Neutron resonances in three-body system in the thermal range

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Abstract

The main objective of the work is to determine the new resonances in three-body system that consists of one neutron and two heavy nuclei. New resonances are formed in the re-scattering of neutron on subsystem of these nuclei. Such neutron resonances become stronger at particular values of the distances between the nuclei and the resonances vanish if distances become larger or less than these resonance distances. Theoretical analysis of the properties of new resonances in three-body systems are given and calculations of the resonance characteristics are provided. Possibilities for experimental studies of new resonance effects are discussed. It is suggested to investigate new neutron resonances in piezo-crystals that contain isotopes, which have resonances in the thermal range. As the sample the isotopes of ^{113}Cd are considered because the corresponding the electric piezoeffect allows to vary the distances between the nuclei.

Subject Classification: 21.10.-k; 25.40Lw; 26.60+c

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1 Introduction

In the recent years new resonance peaks were experimentally observed in the spectra of neutron scattering at various nuclei in the thermal range [9] (see, also https://www.ncnr.nist.gov/resources/activation/resonance.htm).

The interest towards these neutron resonances is stipulated by the nuclear engineering and other applied tasks. Such experiments are informative for nuclear physics, in particular for neutron star physics [11, 5]. The fact that almost impossible to run experiments for nuclear astrophysics in terrestrial conditions, although it is possible to generalize some of the results to areas of extreme conditions. That is why any laboratory experiment even partly related to the phenomena or processes in the named above objects becomes of vivid interest. This statement is equally correct for computer simulations and analysis of processes and reactions in neutron star interiors (see, for example [11, 5, 7]).

The theoretical consideration of the problem is presented below based on a three-body quantum scattering theory [3], the Born-Oppenheimer approximation [4] for a system of two heavy nuclei and one particle with much smaller mass (neutron), and the Breit-Wigner form of scattering amplitudes for pair neutron-nucleus subsystems in the vicinity of their single resonances [2, 1]. In the case when a neutron is scattered at a subsystem of two heavy nuclei, the problem of formation of new type resonances has been considered [13, 14, 15]. It occurs when a third particle (neutron) interacts resonantly with each of the heavy particles. The solutions show the resonance behavior of three body systems. An important feature of such solutions is their resonance dependence on the distance between the heavy particles not only on the energy of the light-mass particle [13, 14, 15, 16].

Obviously, a three-particle resonance effects are based on quantum interference in the states which takes place at specific conditions of the system. These conditions are related to the superposition of the wave processes, and to the mutual influence of the resonance sources.

Within the present work, the resonance scattering of neutron on subsystem of two heavy nuclei has been considered in the low thermal range. New quasi-stationary states formed at neutron scattering at a system of two non-interacting nuclei are of interest in our case [14, 15].

In the next section, the main theoretical computations related to a quantum-mechanical scattering problem for a three-body system (two heavy particles and one particle with small mass) are given in brief form.

Section 3 presents the calculation results of the three-body resonances that obtained on the base the neutron-nucleus resonance data in the low thermal range for selected isotopes $^{149}Sm,^{152}Sm,^{155}Gd,^{157}Gd$ and ^{113}Cd. These three-body resonances appear at distances between these isotopes that are comparable with the interatomic distances in the crystal.

Here the possibility for experiments on thermal neutron scattering at piezocrystalline targets with isotopes of ^{113}Cd are discussed. Since the piezocrystals change their internal spatial parameters due to voltage, the phenomenon can be used to control the alterations of distance between these isotopes.

