ASSOCIATION EURATOM - UNIVERSITY OF LATVIA AEUL







ANNUAL REPORT 2012

Riga 2013

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1. INTRODUCTION

The activities of the Research Unit are continued in fusion science and technology under the Contract of Association and Technology Programme under EFDA. The AEUL in the frame of the EFDA Workprogramme 2008 starts to take part in the Goal Oriented Training Programme - GOT "EUROBREED".

The Physics Programme is carried out at IP UL – Institute of Physics, University of Latvia, and at ISSP UL – Institute of Solid State Physics, University of Latvia. The research areas of the Physics Programme are:

- Preparation of a gallium jet limiter for testing under reactor relevant conditions
- Characterization of the impurity concentration, profiling and erosion in ITER relevant materials using *ex situ* LIBS spectroscopy
- *In situ* tokamak laser enhanced LIBS spectroscopy of the impurity concentration depth profile in wall tiles.

Theory and Code Development:

- On the theory of high-power gyrotrons with uptapered resonators
- Structure and dynamics of sawteeth crashes in ASDEX Upgrade
- Computer modeling of impurity clusters in steels; HPC facilities are effectively used to perform large-scale calculations of ODS steels.

The Technology Programme is carried at ICP UL - Institute of Chemical Physics, University of Latvia. The technology research and development under EFDA JET is focused on:

- Analysis of tritium distribution in plasma facing components
- Release of tritium from neutron-irradiated pebbles
- Radiolysis of plasma synthesized lithium orthosilicate nanopowders.

Several Staff Mobility actions took place in 2011: to IPP Garching, FZK Karlsruhe, UKAEA Culham, ISTTOK Lisbon, and Meriland University.

Finally I wish to thank all the staff members of AEUL for their contribution and Latvian Ministry of Education and Sciences for continuous support.

Riga, 2013

(Andris Sternberg, Head of Research Unit of AEUL)

2. FUSION PROGRAMME ORGANISTION

2.1 Programme Objectives

The Latvian Fusion Programme, under the Association EURATOM-University of Latvia, is fully integrated into the European Programme, which has set the long-term aim of the joint creation of prototype reactors for power stations to meet the needs of society: operational safety, environmental compatibility and economic viability. The objectives of the Latvian programme are: (i) to carry out high-level scientific and technological research in the field of nuclear fusion, (ii) to make a valuable and visible contribution to the European Fusion Programme and to the international ITER Project in our focus areas. This can be achieved by close collaboration with other Associations.

2.2 Association EURATOM-University of Latvia (AEUL)

The Latvian contribution to the European fusion programme began in 2000 in the form of cost-sharing actions (fixed contribution contracts with EURATOM). The Association was established on 19 December 2001 incorporating the existing costsharing actions into its work plan.

2.3 Fusion Research Units

The Latvian Research Unit of the Association EURATOM-University of Latvia consists of three Institutes of University of Latvia.

- IP UL Institute of Physics, University of Latvia
 32 Miera St., Salaspils LV-2169, Latvia.
 Phone +371 6 7944700, Fax. +371 6 7901214
- ISSP UL Institute of Solid State Physics, University of Latvia 8 Kengaraga St., Riga LV-1063, Latvia. Phone +371 6 7187810, Fax. +371 6 7132778
- 3. ICP UL Institute of Chemical Physics, University of Latvia 4 Kronvalda Blvd., Riga LV-1010, Latvia. Phone +371 6 7033884, Fax. +371 6 7033884

2.4 Association Steering Committee

The research activities of the Latvian Association EURATOM-University of Latvia are directed by the Steering Committee, which comprises the following members in 2012:

Mr. Vito Marchese Scientific Officer, Unit RTD - K6

Mr. Rugero Giannella Scientific Officer, Unit RTD - K6

Mr. M. Cosyns, Administration and finance, Unit RTD - K7

Mrs. Irina Arhipova, Ministry of Education and Science

Mr. Ivars Lacis, University of Latvia

Mr. Andrejs Silins, Latvian Academy of Sciences

The Steering Committee had one meeting in 2012. This meeting was organised on July 2, 2012 with remote participation of EU Commission representatives.

2.5 The Latvian Members in the EU Fusion Committees

Consultative Committee for the EURATOM Specific Research and Training Programme in the Field of Nuclear Energy-Fusion (CCE-FU) Mr. Andris Sternberg, ISSP UL

EFDA Steering Committee Mr. Andris Sternberg, ISSP UL

Governing Board for the Joint European Undertaking for ITER and the Development of Fusion Energy, "Fusion for Energy" (F4E GB) Mrs. Maija Bundule, Latvian Academy of Sciences Mr. Andris Sternberg, ISSP UL

EFDA Public Information Group(recently – Public Information Network – PIN) Mr. Maris Kundzins, ISSP UL

2.6 Public Information

Conferences

Results of fusion research were presented at:

- The annual scientific conference of University of Latvia.
- The 27th and 28th Scientific Conferences of Institute of Solid State Physics, University of Latvia.
- International Conferences "Functional Materials and Nanotechnologies" (FM&NT-2012, FM&NT-2011) Riga, Institute of Solid State Physics, University of Latvia

Educational activities

Excursions at ISSP UL from schools were organized two to three times a month for PhD students from Latvian universities. Booklets about ISSP UL and EFDA were distributed.

Television, press

Presentation in the television broadcasts TV1, TV7, TV24 and interviews in the newspapers "Neatkarīgā rīta avīze" and "Latvijas avīze". Presentations in Radio – popular science broadcast.

Popularization of science

Presentation in the TV programme "Science in Latvia", Presentation in the programme "Researchers Night in Latvia" on 28th of September, 2012.

2.7 Funding and Research Volume 2012

In 2011 the expenditure of the Association EURATOM-University of Latvia was:

Item	Expenditure (EUR)
General Support (20% EU contribution) Physics	427 917
TOTAL GOT EOROBREED HYDOBE Priority Actions (Additional 20% EU contribution)	427 917 11 251 25321
Missions and Secondments under the Agreement on Staff Mobility (100% EU contribution)	5709

3. PHYSICS PROGRAMME – FUSION PHYSICS

3.1. Stability of metal droplets jets in tokamak eviroment

WP12-PEX-04-TO3-01/University of Latvia/BS

Principal investigator: E.Platacis.

Staff members: O.Lielausis, A.Shishko, A.Klukins, K.Kravalis, G.Lipsberg, J.Peinbergs.

Introduction

Historically three types of free surface liquid metal flows have been considered as promising means for high heat flux removal in fusion applications, namely, capillary motions, jet/droplet streams and film flows. Three are also the main candidates of materials - lithium, gallium and tin. The given work belongs to a direction characterized by the fact that as a working medium a high-z material, namely Ga, is chosen. First publications here are bringing us back to the 1980th, for example [1]. However, in a definite sense decisive are the recent results gained on ISTTOK [2, 3, 4, 5]. In general, these results should be classified as clearly positive. It has been shown that not especially complicated techniques are needed for the preparation of the material, for its introduction in the discharge chamber, for a long-standing prevention of the workability of Ga. Next, confirming information has been presented that in the presence of a direct contact of Ga with the plasma the discharges remain feasible, practically unchanged. At the end, the power extraction capacity of a fast flowing stream of Ga was directly measured. Numbers were gained fully relevant to the conditions on the surface of real highly loaded divertor. It is worth mentioning that these are results of a rather general meaning, not connected with the concrete form of material motion.

