2012)
^{27}Al(d,*x*)	−16.25*	17.46*	Ring and Litz (1955), Karpeles (1969a), Martnes and Schweimer (1970), Takács et al. (2001), Hagiwara et al. (2004), Nakao et al. (2006), Hermanne et al. (2012)
^{21}Ne(p,γ)	6.73	0	–
^{22}Ne(p,n)	−3.62	3.79	Saam et al. (1989), Takács et al. (1996), Wrean and Kavanagh (2000)
^{23}Na(p,d)	−10.19	10.64	Meadows and Holt (1951), Cohen et al. (1955)
^{24}Mg(p,*x*)	−16.39*	17.08*	Meadows and Holt (1951), Bodemann et al. (1993)
^{25}Mg(p,*x*)	−3.14*	3.27*	Meadows and Holt (1951)
^{26}Mg(p,*x*)	−14.24	14.79	Meadows and Holt (1951)
^{nat}Mg(p,*x*)	−3.14*	3.27*	Batzel and Coleman (1954), Furukawa et al. (1971), Lagunas-Solar and Carvacho (1990), Bodemann et al. (1993)
^{27}Al(p,*x*)	−20.28*	21.04*	Hintz and Ramsey (1952), Batzel and Coleman (1954), Gauvin et al. (1962), Cumming (1963), Williams and Fulmer (1967), Miyano (1973), Aleksandrov et al. (1988), Lagunas-Solar et al. (1988), Steyn et al. (1990), Bodemann et al. (1993), Buthelezi et al. (2006), Khandaker et al. (2011), Titarenko et al. (2011)

explain nuclear reaction mechanisms and the properties of the excited states for different energy ranges (Tel et al., 2007).

This study explores producing the ^{22}Na via more than thirty light charged-induced nuclear reactions. These nuclear reactions are studied by using the nuclear reaction model codes TALYS-1.4 (Koning et al., 2008a) and ALICE/ASH (Broeders et al., 2006) with a number of model options such as selective reaction mechanism and level density. Besides, the theoretical calculations are compared with the reported experimental data from different laboratories.

2. Nuclear reaction models and calculation methods

2.1. Pre-equilibrium mechanism

At incident energies from 10 MeV up to 200 MeV, a significant part of the reaction flux is emitted in the pre-equilibrium stage taking place after direct mechanism but long before statistical equilibrium of the compound nucleus (Griffin, 1966; Blann, 1971, 1975). It is imagined that the incident particle step by step creates more complex states in the compound system and gradually loses its memory of the initial energy and direction (Koning and Rochman, 2012).

2.1.1. Exciton model

The exciton model was first proposed by Griffin (1966) for explaining various experimental nuclear reaction data. In exciton model, the composite nucleus states are characterized by the number of excited particles and holes at any stage of the nucleon-nucleon cascade. The basic formula for the exciton model cross section is,

$$\frac{d\sigma_k^{EM}}{dE_k} = \sigma^{CF} \sum_{p_\pi=p_\pi^0}^{p_\pi^{eq}} \sum_{p_\nu=p_\nu^0}^{p_\nu^{eq}} W_k(p_\pi, h_\pi, p_\nu, h_\nu, E_k) \times S_{pre}(p_\pi, h_\pi, p_\nu, h_\nu), \quad (1)$$

where p_π (p_ν) is the proton (neutron) particle number and h_π (h_ν) the proton (neutron) hole number, σ^{CF} is the compound formation cross section, calculated with the optical model potentials (Koning and Delaroche, 2003), W_k is the emission rate for ejectile *k* (Dobeš and Běták, 1983; Cline and Blann, 1971) and S_{pre} is the time-integrated strength which determines how long the system remains in a certain exciton configuration. The initial proton and neutron particle numbers are denoted $p_\pi^0 = Z_p$, and $p_\nu^0 = N_p$ with Z_p (N_p) being the proton (neutron) number of the projectile. In general, $h_\pi = p_\pi - p_\pi^0$ and $h_\nu = p_\nu - p_\nu^0$, so that the initial hole numbers are zero. This follows $h_\pi^0 = h_\nu^0 = 0$ for primary pre-equilibrium emission. p_π^{eq} and p_ν^{eq} are the equilibrium particle numbers, whereas the part of the reaction flux is distributed through the Hauser–Feshbach model (Hauser and Feshbach, 1952) for compound nucleus reactions.

2.1.2. Hybrid and geometry dependent hybrid (GDH) models

The hybrid model for pre-equilibrium emission is given by Blann and Vonach (1983) as,