2 Theoretical background

The quantum scattering theory for systems of three and more particles is based on Faddeev equations [3], where the existence and uniqueness of solution conditions are satisfied. An important peculiarity of the Faddeev equations is the sequential order where the equations for the components of the three-particle T-matrices are expressed through the solutions for the two-particles t-matrices:

$$T_{i,j} = t_i\, \delta_{ij} + \sum t_i\, G_0(E)\, \bar{\delta}_{i,l}\, T_{l,j}, \tag{1}$$

where t_i matrices are given as known quantities, $t_i = V_i + V_i G_0\, t_i$ are associated with pair interaction potentials V_i and determined in the space of three particles, $(i, j, l = 1, 2, 3)$. In Eq. (1) $G_0(E)$ is the Green's function for three free particles and $\bar{\delta}_{i,j} = 1 - \delta_{i,j}$, where $\delta_{i,j}$ is the Kronecker symbol. The total T-matrix is the sum over the indices i and j; $T = \sum T_{i,j}$.

Formally, the index i on the element $T_{i,j}$ corresponds to the number of the last surviving pair in the left asymptotic region - that is, it corresponds to the number of the particle that leaves the interaction region first. Similarly, the index j corresponds to the number of the last interacting pair in the right asymptotic region. The Faddeev equations (1) guarantee uniqueness and existence of solutions [3].

Our model related to the description of resonant phenomena at low energies is based on two simplifying assumptions: the pair t-matrix considered at energies close to the neutron-nuclei resonance energy is considered in the Breit-Wigner form; a description of neutron scattering at a system of two nuclei is taken in the Born-Oppenheimer approximation.

So, for the ratio of the neutron mass m to the nucleus mass M we can accept $m/M \to 0$, assuming that the effective mass, like in the Mössbauer effect, is equal to the mass of the whole crystalline domain. Assume that the crystalline target is kept at very low temperature so thermal oscillations in the crystal are minimal. Then the total kinetic energy of the system equals to the kinetic energy of the neutron $E = p_0^2/2m$, where $\vec{p_0} = \hbar\vec{k_0}$. We use below the units $c = \hbar = 1$; then $V_{i=2,3} = V_{nA}(\vec{k}, \vec{k'})$.

Restrict our analysis by the elastic channel assuming the inelastic one be closed or suppressed. In reality, consideration of other channels is not a big challenge, since the inelastic channel (for instance, at neutron capture and emission of gamma by excited nucleus) transforms the nucleus into a different one with other properties. In this case the process of resonance re-scattering of neutrons at given nuclei is aborted.

Neutron resonance scattering. Breit-Wigner t-matrix

For the non-relativistic two-body problem one can write the expression for the S-matrix in the vicinity of resonance as [2]

$$S = \frac{E - E_R - i\Gamma/2}{E - E_R + i\Gamma/2} = I - 2\pi i\rho(E)t(E) \tag{2}$$

and

$$t(E) = \frac{1}{\pi\rho(E)}\frac{\Gamma/2}{E - E_R + i\Gamma/2}, \tag{3}$$

where $\pi\rho(E) = 2mk_0/4\pi$, $E = k_0^2/2m$.

In the case when low-energy neutron scattering at a nucleus is determined by potential and resonant channels, then the complete t-matrix in the coupled channel method can be written for the S-wave in the well-known form [1]:

$$t(E) = \frac{2\pi}{mk_0}\left[(1 - exp(2i\delta_{pot}))/2i + \frac{\Gamma/2}{E - E_R + i\Gamma/2}\cdot exp(2i\delta_{pot})\right] , \tag{4}$$

where δ_{pot} is the phase shift of elastic potential scattering and can be written at low energy in the form $\delta_{pot} = -k_0 a$, a is a scattering length. The second term in (4) corresponds to the interference of the resonance and the potential parts of the t-matrix.

At the very low energies limit $k_0 \to 0$, the t-matrix (4) reduces to:

$$t(E) \to \frac{2\pi}{m}\left[\frac{1}{\kappa + ik_0} + \frac{1}{k_0}\frac{\Gamma/2}{E - E_R + i\Gamma/2}\right] , \tag{5}$$

where $1/\kappa$ is the neutron scattering length at the nucleus and in the case of low energy, κ corresponds to the wavenumber of the neutron-nucleus bound ($\kappa > 0$) or virtual ($\kappa < 0$) state.