In the last phase of work on ISTTOK a definite deflection of the downwards directed Ga stream was detected, caused by the discharge. It is not a trivial task to clear up this phenomenon. Forces should be found, comparable with the gravity force. Especially complicated is the situation when the flow fully consists of small scale droplets.

Stability of liquid metal jets trajectory in strong non homogeneous magnetic fields.

The performance of the described below experiment was motivated by the deflection of the jet/droplet stream observed during the tests on ISTTOK. The question was could not the shift be caused by the non-uniformity of the magnetic field. Our superconducting magnet, inclined for 30^{0} , served as a base for the experiment (Fig.3.1.1). A containing the jet cylinder (D=6cm; L=24 cm) can be placed in two positions. First, in the central plane of the magnet when only two components of the field are present, second, in a shifted position when all the three components of the field are included in the action. A reference [6] can be mentioned here showing that the presence of all the three components of field is essential. Important is the distribution of the component B_x reaches a remarkable value, close to 9 T/m. If the cylinder is shifted the gradient of the jet has been shown in a sequence of video frames (Fig.3.1.3). The jets trajectory remains

practically unchanged. The conclusion is that the gradient magnetic fields can not be considered as remarkable actors at the consideration of the mentioned deflection. An additional experimental confirmation of old theoretical estimates has been given.



Fig.3.1.1 Superconducting magnet, inclined for 30°



Fig. 3.1.2 Distribution of the components of the field along the axis of the jet.



Fig.3.1.3. The paths of the jet, shown in a sequence of video frames.

Influence of a non-homogeneous magnetic field on the stability of the break-up length.

If it is necessary to describe the "healthy' of a jet quantities the break-up length can be considered as one of the characteristics. Previously we have shown that under the influence of a magnetic field the break-up length of a liquid metal jet can remarkably grow [7]. However, in the corresponding experiments the transverse magnetic field was applied only to the origin of the jet. Directly the nozzle was placed in the space between the magnetic poles with permendure pole-shoes. Values of the field up to 3.5 T were reached. After passing the nozzle the jet had to penetrate a region characterized by a very high gradient of the field, of the order of 50 T/m. Under such conditions the structure of the jet becomes essentially influenced by the e.m. forces, even the cross section of the jet is changing, etc [7]. In spite of such additionally introduced perturbations the break-up length was growing. It is a direct indication that the influence of the field on the jet can be clearly stabilizing. Without any doubts, this phenomenon is worth a deeper investigation. In the given case not only the nozzle but the full path of the jet was placed in a magnetic field, non homogeneous, but characterized by the mentioned in Chapt.2.1 gradients. In a rather wide range of velocities the break-up length was measured. Mainly because of the strong stray fields around the magnet it was not an easy task.

In Fig.3.1.4. photos of the jet at two different velocities have been presented. At v=54 cm/s a clear sequence of jets distortion can be fixed. The first break-up point was considered as characteristic. At v= 108 cm/s only this first break-up point remains in the field of vision.



V = 54.2 cm/s

Fig.3.1.4. Photos of the jet at two different velocities

The main result is represented in Fig. 3.1.5a,b. For two situations the break-up length in dependence on the velocity can be compared. First, in the initial zero-version (B=0T), second, in the case of a 4T.



Fig.3.1.5. Break-up length in dependence on the velocity, a: B=0T, b: B=4T

Pathway of a LM jet over a solid substrate in the presence of a strong magnetic field.

The ISTTOK results have triggered the resumption of the old discussions about the stability/applicability of free-flying LM formations. The introduction of LM droplet screens [1] could be reminded as a direct initial result of these discussions. However, these applications caused a number of new problems. It was difficult to generate the droplets with the necessary velocity; it was difficult to define the amount/number of droplets which are reacting with the plasma during the short discharge, etc. At the experiments on ISTTOK a new physical phenomenon was introduced in the consideration - the break-up of a jet in droplets. Accordingly, new experimental opportunities appeared. The determination of the high power transfer capacity of a free surface LM flow should be named as an essential result in this direction. To explain the measured deflection the necessity in high acting force should be underlined - during the short pulse of the order of the gravity force. It is not easy to find a source for forces of such a value, especially in the case of a pure droplet flow.

In the given Chapter we are speaking about additional opportunities connected with the specific behaviour of LM jets doing their path over solid substrates in the presence of strong magnetic fields. Purposeful investigations in this direction were started in 2011, the corresponding results can be found in the Annual report 2011 of our Association [8]. Let us start with a picture from this report (Fig.3.1.6) where the scheme of the experiment is presented. Three d=2.2 mm jets were targeted along a flat plate under the angle of 12^{0} . The magnet was inclined for 10^{0} . In such a way a typical to a divertor configuration of the field was achieved – 90% coplanar with the plate, 10% perpendicular to the plate.



Fig.3.1.6. Tree v = 2 m/s jets touching the plate in the presence of a B=1T field.

Fig. 3.1.6b. illustrates also a typical to the experiment situation – three jets touching the plate with the velocity of 2 m/s in the presence of a B=1T field. The field reached the value of 4T. A specific feature was clearly fixed, namely, the tendency of the jets to rebuild and preserve their individuality under the influence of orthogonal magnetic field. It was stated that the structure of the generated flow depends essentially on the boundary conditions. Non wetted /wetted substrates were compared. In a number of experiments the conducting nozzles were electrically shorted with the outlet of the plate, etc.

In 2012 the experiments were extended to the case of curved substrates. It is well known that the curvature of the path can essentially influence the structure and stability of the flow. The scheme of the experiment is presented in Fig. 3.1.7a and Fig. 3.1.7b.



(a)





Fig.3.1.7. Scheme of the experiment



Fig. 3.1.8. Design of the nozzles









V = 141 cm/s

V = 214 cm/s

V = 261 cm/s

B= 2 T







V = 110 cm/s



V = 150 cm/s

B= 4T







Fig. 3.1.9. Paths of the jets over a curved substrate.

The design of the nozzles should also been mentioned. In the previous 2011 experiments the nozzles were fully metallic, made of a SS monolith. In the new 2012 experiments the jets were formed by 40 mm long SS needles issuing from a cylindrical Plexiglas extension (Fig.3.1.8). The bare SS contacting surface was not specially prepared. The boundary conditions can be described in a following way – a non wetted wall, with a bad electric contact to the liquid metal. The jets are attacking the wall at an angle of $\approx 30^{\circ}$. The initial situation without the field can be characterized by Fig. 3.1.9a. In this purely hydro-mechanical case a definite spreading or diffuseness of the material is clearly present; this structure is essentially time dependant. When a 2T magnetic field is applied drastic changes in the process of collision can be fixed (Fig. 3.1.9b.). The jets are clearly tending to preserve their individuality, to remain standing apart. In the presence of a 4T field this tendency be comes even more expressed (Fig. 3.1.9c).

Conclusion

The non-uniformity of the magnetic field can not remarkably influence or explain the measured on ISTTOK shift of the LM jet / droplet stream.

Under conditions when the jet (including the nozzle) is placed in a non-uniform magnetic field the break-up length of the jet is not reduced, remains practically unchanged.

Solid substrates or rails can be used for the control of the pathway of LM jets in the presence of strong magnetic fields. The corresponding physical processes can depend essentially on the boundary conditions.

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Cooperation

- 1. ISTOK Lisbon, Portugal
- 2. EURATOM Association of Hellenic Republic

3.2. Theory and code development

3.2.1 EU Topical Groups: TG-MHD (MHD), TG-H&CD (Heating and Current Drive)

Principal investigator O. Dumbrajs

Research Topics

3.2.1.1. Analysis of equations arising in gyrotron theory.

The gyrotron is a microwave source whose operation is based on the stimulated cyclotron radiation of electrons oscillating in a static magnetic field. Powerful gyrotrons can be used to heat nuclear fusion plasma. In addition, they have found a wide utility in plasma diagnostics, plasma chemistry, radars, extra-high-resolution spectroscopy, high-temperature processing of materials, medicine, etc. However, the main application of gyrotrons is in electron cyclotron resonance heating in tokamaks and stellarators. Equations describing gyrotron operation are ordinary differential equations and Schrödinger type partial differential equations. The present paper provides a survey of the analytical and numerical results concerning these equations obtained by our group in the last decade.

3.2.1.2 Regions of azimuthal instability in gyrotrons.

This paper is devoted to the analysis of the instability of operating modes in highpower gyrotrons with cylindrically symmetric resonators. This instability manifests itself in destruction of the azimuthally uniform wave envelope rotating in a gyrotron resonator having a transverse size greatly exceeding the wavelength. The appearance of azimuthally nonuniform solutions can be interpreted as simultaneous excitation of modes with different azimuthal indices. This problem is studied self-consistently, i.e. taking into account the temporal evolution of both the azimuthal and axial structures of the wave envelope. The region of gyrotron operation free from this instability is identified. The efficiency achievable in this region can be only 1-2% lower than the maximum efficiency. It is also possible to address the difference between the theory of mode interaction developed under assumption that all modes have fixed axial structure and the self-consistent theory presented here. As known, for fixed axial mode profiles, single-mode high-efficiency oscillations remain stable no matter how dense is the spectrum of competing modes, while the self-consistent theory predicts stable highefficiency operation only when the azimuthal index does not exceed a certain critical value. It is shown that the azimuthal instability found in the self-consistent theory is caused by excitation of modes having axial structures different from that of the desired central mode.



Fig. 3.2.1. Lines of equal orbital efficiencies and the boundary of the region of stable operation in the plane of gyrotron parameters "beam current versus cyclotron resonance detuning" for two values of the normalized cavity length. Dashed lines show the efficiency contours of central mode oscillations which exist at small azimuthal parameter W, but are unstable at large W. Dash-dotted lines show the boundary of the region where oscillations of the central mode exist.

3.2.1.3. Analysis of aftercavity interaction in European ITER gyrotrons and in the compact sub-THz gyrotron FU CW-CI.

Possibilities of arising of aftercavity interaction (ACI) are analyzed in the ITER 170 GHz 2 MW coaxial cavity gyrotron and the 170 GHz 1 MW cylindrical cavity gyrotron, as well as in the compact 394.5 GHz low power gyrotron FU CW-CI. Also, the simulations for the gyrotron efficiency in the presence of aftercavity interaction are performed in the cold cavity approximation. Results of the analysis illustrate the subtle interplay between the geometry of the output taper and the profile of the magnetic field. ACI can have a noticeable influence, both positive and negative (as shown in the figure below), on the efficiency of the tube. Subtle interplay between the geometry of the output taper and the geometry of the output taper and the magnetic field profile should be analyzed in detail for each chosen set of gyrotron operating parameters best of all self-consistently. Since it is much easier (cheaper) to modify the geometry of the output taper than the profile of the given magnetic field and then optimize the geometry of the output taper, in order to achieve the highest possible efficiency for the desired operating parameters of the gyrotron.



Fig. 3.3.2. Efficiency as a function of longitudinal coordinate. The vertical dashed line marks the middle of the cavity.

Calculations of starting currents and frequencies in frequency- tunable gyrotrons.

In recent years, much attention has been paid to the development of frequency-tunable low-power high-frequency gyrotrons. Such gyrotrons can be used to study dynamic nuclear polarization, nuclear magnetic resonance, the hyperfine split of positronium, and for plasma diagnostics measurements. Here, the tuning scheme is based on the excitation of cavity modes that only differ by their number of axial variations on their field profile, which may lead to continuous tunability.

In this paper, we summarize cold cavity and self-consistent formalisms for calculating starting currents and frequencies. A comparison of the obtained results shows that they are very different and that for a reliable design the use of the self- consistent approach is mandatory.



Fig. 3.2.3. Starting current as a function of magnetic field.

3.2.1.4. On optimization of sub-THz gyrotron parameters.

The theory is developed describing how the optimization of gyrotron parameters should be done taking into account two effects deteriorating the gyrotron efficiency: the spread in electron velocities and the spread in the guiding center radii. The paper starts from qualitative analysis of the problem. This simplified theory is used for making some estimates for a specific gyrotron design. The same design is then studied by using more accurate numerical methods. Results of the latter treatment agree with former qualitative predictions.

Collaborations

Institute of Mathematics and Computer Science, University of Latvia, LATVIA Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, USA Research Center for Development of Far-Infared Region, University of Fukui, JAPAN

3.2.2. *Ab initio* simulations of the reduced activation steels strengthened by yttria precipitates

WP11-MAT-REMEV-01-01/University of Latvia

Principal investigator: Dr. V. Kuzovkov Staff members: Yu.F. Zhukovskii, A. Gopejenko, Yu.A. Mastrikov,

Problem and Motivation

Studies of oxide dispersion in steels performed, in order both to strengthen them mechanically and to increase their working temperatures, were started in 1950's being permanently improved then. Current generation of reduced activation ferritic-martensitic steels (RAFM) strengthened by oxides allows a growth of the operating temperature for future fusion and advanced fission reactors by 100°C, up to 650°C, or even higher. The most commonly used oxide for the strengthening of RAFM steels is Y_2O_3 . It is one of the most stable oxides with melting temperature higher than that of the steels, which might play a significant role in the formation of oxide nanoparticles in the oxide dispersion strengthened (ODS) steels. These materials are produced by mechanical alloying for several tens of hours, followed by a hot isostatic pressing (hipping) at temperature around 1000-1200°C and pressure ~100 MPa. Experimental evidences suggest that a significant part of Y and O atoms were observed in steel matrix with concentrations above their equilibrium solubility. This might mean that precipitation of Y_2O_3 nanoparticles occurs already during the hipping stage.

Mechanical properties and radiation resistance of ODS steels are strongly affected by a size and distribution of oxide particles. Atomic-scale calculations provide a valuable information on the details of the ODS particles formation process. Depending on the concentration of Cr, steel may go or may not go through the phase transformation. Low-Cr (9-12%) steels might be considered as better candidates for application in future fusion and advanced fission reactors as under irradiation at low temperatures while higher concentration of Cr (>12%) cause the formation of the δ ferrite and Cr-rich α '-phase which negatively affect the impact toughness of the material. This is why, the process of ODS particle formation has to be studied in both phases – α (*bcc*) and γ (*fcc*).