One can present the resonance and potential parts of the t-matrix in a separable form. Let us take into account the S-wave component only. The potential part of the t-matrix can be written in the form:

$$t(E; k, k') = \overline{\nu}(k)\eta_{pot}(E)\nu(k'), \tag{6}$$

where $\overline{\nu}(k) = \nu(k) = \sqrt{2\pi/(m\beta)}/(1 + k^2/\beta^2)$, $\eta_{pot} = \beta/(\kappa + ik_0)$. The value β^{-1} corresponds to the radius of nuclear forces, i.e. this value is many times less than the atomic size, therefore for thermal neutrons we can neglect k/β in the expression for $\nu(k)$.

Generalizing the expression (3), one can write the resonance t-matrix as:

$$t_{a,b}(E; k, k') = \overline{\nu}_a(k)\eta_{res}(E)\nu_b(k'), \tag{7}$$

where $\overline{\nu}_a(k) = \sqrt{2\pi\Gamma_a/mk\Gamma}$, $\nu_b(k) = \sqrt{2\pi\Gamma_b/mk'\Gamma}$, and $\eta_{res}(E) = (\Gamma/2)/(E - E_R + i\Gamma/2)$. Here the indexes a and b denote inlet and outlet channels; and Γ is the total width of the open channels.

Note that the sum of a finite number of separable terms can describe the short-range potentials of complicated forms. The solutions in these cases can also be written in an analytical form.

Within this work we do not consider contributions from the neighboring resonance levels, coupled or virtual states located far from the considered low-energy resonance. It would be noted that their contributions to the considered effects should be small.

Solution of the problem for neutron scattering at a system of two nuclei

In the case of the separable form of pare t-matrices (6) and (7) the three-body T-matrix can be written in the following form [13]:

$$T_{i,j} = \overline{\nu}_i \eta_i \delta_{i,j} \nu_j + \overline{\nu}_i \eta_i M_{i,j} \eta_j \nu_j, \tag{8}$$

and one can get the system of simple equations for the components $M_{i,j}$:

$$M_{i,j} = \Lambda_{i,j} + \sum_{l=2,3} \Lambda_{i,l}\ \eta_l\ M_{l,j}, \tag{9}$$

where

$$\Lambda_{i,j} =< \nu_i | G_0(E) | \nu_j > \bar{\delta}_{i,j} \quad . \tag{10}$$

Here $\Lambda_{i,i} \equiv 0$, what excludes repeated interactions in the pairs and creates sequential inclusions of interactions from different pairs. When a neutron is scattered at two fixed nuclei in the lattice nodes, the equation (9) describes a sequential scattering of a neutron at each of these two nuclei. It is assumed that the nuclei in the lattice do not interact with each other via nuclear forces.

Using the conservation of the total momentum in three body system, $\vec{k} = \vec{k}_1 = -\vec{k}_2 - \vec{k}'_3$, one can write Eq. (10) in the integral form

$$\Lambda_{i,j}(\vec{k}_2, \vec{k}'_3; k_0) = \int d\vec{r} \exp(i\vec{r}\vec{k}_2) J_{i,j}(\vec{r}) \exp(i\vec{r}\vec{k}'_3) \ , \tag{11}$$

where

$$J_{i,j}(\vec{r}; k_0) = 2m \int d\vec{k} \exp(i\vec{k}\vec{r}) \frac{\nu_i(k)\overline{\nu}_j(k)}{k_0^2 - k^2 + i\gamma} \ . \tag{12}$$