Method

We propose a two-step approach for the atomistic simulation of the oxide nanoparticle formation. The first step described in this study includes large-scale ab initio calculations of different defect complexes (vacancies, yttrium and oxygen atoms) in various spatial configurations. Defect interaction energies and diffusion barriers of solute atoms extracted from these calculations are used in further atomistic simulations. The second step includes the lattice kinetic Monte Carlo (LKMC) simulations based on the results of *ab initio* calculations, in order to study the kinetics of the growth of the precipitates. Our previous first principles calculations performed for fcc-Fe phase clearly show that vacancies might play the significant role in the formation of the ODS precipitates in the steel matrix.

The first principles calculations have been performed using the *VASP 5.2* computer code. This is based on the Density Functional Theory (DFT) approach with a plane-wave (PW) basis set as well as the Perdew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA) and Perdew-Wang-91 GGA [13] non-local exchange-

correlation functional for α - and γ -Fe lattices, respectively. The core electrons are described using the Ultra Soft Pseudopotentials (USPP) within the Projector-Augmented Wave (PAW) method.

A series of preliminary *ab initio* calculations has been performed, to define the parameters of calculations necessary to reproduce the basic experimental data (lattice constant, cohesive energy *per* atom) for both α -Fe and γ -Fe. This includes an analysis how the convergence of the results depends on the supercell size, the cut-off energy and the *k*-point set in the corresponding Brillouin zone. Our model supercells are cubic for both phases, with the extension $4a_0 \times 4a_0 \times 4a_0$. It provides the lowest volume and, at the same time, the largest distance along the direction of the strongest interaction in both lattices. Lattice parameters have been optimized for perfect *bcc*- and *fcc*-lattices being fixed for the calculations on defective lattices. For arbitrary configuration of defective iron supercells, positions of all atoms have been optimized by a minimization of the total energy. Since the magnetic properties have certain impact on several parameters of defective lattice, different configurations of *bcc*-Fe have been calculated in the ferromagnetic state while *fcc*-Fe phase attributes to paramagnetic state. The *k*-point sets in the Brillouin zone should be at least $16 \times 16 \times 16$ -mesh for unit cell model (UC) and $9 \times 9 \times 9$ -mesh for supercell (SC).

Progress in 2012

1. ODS simulation in α *-Fe lattice*

A. Atomic radius of Y atom is larger than that of Fe atom (0.18 and 0.14 nm respectively), which creates a strong repulsion between them inside an iron matrix. On the other hand, impurity Y atom can stably exist in iron lattice as a substitute only (Y_{Fe}) . The repulsion between the two Y_{Fe} atoms could be reduced by creation of Fe vacancies (V_{Fe}). Stabilization of Y atom inside iron lattice could require more than one vacancy *per* solute atom. In such a case, not only substitute Y_{Fe} atom is stable but also yttrium atom in interstitial sites (Y_i). The reference energy state for the isolated cluster of N vacancies as well as isolated Y_{Fe} and Y_i atoms could be estimated if the impurity yttrium atom is positioned in the center of vacancy cluster:

$$-E_{bind}(N) = E_{cluster}(N) + N \times E_{Fe_UC} - N \times E_{single_{V_{Fe}}} - E_{single_{Y_{Fe}}}.$$
 (1)



Fig. 3.2.2.1. Energetic stabilization of yttrium atom surrounded by different number of vacancies in *bcc* iron lattice.

Size of vacancy cluster in the bcc iron lattice has been varied from one to nine vacancies in the 128-atom supercell (Fig. 1). A single Y solute atom incorporated in different vacancy clusters has been considered. As the reference energies, there are used isolated vacancies and isolated Y_{Fe} , Eq. (1). In all the configurations, yttrium atom is positioned in the middle of $N \times V_{Fe}$ cluster and all the defect complexes have been found to be energetically more

stable. As in the case of pure vacancy clusters, incorporation of additional vacancy to the cluster containing Y_i atom and six vacancies in octahedral coordination around it (Fig. 1) is energetically less favorable. Although the complex of Y_{Fe} atom and eight vacancies in cubic coordination around it has been found to be stable too, the binding energy for this configuration is smaller, than that for clusters containing six and eight vacancies with interstitial Y*i*.



Fig. 3.2.2.2. Interstitial O_i atom localized at a) octahedral and b) tetrahedral sites of α -lattice.

B. There are two stable interstitial positions for oxygen in the *bcc* Fe lattice: octahedral and tetrahedral (Fig. 2): Interstitial O_i atom localized at a) octahedral and b) tetrahedral sites of α -Fe lattice. Interactions between the two O atoms at both octahedral and tetrahedral positions are repulsive. The strongest repulsion has been observed for the 4NN and the 11NN O_i - O_i distances (-1.81 eV and -2.28 eV, respectively), *i.e.*, the former is energetically more favorable (by 0.47 eV).

2. ODS simulation in γ -Fe lattice

A. Different configurations of defective clusters containing O and Y impurity atoms as well as vacancies in fcc Fe lattice were considered by us earlier. The results obtained by us recently clearly show noticeable influence of vacancies on the binding energies of impurity atoms which lead to the study of the interactions between increased number of vacancies (three and four vacancies were placed in the closest positions). Very small binding energy was found between three vacancies (0.36 eV), however, noticeable binding energy was found between four vacancies (1.36 eV), which qualitatively corresponds to results obtained by us for clusters of vacancies in bcc-Fe lattice. Analogous conclusion can be drawn when comparing bonding of Y atoms in vacancy clusters of different sizes and configurations inside bcc- and fcc-Fe lattices (Table 1), results obtained for fcc-Fe lattice are qualitatively similar to those obtained for bcc-Fe.

Table 3.2.2.1. Binding energies between Y and multiple vacancies inside γ -Fe lattice.

	1NN					2	2NN	1	
•	٠		Configuration	E_{bind} , eV		•		٠	
		•	$Y_{\rm Fe}$ -2 $V_{\rm Fe}$ (1NN)	4.75	-	•	•	-	•
•			$Y_{Fe}-2V_{Fe}(2NN)$	4.14					
	•	•	$Y_{\rm Fe}$ - $3V_{\rm Fe}$	7.55			0		

B. The calculations of the two Y atoms and V_{Fe} vacancy were performed for configurations where two Y atoms were located at the increased distances 2NN, 3NN and 4NN (Table 2). The binding energies increased with growth of the distance between two Y atoms, analogously with the results obtained for $Y_{\text{Fe}}-V_{\text{Fe}}-Y_{\text{Fe}}$ configuration in *bcc*-Fe lattice.

Table 3.2.2.2. Binding et	nergies between the two	• Y _{Fe} atoms at di	fferent distances and
$V_{\rm Fe}$ inside γ -1	Fe expressed via nearest	t-neighbor (NN)	spheres.

Configuration	E_{bind} , eV
Y_{Fe} - V_{Fe} - Y_{Fe} 2NN	1.76
Y_{Fe} - V_{Fe} - Y_{Fe} 3NN	2.26
Y_{Fe} - V_{Fe} - Y_{Fe} 4NN	2.32

C. It is also important to study how O impurity might affect the binding energies between two Y atoms. Calculations of different impurity clusters containing two Y_{Fe} atoms and O atom have been performed: two Y atoms are either 1NN (*i*) or 2NN (*ii*) neighbors while oxygen atom is either located at O site closest to both Y (*iii*) or O_{Fe} substitute closest to them (*iv*). The results of these calculations (Table 9) show that no bonding exists for both (*i*) and (*ii*) configurations whereas the large binding energies are found for the configuration where O atom is in the substitution position with the highest binding energy assessed for the (*iv*) configuration. Thus, a quite complicated field of the interactions is formed at the initial stage of Y₂O₃ precipitate growth inside the iron lattice, and location of the impurity atoms in their equilibrium sites found for single atoms does not result in their stable co-existence in Y_mO_n clusters.

Table 3.2.2.3. Interactions in $Y_{Fe}-O_{Fe}-Y_{Fe}$ and $Y_{Fe}-O_i-Y_{Fe}$ clusters inside γ -Fe.

Configuration	E_{bind} , eV
Y_{Fe} - O_{Fe} - Y_{Fe} (2NN)	3.11
Y_{Fe} - O_{Fe} - Y_{Fe} (1NN)	2.23
Y_{Fe} - O_i - Y_{Fe}	no bonding

Collaboration

1. Dr. A. Möslang and Dr. P.V. Vladimirov (IAM, Forschungzentrum Karlsruhe, Germany)

4. EFDA FUSION TECHNOLOGY PROGRAMME

4.1. Analysis of accumulated tritium and microstructure of carbon based jet divertor tiles JW11-FT- 1.19 and JW12-FT-1.20

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Staff members: L. Avotina, M. Halitovs, J. Jansons, L. Baumane, R. Zauls, D.Kurgs, J. Lapins

The tasks JW11-FT-1.19 and JW12-FT-1.20 are related to the estimation of the tritium distribution in the carbon based tiles – tungsten uncoated, coated and laser cleaned. Both tasks are continuation of the EFDA JET Technology Tasks on the tritium in tokamaks. Besides mentioned tasks laboratory additionally investigated microstructure of tiles.

The tasks were realized in cooperation with association of EURATOM and Romania, MEdC, as well as with Finland, TEKES and Estonia.

The use of the materials with high mechanical, thermal stability and low tritium inventory is of great importance in the devices foreseen for the power generation. Particularly high demands on the properties of the materials are for those used in fusion devices, because of the severe conditions they will be exposed to. The surface temperature of divertor materials, used in fusion reactors, in some moments reaches even 2000°C.

Carbon fibre composites (CFC) are one of the considered materials for the applications in fusion devices. Besides its high stability, CFC is a material with low mass number and therefore with small effect on plasma and fusion reaction in contrary to high Z materials. Nevertheless, erosion, tritium co-deposition and high tritium retention in CFC material is an important problem.

Tungsten, due to its small physical and chemical sputtering and low tritium permeability, will be used as the main material for divertor of fusion devices such as International Thermonuclear Experimental Reactor (ITER). Joint European Torus is now operated with an ITER like wall (ILW) in which tungsten coatings on (CFC) tiles are also presently tested in the divertor area while CFC-only tiles were used previously. The effects of W coating are evaluated in terms of tritium retention analysing the tritium inventory in the divertor tile samples. The results are meant to be used for the development of divertor tiles in ITER.

Tritium accumulation in co-deposited layers of CFC on surface of a tile is an important problem for resolution, as inventory of tritium be limiting phase for the operation a fusion device. One of the methods for cleaning CFC tiles from tritium is removal of deposited layers with laser ablation. Tritium amount in laser cleaned and uncleaned surface of a tile and in a bulk is compared.

Goals of the tasks are to estimate influence of tungsten layer on a surface of a tile on tritium accumulation on the first layers of a tile and deeper, to determine depth profiles of tritium trapped in the bulk of CFC tiles, to make comparison of tritium amount in the bulk and surface layers, to estimate changes of structure of a tile and to investigate properties of the tritium trapped in CFC tiles.

The slices for analysis of tritium amount were prepared by standard method, at first a cylinder sawing and after cutting of the cylinder in slices were done.

Determination of tritium in a separate sample was realized by full combustion or wet oxidation method and liquids scintillation method. Selected samples were analysed with the methods of powder X-ray diffractometry (PXRD), Raman spectroscopy and Fourier transformation infrared spectroscopy (FT-IR).

4.1.1. Tritium inventory in tungsten coated and uncoated tiles of divertor MkII-HD

Tungsten coated and uncoated tiles of the MkII-HD divertor configuration used in JET during the experimental campaign in 2007-2009 were compared. Tile 20WG7B and 20NG8A tungsten coated and uncoated tile 2IWG1A had been analysed. Tile 20WG7B and 20NG8A have $\sim 25 \,\mu m$ tungsten coating with molybdenum interlayer.



Fig. 4.1.1. Tungsten coated divertor tiles 20W G7B (a) and 20N G8A (b)



Fig.4.1.2. Drill holes of sample cylinders in tiles 2OW G7B (a) and 2ON G8A (b and c)



Fig.4.1.3. Some of the analyzed samples with W coating (a), with W coating and erosion material film (b), without coating in the bulk of cylinder (c)

Analysis of tritium distribution in the cylinders of tungsten uncoated and coated tiles show the same regularity of tritium distribution as in previously analyzed samples but was observed difference that changes amount of tritium and ratio between tritium amounts in plasma facing part slices and in the bulk slices.

Analysis of surface activity of tritium once more confirms the fact that main part of tritium is accumulated in a deposited layer. Thickness of the first analyzed layer is about 1 mm for full combustion technique. In the next slice, which is 2-3 mm deeper from plasma facing part, tritium amount sharply decrease up to order of 1-1.5 magnitude.

The results of experiments are as following.



Fig.4.1.4. Tritium mass activity comparison in tungsten coated tile 2ON G8A and scheme of positions of the cylinders

Distribution of tritium amount depends on position of tile against plasma reaction zone. Anyway the difference between activity of tritium amount for cylinders Cyl 2a, 6a and 8a of tungsten coated tile 2ON G8A is not substantially different, but in the first slice of Cyl 10a amount of tritium is the larger. It is understandable as the Cyl 10a is not placed straight against plasma zone. In the bulk of tile 2ON G8A in the slices 2, 3,4 5, which are 2-9 mm deep from plasma facing surface, for all investigated cylinders Cyl 2a, 6a, 8a and 10a tritium amount has one order magnitude.



Fig.4.1.5. Tritium mass activity comparison in tungsten coated tiles 20WG7B (blue color) and 20N G8A (orange color)

Tritium amount in tungsten coated tiles 7 and 8 (20WG7B and 20N G8A) is one magnitude. Comparison of tritium amount in tile 7 and 8 shows clearly, that tritium is more accumulated in tile 8 -20N G8A. Observed that in both cases as in the first slice and in the bulk of tile tritium accumulated more in tile 20N G8A.

Samples of uncoated divertor tile **2IWG1A** used in the same JET experimental campaign in 2007-2009 with an MkII-HD divertor configuration was analyzed in comparison to W-coated tiles, resulting in following:



Fig.4.1.6. Tritium mass activity comparison in cylinders of uncoated and tungsten coated tiles:

- cylinders Cyl 1b, Cyl 2b, Cyl 5b of uncoated tile 2IW G1A tile
- cylinder Cyl 2a of tungsten coated tile 2ON G8A
- cylinders Cyl 1a, Cyl 5a of tungsten coated tile 2OW G7B

As observed in this and previous studies for uncoated divertor tiles, there is up to 3 orders of magnitude difference between the tritium activity in plasma exposed surface upper layer and the bulk. For the W-coated tiles retrieved from the same divertor area this difference appears to be smaller –about 1-2 orders of magnitude – compare with the bulk activity of tile.