Using the Fourier transformation for $M_{i,j}(\vec{k}, \vec{k}')$

$$M_{i,j}(\vec{r}, \vec{r'}) = \int\int d\vec{k} d\vec{k}' \exp(-i\vec{r}\vec{k}) M_{i,j}(\vec{k}, \vec{k}') \exp(i\vec{r'}\vec{k}') \ , \tag{13}$$

and taking into account relations Eqs. (11) and (12) we rewrite Eq. (9) for the re-scattering matrixes in the coordinate form [13]:

$$M_{i,j}(\vec{r}, \vec{r'}) = J_{i,j}(k_0; \vec{r}) \delta(\vec{r} + \vec{r'}) + \sum_l J_{i,l}(k_0; \vec{r}) M_{l,j}(-\vec{r}, \vec{r'}) \ , \tag{14}$$

where for simplicity, we omit indexes for $\vec{r}$ and $\vec{r'}$.

The coordinates $\vec{r}$ and $\vec{r'}$ correspond to the locations of the nuclei which take place in neutron re-scattering and are taken relative to the center of symmetry in the system of two heavy nuclei. The amplitudes $M_{i,j}(\vec{r},\vec{r'})$ represent an effective interaction of nuclei created by re-scattering of a light particle (neutron) at them. $M_{i,j}(\vec{r},\vec{r'})$ can be written in the form:

$$M_{i,j}(\vec{r},\vec{r'}) = M^{+}_{i,j}(\vec{r})\delta(\vec{r}+\vec{r'}) + M^{-}_{i,j}(\vec{r})\delta(-\vec{r}+\vec{r'}). \tag{15}$$

Since Eq. (15) includes the delta-functions, they eliminate integrations in the right part of (13) and (14). Then, the equations for the matrices $M^{\pm}_{i,j}(\vec{r})$ take the following simple forms:

$$M^{+}_{i,j}(\vec{r},k_0) = \frac{1}{D_{i,i}(\vec{r};k_0)} J_{i,j}(\vec{r},k_0)\ , \tag{16}$$

and

$$M^{-}_{i,i}(\vec{r},k_0) = \frac{1}{D_{i,i}(\vec{r};k_0)} J_{i,l}(\vec{r},k_0)\eta_l(k_0)J_{l,i}(-\vec{r},k_0). \tag{17}$$

In Eq. (16) and (17) the matrix D is a diagonal one

$$D_{i,i}(\vec{r};k_0) = 1 - \sum_l J_{i,l}\eta_l(k_0)J_{l,i}(-\vec{r},k_0)\eta_i(k_0) \tag{18}$$

and its non-diagonal elements when $i \neq j$, are equal to $D_{i,j}(\vec{r};k_0) = 0$

Consider the simple case when two nuclei are located in neighbor nodes of a crystal lattice. The wave functions of these heavy particles could be written in the form

$$\Psi_i(\vec{r}) = C\exp[-\frac{(\vec{r}-\vec{r_i})^2}{2\Delta^2}], \tag{19}$$

where i is the number of nucleus, $\vec{r_i}$ is the coordinate of the node, C is the normalized factor satisfying the normalization condition $<\Psi_i|\Psi_j>=0$ if $i \neq j$ and $<\Psi_i|\Psi_i>=1$, so that $C^2 = \Delta^{-3}\pi^{-3/2}$. The limit $\Delta \to 0$ means that nuclei will be strictly fixed at the points $\vec{r_2}$ and $\vec{r_3}$. It is convenient to take the starting point at the center of symmetry of the system. In this case, one nucleus will be located at the point $\vec{r}$ and the another one at the point $\vec{r'} = -\vec{r}$.

As a result, the total T-matrix for neutron scattering on the system of two nuclei takes the form:

$$<T>= \sum_i \overline{\nu}_i\eta_i\nu_i + \sum_{i,J} \overline{\nu}_i\eta_i < M_{i,j} > \eta_j\nu_j\ . \tag{20}$$

Here, the first term on the right-hand side of Eq. (20) corresponds to the sum of independent neutron scatterings t_i-matrix on every separate nucleus of the considered pair, while the second term corresponds to the neutron scattering on the two-center system. The $< M_{i,j} >$ form means that the matrix is taken in the brackets of the wave functions Ψ_i and Ψ_j: $< M_{i,j} >= M_{i,j}(\vec{r_i}) = M_{i,j}(-\vec{r_j})$. For simplicity, we omit indices, take the form: $\vec{r_i} = \vec{r}$ and $\vec{r_j} = \vec{r'} = -\vec{r}$.