Experimental work provides confirmation that tungsten coating of divertor tiles has a beneficial effect reducing the tritium retention on both, on the plasma exposed area of as well as in the bulk of tile. Therefore, from the point of view of tritium retention, tungsten can be efficiently used in the divertor region of any fusion machine such as ITER or DEMO.

4.1.2. Tritium in laser cleaned tiles of divertor MkII-SRP

Effects of divertor **tile surface laser** treatment were evaluated. Divertor laser cleaning is one of the fusion device maintenance methods that would be used to prolong the usage of divertor material, decrease tritium accumulation in the divertor materials and provide less erosion materials that might interact with plasma.

Samples of tiles 14ING3B with part of the plasma facing surface area $(25 \cdot 10^{-4} \text{ m}^2)$ cleaned by Yb-doped 1070 nm fibre laser from JET experimental campaign in 2001-2004 with an MkII-SRP divertor configuration were tested. Parallel samples were tested from cleaned and non-cleaned sides of the divertor tile.



Fig. 4.1.7. Divertor tile 14ING3B with drill holes and laser-cleaned side, MkII-SRP divertor configuration



As observed in the experiments, laser treatment of divertor tile top layers indeed decreased the amount of accumulated tritium in the analyzed samples. Due to the fact that vast amount of accumulated tritium is located in the top layer of divertor (in depth less than 1 mm), and as cleaned side of the tile had approximately 50 μ m of material removed, the experimental results have proven effect of laser cleaning. Total accumulated tritium activity is reduced by 10 – 100 times and it means that the method is efficient enough to be used for the maintenance of fusion device divertor.

4.1.3. Microstructure of MkII-SRP divertor tiles comparing with amount of accumulated tritium

Studies were realized for selected tiles of the JET divertor configuration MkII-SRP (SRP – septum replacement plate) of campaign during period 2001.-2004. Tile samples (slices cut from a tile) were taken in order to characterize the structure of material in bulk of a tile and to find possible bonding with accumulated tritium. The samples were analyzed with the methods of powder X-ray diffractometry (PXRD), Raman spectroscopy and Fourier transformation infrared spectroscopy (FT-IR). In order to understand is tritium accumulation in bulk of CFC related with microstructure of a tile we chose for analysis base wide tile 4 - 14BWG4B and inner narrow tile 3 - 14ING3B. Several cylinders, considering to poloidal and toroidal direction in a tile, were sawed from different parts of it (Figs. 4.10, 4.12). Cylinders were afterwards cut in two parts and sliced in separate slices of thickness of 0.7 - 1.2 mm and the diameter of about 1.5 cm, sawing way - 1 mm (Figs. 4.13, 4.15). One part slice was send to accelerated mass spectrometry analysis (AMS).

The positions of analyzed cylinders of tile 14BWG4B are done in the Fig. 4.10 and characterization of tile 14ING3B – in Figs. 4.11 and 4.12.



Fig.4.1.10. Positions of analyzed cylinders of tile 14BWG4B, the JET MkII Septum Replacement Plate divertor (SRP)



Fig.4.1.12. Scheme of divertor fragment exploited in JET (2001.-2004.)



Fig.4.1.13. Tile 14ING3B, exploited in JET (2001.-2004.), top view





Fig.4.1.14. Slices of tile 14ING3B

Fig.4.1.15. SEM image of slice 3f-6N from tile 14ING3B, dimensions approx.0.1x0.1 mm)

X-ray diffractometry was used for structure analysis. It is known that changes of the reflex intensity show heterogeneity and crystallinity of sample. In diffractrogramms observed diffraction reflex at $26.5^{\circ}2\Theta$ characterises graphite structure in CFC material. The mentioned reflex is observed in all analyzed CFC slices.



Fig. 4.1.16. X-ray diffractogramms of slice 1f-6a from tile 14ING3B

Position of cylinder 1f of tile 14ING3B and diffractogramms of half-slice 6a are shown in Fig. 4.16.

Interaction between amount of accumulated tritium (Figs.4.17and 4.18) and material of tile 14BWG4B taken from two parallel rows shows that amount of accumulated tritium and changes of structure correlates. Material is more amorphous (Fig. 4.18.) in parts of tile where the amount of accumulated tritium is higher. Differences in structure depend on plasma processes in vacuum camera and are linked to position of tile in vacuum chamber and geometry of tile.



Fig.4.1.17. Tritium distribution in slices in poloidal direction in the I and II row of tile 14BWG4B (in depth 3-4 mm from plasma facing surface-PFS)



Fig.4.1.18. Intensities of diffraction reflexes in poloidal direction in the I and II row of tile 14BWG4B (in depth 2-3 mm from PFS)

The structure of material was also investigated with Raman spectroscopy. Raman spectra were taken for the half-slice from the middle part of tile – half-slice 3f-6a, tile 14ING3B. If in the spectrum is a single high-frequency line at about 1580 cm⁻¹ it is attributed to large single crystal graphite. In case of analyzed CFC two peaks are observed in spectra. The G-peak, at about 1580 cm⁻¹, is due to the bond stretching of all pairs of sp² atoms in both rings and chains (C-C bonds of graphite). A peak at about 1350 cm⁻¹ (D-peak) is due to the breathing modes of sp² atoms in rings.

The presence of the D-peak in Raman spectra points to disorder related structures in material. That matches with results of X-ray diffractometry, which shows a presence of amorphous structures in the investigated tiles (Fig.4.19). The differences between Raman spectra of samples could be explained with different plasma exposure to different parts of the tile.



Fig. 4.19. Raman spectra of the slice 6a from cylinder 3f of tile 14ING3B and position of these in the divertor

In the sloping part of tile 14BWG4B (positions see Fig.4.10, Cyl 6 to Cyl 8) tritium activity is higher as in cylinders of the SRP and of the shadowed part (Fig. 4.20).



Fig. 4.1.20. Tritium activity in slices of tile 14BWG4B into depth 4-5 mm from PFS



Fig.4.1.21. Intensity ratio I_D/I_G in slices of tile 14BWG4B in depth 2-3 mm from plasma facing surface

Intensity ratios I_D/I_G calculated from Raman spectra are lower in sloping part as in shadowed area and SRP part (Fig.4.1.21), which points to structure changes in severe parts of tiles, that is analogous to tritium distribution.

Structure, including microcrystalline structure, of the tiles is not homogeneous and depends on a position of a tile, against plasma interaction. Consequently, it might be assumed that different mechanisms of tritium migration and deposition are possible in different parts of tile.

4.2. Tritium release from high dose neutron irradiated HIDOBE-01 beryllium pebbles

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The helium-cooled pebble bed (HCPB) is one of the concepts developed in Europe for the breeding blanket of the future DEMO/Power Plant. In the HCPB blanket, beryllium or beryllide pebbles ($\emptyset \approx 1$ mm) are used as a neutron multiplier. As a result of neutron induced transmutations of beryllium helium and tritium gas is produced in considerable amounts. The global tritium production in the whole of the blanket (390 tons of beryllium) is 23.8 kg.

Under the real operating conditions of the HCPB of different designs, the multiplier Be pebbles will be subjected to action of a high temperature up to 920 K or even higher – 700-1050 K or up to 1170 K. Tritium release is governed by several mechanisms:

diffusion, surface desorption, trapping. For modeling tritium behaviour in beryllium it is necessary to know a lot of parameters solubility, trapping energies and diffusivity. Tritium and helium thermo-desorption spectra had been analyzed widely in order to get comprehensive overview of the processes occurring during thermo annealing of irradiated beryllium, but in real exploitation conditions materials will be under simultaneous action of some external energetic factors - temperature, irradiation and high magnetic field. Laboratory investigated tritium release under temperature, fast electron irradiation and magnetic field. Results of these experiments will provide better understanding on tritium behaviour in the conditions similar to magnetic confinement fusion devices and give possibility to compare material reliability for fusion applications regarding the detritiation options.

4.2.1. Determination of tritium amount and its chemical forms in the HIDOBE-01 pebbles

In order to determine total tritium activity, bulk distribution and abundance ratios of chemical forms (T_2 , T^0 , T^+) in irradiated beryllium samples, chemical scavenger and dissolution method was used. This method had been originally developed in the Laboratory of Radiation Chemistry of Solids of the University of Latvia (UL). Tritium accumulated in the HIDOBE-I beryllium pebbles has been localized in forms of the gas T_2 , radicals T^o and ions T^+ . Two different dissolution systems were used for analysis of a pebble:

• $2 \text{ mol/L H}_2\text{SO}_4$.

The dissolution of a separate pebble in pure acid transfer the T_2 and T^0 localized in the Be pebbles as T_2 +HT into a gas phase.

 T^+ localized in a Be pebble remains in the solution.

• $2 \text{ mol/L H}_2\text{SO}_4 \text{ with } 0.5\text{-}1 \text{ mol/L N}_2\text{Cr}_2\text{O}_7.$

The dissolution of a pebble in acidic solution in a presence of $Na_2Cr_2O_7$ gives additional data in order to determine the chemical forms of tritium T^0 and T_2 separately. Experiments with non-irradiated beryllium pebbles were performed in order to estimate the time of dissolution.

The rate of tritium release was measured continuously with a tritium monitor TEM 2100A with a gas flow proportional detector DDH 32. Tritium T^+ localized in the solution was analyzed by liquid scintillation method. Distillation of the solution was performed before analysis of amount of tritium. The contents of T^0 , T_2 and T^+ (Bq g⁻¹) in the sample were calculated from the tritium activities in a gas phase and in the solution. Analysis of tritium distribution in a pebble has some problems because a pebble has not perfect spheres, ideal surface and bulk structure. In the method it is assumed that tritium concentration in all points of a sphere with radius is equal. Therefore only an overall tendency of tritium distribution could be obtained. The residual amount of tritium remained in the Be pebble after its annealing was determined also by dissolution method. The initial total tritium amount in the HIDOBE-01 pebbles was determined as the sum of the total tritium activity released on annealing and the residual amount of tritium remained in the pebble after its annealing.

4.2.2. Remaining tritium in pebbles after the HIDOBE-01 neutron irradiation

At low irradiation temperature (425°C, 525°C) about 90% of produced tritium has remained in the bulk of the pebble (Fig.4.2.1.). Chemical form analysis shows that most of tritium is

accumulated as molecular T_2 . At 750°C most of the tritium is released already during the irradiation (~99%) and remaining tritium is mostly chemically bonded, could be more likely to the oxygen containing compounds.



Fig.4.2.1. Remaining tritium in beryllium pebbles of 0.5 mm size after irradiation at different temperatures



Fig.4.2.2. Distribution of tritium chemical forms in pebbles of 0.5 mm size after irradiation

Tritium bulk distribution was measured for pebbles irradiated at low temperatures, at high temperatures (750 0 C) there were insufficient tritium concentration for this method. Tritium bulk distribution measurements indicate that except for the surface layer where tritium concentration is comparably low in remaining bulk of the pebbles tritium is evenly distributed **Fig.**4.2.3.



Fig.4.2.3. Tritium distribution in the bulk of the 0.5mm pebbles irradiated at 425°C and 525°C temperature.

At low irradiation temperature (425° C) all of produced tritium remains in the bulk of the pebble. At 650°C tritium release during the irradiation has started and only 37% has remained in the bulk of the pebbles. At 750°C ~95% of the tritium is released already during the irradiation. In contrast to 0.5 mm pebbles most of the remained tritium is molecular. Therefore it might be concluded that from 1.0 mm pebbles at this temperature not all of gaseous products are released during irradiation. Tritium distribution in the bulk of the 1.0 mm pebbles after irradiation at 650°C was found to be uneven– tritium concentration increases towards centre of the pebble.

4.2.3. Thermal desorption of tritium up to 1040 °C

In order to obtain better understanding of tritium desorption, it was carried out up to 1040 °C. Tritium release experiments were performed in a quartz tube, consisting of two compartments – one for the sample and one for a bed of granulated zinc. One Be pebble was investigated in each tritium release experiment. The tritium release was performed in a continuous flow of the purge gas He + 0.1% H₂. The sample temperature was initially increased linearly with time at a constant rate of 2.3-4.8 °C/min from room temperature up to an end temperature of 1040 °C, which was kept constant for 1 h.

A stage of gradual release and a stage of abrupt release peaks (burst release) can be distinguished in the histograms of the tritium release rate. These two stages may be related to the tritium release by atomic diffusion and bubble venting, respectively. Fig.4.2.4. shows tritium release histograms from three pebbles of the same batch. Tritium release even from three beryllium pebbles of one batch is very dissimilar.



Fig.4.2.4. Tritium release rate and tritium sum release from the HIDOBE-01 beryllium pebbles having lower level tritium activity heated at the given temperature.

4.2.4. Tritium release under action of irradiation with fast electrons and magnetic field

Tritium release experiments under action of temperature, radiation and magnetic field (MF) were realized in irradiations for 3 h each with 5 MeV fast electrons for one pebble with an increasing pebble temperature: 190-250 °C (without additional heating), 500 °C, 550 °C, 600 °C, 650 °C, 700 °C, 750 °C and 800 °C. The upper limit of the annealing time of 3 h is determined mostly by the working capacity of the linear electron accelerator ELU-4 having the power consumption of 100 kW and by the aim not to increase the total time for one annealing experiment with electron radiation above 24 h. It is worth emphasizing, that the annealing experiments have high gas consumption rates – 14-15 L/h and 42-45 L/h for the purge gas He+0.1% H₂ and the counting gas 90% Ar + 10% CH₄, respectively.

A sample of tritium release from a pebble under action of irradiation without and with magnetic field is shown for a pebble irradiated with neutrons at 525 °C temperature. Such tritium release from the pebble 38sPC/3/21 (525 °C) without magnetic field and from the pebble 38sPC/3/22 (525 °C) in presence of magnetic field (MF) of 1.5-1.7 T is shown in the Figs.4.2.5-4.2.6. Forward in all figures abbreviation TR means following – T temperature, R -irradiation with fast electrons, TRM – T-temperature, R-irradiation with fast electrons and M- Magnetic field.