This approach brings us to the effect related to interference of two close resonance sources which generate additional resonance levels [14, 15, 16]. New resonance levels occur at specific distances between these sources $L = L_{res}$, where $L = |\vec{r} - \vec{r'}| = 2r$. One should note here that at lower, or, vice versa, larger distances these resonances disappear abruptly.

3 Calculations of new neutron resonances in the low thermal range

There are only few isotopes, which have the single neutron resonances in the low thermal range (See Table 1 and details at the site https://www.ncnr.nist.gov/resources/activation/resonance.html).

Table 1: Isotopes with low resonance energy

Isotope	Neutron wavelength ($\mathring{A}$)	Energy (meV)	k_{res} in $\mathring{A}^{-1}$
^{155}Gd	6.44	1.97	0.975
^{157}Gd	6.18	2.14	1.016
^{149}Sm	6.02	2.26	1.044
^{113}Cd	5.44	2.77	1.157
^{152}Sm	2.72	10.93	2.298

These data are taken as basic ones in our assessments of resonance neutron scattering at a subsystem of two neighbor nuclei in the crystalline lattice. Take into account only the selected isotopes that have resonances in the lowest thermal range [12, 6, 10]. The contribution of other isotopes, which can be incorporated into the crystal structure, is very small and could be disregarded. In Table 1 and Figs 1-4, wavenumbers are given in $\mathring{A}^{-1}$.

The dependences of structure neutron resonances on the distances between two the same or different heavy isotopes were calculated.

Determine the enhancement factor $F(k_0, r)$ in the following form:

$$F(k_0; \vec{r}) = |\sum_{i,j} \overline{\nu}_i \eta_i M_{i,j} \eta_j \nu_j / (t_i \delta_{i,j}|^2 \quad , \tag{21}$$

in order to estimate the action of three-body resonances in comparison with two-body one. This expression could be obtained using the relations given in (18 - 20).

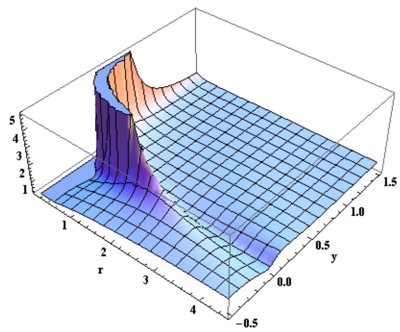

Figure 1: $F(k_0, r)$ for the system $n +^{113} Cd +^{113} Cd$; $k_{res} = 1.157$ is the wavenumber of the $n +^{113} Cd$ resonance; $y = k_0/k_{res} - 1$

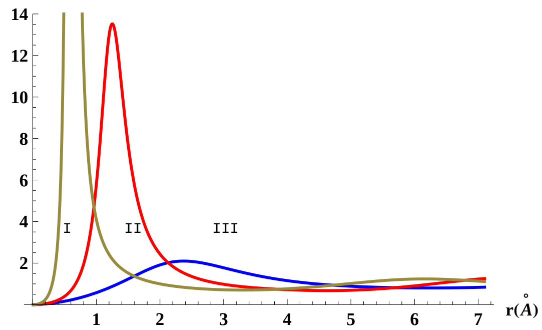

Figure 2: $F(k_0, r)$; the system $n +^{155} Gd +^{157} Gd$; the curves I, II, III correspond to $k_0 = 0.87; 1.013; 1.126$, accordingly

The factor $F(k_0, r) = \sigma_3/\sigma_2$, where σ_3 means the three-body cross-section and σ_2 is a sum of two-body cross sections. If the re-scattering of a neutron on two-nuclei subsystem becomes negligible, then $F(k_0, r) \to 1$. We mark the cross sections as σ_2 in the case when every nucleus interacts with neutron independently, for instance, at large r. The results of the calculations are shown in Fig. 1-4, which demonstrate that $F(k_0, r)$ has a resonance behavior at the certain values of the distance between two neighbor isotopes.

Table 2 contains the parameters of CdS and $CdSe$ crystals with a hexagonal (h) and a face-centered cubic (c) structures [12, 18]. The parameter L is the distance between two neighbor Cd nuclei.

The estimation of minimal distances between Cd nuclei is in agreement with the results obtained using the VESTA program [8] and experimental data [18, 17]. It is noteworthy that the values for the distances L between the nuclei of cadmium proved to be close to the values of the area for new neutron resonances (Fig. 1 - 3).

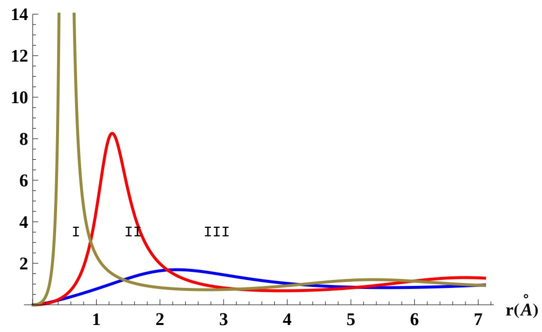

Figure 3: $F(k_0, r)$; the system $n+^{113}Cd+^{113}Cd$; here I, II, III mark the cases with $k_0 = 0.988; 1.15; 1.278$

Table 2: Parameters of Cd crystals

Phase	a = b (Å)	c (Å)	L (Å)
CdS; h	4.13	6.71	4.116
CdS; c	5.3	5.3	3.748
CdSe; h	4.29	7.01	4.292
CdSe; c	5.54	5.54	3.917

Note that at high energy the new neutron resonances disappear because their wavelengths become very small in comparison with lattice parameters. But in the case of overdense crystall the lattice parameters become comparable again with resonance neutron wavelengths that exist up to 1 MeV. And the neutron resonances should be significantly reinforced.

Of course, the neutron resonance in the crystalline structure depends on parameters of neutron resonances, including the resonance energy and width, its quantum numbers etc.

4 Conclusion

We have performed the calculations of the new neutron resonance at systems of two nuclei in the energy range close to conventional neutron-nucleus resonances. Our goal is the study of the three-body resonance effects in the scattering of neutrons at subsystem of two isotopes in the dependence of distances between these nuclei.

Three-dimensional picture (Fig. 1) demonstrates the behavior of the enhancement factor for the system $n + Cd^{113} + Cd^{113}$. Remarkable that when the neighbor isotopes have the resonance levels with nearby energy, the enhancement factor for structural resonance (Fig. 2) becomes more significant at certain distances. In the opposite case (Fig. 4) the enhancement factor is

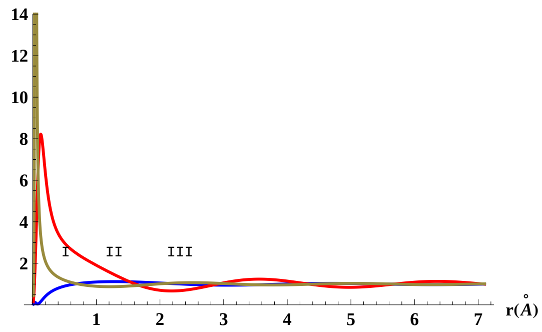

Figure 4: $F(k_0, r)$; the system $n +^{149} Sm +^{152} Sm$; I, II, III correspond to $k_0 = 1.954; 2.275; 2.528$, accordingly

small.

All stated above opens up opportunities to use the specialized piezo-crystals and provide the control over the target's parameters in the experiments with thermal resonance neutrons. For example, it is possible to provide the experiments with different targets: the thermal neutron scattering at CdS and $CdSe$ crystals.

The calculated data indicate that there is the real possibility to investigate the new resonance effects in the neutron scattering in the thermal range at different crystals containing the selected isotopes.

It must be noted that the new neutron resonances are created by interactions in three-body systems. They supplement the well-known phenomena as Bragg's scattering (Bragg's law and neutron diffraction) or the crystal vibrations at neutron scattering. The influence of new resonances would increase and become very important in the case of overdense matter, for example in neutron stars.

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References

[1] V.V. Balashov, *Interaction of Particles and Radiation with Matter* (Springer-Verlag Berlin Heidelberg, 1997) ISBN 978-3-642-64383-5

[2] A.I. Baz′, Ya.B. Zeldovich, A.M. Perelomov, *Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics* (Jerusalem, 1969) ASIN: B0006C7UF0, ISBN-10:5458262298

[3] L.D. Faddeev, *Mathematical Aspects of the Three-Body Problem in Quantum Scattering Theory* (Davey, New York, 1965)

[4] W.H. Flygare, *Molecular Structure and Dynamics* (Engewood Cliffs, New Jersey, 1978) ISBN-13: 978-0135997536

[5] P. Haensel, A.Y. Potekhin, D.G. Yakovlev, *Neutron Stars* (Kluwer Academic Publishers, 2007) ISBN 0387335439

[6] D. Kuciauskas, A. Kanevce, J.N. Duenov, P. Dippo, M. Young, J.V. Li, D.H. Levi, T.A. Gessert, Appl. Phys. Lett., **102**, 173902 (2013); http://dx.doi.org/10.1063/1.4803911

[7] J.M. Lattimer, *Neutron stars* (Springer Science+Business Media New York 2014) DOI 10.1007/s10714-014-1713-3

[8] Koichi Momma, Fugio Izumi, *VESTA: a Three Dimensional Visualisation System for Electronic and Structural Analysis*, Japan, 2011; URL:http://jp-minerals.org/vesta/en/

[9] B. Pritychenko, S.F. Mughabghab, *Neutron Thermal Cross Sections, Westcott Factors, Resonance Integrals*, (Evaluated Data Libraries, BNL Report, 2013) arXiv:1208.28793v3 [astro-ph.SR], 2013, 145 pp.

[10] A. Sayede, E. Bruyer, M. Springborg, Phys. Rev. B, **86**, 125136 (2012)

[11] S. Shapiro, S. Teukolsky *Black Holes, White Dwarfs, and Neutron Stars* (United States: John Wiley /Sons 1983) ISBN 0-471-87317-9

[12] D. Shvydka, J. Drayton, A.D. Compaan, V.G. Karpov, Appl. Phys. Lett., **87**, (2005) 123505

[13] N.Zh. Takibayev, Physics of Atomic Nuclei **78**, (2008) 405

[14] N.Zh. Takibayev, EPJ Web of Conference **3**, (2010) 050028, DOI:10.1051/epjconf/20100305028

[15] N.Zh. Takibayev, Few-Body Systems **50**, (2011) 311-314, DOI 10.1007/s00601-010-0207-4

[16] N. Takibayev, K. Kato, M. Takibayeva, A. Sarsembayeva, D. Nasirova, Few-Body Systems **54**, (2013) 447-450, DOI: 10.1007/s00601-013-0598-0

[17] P. Villars, K. Cenzual, *Pearson's Crystal Data: Crystal Structure Database for Inorganic Compounds*, Release 2014/15, ASM International Materials Park, Ohio, USA

[18] Yong-Nian Xu, W.Y. Ching, Phys. Rev. B, **48**, 4335 (1993)