Fig.4.2.5.Tritium release from pebble 38sPC/3/21 (525 °C), in the flow of He+0.1% H₂. The maximum temperature 804 °C; without MF; electron irradiation for 3 h with the estimated dose 33.1 MGy. Final tritium sum release: 14.25 GBq/g (74.2% of the estimated initial total tritium 19.2 GBq/g). The current collected with the probe (the light blue curve) indicates the presence of the 5 MeV electron radiation during the annealing.



Fig.4.2.6. Tritium release from pebble 38sPC/3/22 (525 °C), m=0.16 mg, \emptyset 0.53 mm, in the flow of He+0.1% H₂ of 14-15 L/h. The maximum temperature 806 °C; in a MF of 1.5-1.7 T; electron irradiation for 3 h with the estimated dose 34.0 MGy. Final tritium sum release: 22.21 GBq/g (116% of the estimated initial total tritium 19.2 GBq/g). The current collected with the probe (the light blue curve) indicates the presence of the 5 MeV electron radiation during the annealing.

Successive irradiations at the increasing sample temperature were performed also with pebbles 46sPC/3/08 and 46sPC/3/09 without magnetic field and in a magnetic field of 1.5-1.7 T respectively. The results of these irradiations have been summarized and compared with results of the pebbles 38sPC/3/21 (525 °C) and 38sPC/3/22 (525 °C) in Fig.4.2.7



Fig.4.2.7. Cumulative activity of the tritium released in successive irradiations for 3 h with increasing temperature without magnetic field (pebble 46sPC/3/08) and in a magnetic field of 1.5-1.7 T (pebble 46sPC/3/09) as a function of the maximum temperature in the given irradiation. Values of the tritium cumulative release from pebbles 38sPC/3/21 and 38sPC/3/22 are given for comparison.

We can observe that below 600 °C tritium release was little in comparison to the total amount of tritium in the pebbles. Tritium release rate significantly increased above 600 °C. This phenomenon is in line with the fact that a considerable tritium release was observed only at 650 °C and 750 °C of the HIDOBE-01 neutron irradiation, rather than at 425 °C and 525 °C. No quantitative estimation of a possible stimulating effect of the 5 MeV fast electron radiation on the tritium release can be made from the present set of the experimental results obtained because of lack of respective annealing experiments without electron radiation. Regarding the magnetic field effect on the tritium release on annealing with simultaneous 5 MeV electron radiation, we compare two couples of pebbles irradiated with neutrons in HIDOBE-01 at 525 °C: 46sPC/3/08-46sPC/3/09 (Ø 1 mm, Fig.4.2.7) and 38sPC/3/21-38sPC/3/22 (\emptyset 0.5 mm, Fig.4.2.5 and Fig.4.2.6). In the case of the couple of pebbles with \emptyset 1 mm 46sPC/3/08-46sPC/3/09, an appreciable facilitating effect of a magnetic field of 1.5-1.7 T was observed at temperatures above 700 °C as by about 60% larger tritium release at 767-808 °C. In the case of the couple of pebbles with \emptyset 0.5 mm 38sPC/3/21-38sPC/3/22, the tritium release of 22.2 GBq/g at 799-806 °C in a magnetic field of 1.5-1.7 was by about 56% larger than that of 14.3 GBq/g at 797-804 °C without magnetic field. Experimental results indicating a facilitating effect of a magnetic field of 1.5-1.7 T with the simultaneous 5 MeV fast electron radiation on the tritium release were obtained for pebbles 9sPC/3 (Ø 1 mm (2001) 750 °C), 46sPC/3 (Ø 1 mm (2001) 525 °C) and 38sPC/3 (Ø 0.5 mm 525 °C). However, because of the fact that only one couple of pebbles was investigated on the magnetic field effect from each batch, the ability to draw general quantitative conclusions about the magnetic field effect is very limited by possible dissimilarity of the pebbles within the batch with respect to their initial total tritium amount and their tritium release properties

4.3. Influence of chemisorption products on radiolysis of lithium orthosilicate

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Lithium orthosilicate pebbles with excess of SiO₂ (90 mol% Li₄SiO₄, 10 mol% Li₂SiO₃) are the European Union's designed reference tritium breeder for the Helium Cooled Pebble bed blanket module. On surface of Li₄SiO₄ pebbles after annealing (T_{max} =1243 K, t_{max} =168 h) in air may accumulate chemisorption products of CO₂ and H₂O vapor, i.e, Li₂CO₃ and LiOH. The aim of these investigations was to estimate influence of chemisoprtion products on the radiolysis of Li₄SiO₄ pebbles. Due to high surface area and small grain size, nano-structured Li₄SiO₄ powders with different composition and different surface area was selected as investigation materials to compare with pebbles as reference. Research work was done in cooperation with Karlsruhe Institute of Technology, Institute for Applied Materials.

4.3.1. Characterization of samples and analytical methods

Li₄SiO₄ pebbles with 2.5 wt% of SiO₂ ($\emptyset_{pebb} \approx 500 \ \mu m$) were produced with standard melt-spraying method in Scoot Glass (Mainz, Germany) - batch Obi 07/M. Pebbles

were annealed up to 1243 K for 168 hours in air, to obtain homogenous microstructure. Three types of nana-structured Li_4SiO_4 powders with different composition and specific surface area were selected for investigation together with pebbles as reference (Table 1).

Table 4.3.1

Characterization	Pebbles	Nano-structured powder		
Title in text	Annealed Li ₄ SiO ₄ pebbles with SiO ₂	"Pure" Li ₄ SiO ₄ powder	Li ₄ SiO ₄ powder with SiO ₂	Annealed Li ₄ SiO ₄ powder with SiO ₂
Fundamental thermal treatment	1243 K 168 h			920 K 3.5 h
Chemical composition	90±3 mol% Li ₄ SiO ₄ 10±3 mol% Li ₂ SiO ₃	95±3 mol% Li ₄ SiO ₄ 5±3 mol% Li ₂ SiO ₃	$\begin{array}{c} 92{\pm}3 \ mol\% \\ Li_4SiO_4 \\ 3{\pm}3 \ mol\% \\ Li_2SiO_3 \\ 3 \ mol\% \\ SiO_2 \end{array}$	92 \pm 3 mol% Li ₄ SiO ₄ 9 \pm 3 mol% Li ₂ SiO ₃
Grain size (av.)	10 µm	200-300 nm	200-400 nm	300-600 nm
Specific surface	$0.2-0.3 \text{ m}^2 \text{ g}^{-1}$	$23\pm2 \text{ m}^2 \text{ g}^{-1}$	$22\pm2 \text{ m}^2 \text{ g}^{-1}$	$17\pm2 \text{ m}^2 \text{ g}^{-1}$

Characterization of investigated lithium orthosilicate samples

Nano-structured "pure" Li₄SiO₄ powder was obtained by method of plasma synthesis and synthesis was performed by high-frequency plasmatron in the Institute of Inorganic Chemistry of the Riga Technical University. Raw materials were mixture of ultra-disperse Li₂CO₃ and silicon powder (\emptyset_{grain} =20-60 nm). In plasma formed nano-structured Li₄SiO₄ powder was annealed up to 890 K in air, to eliminate unreached phases of raw materials.

 $2 \operatorname{Li}_2 \operatorname{CO}_3 + \operatorname{Si} + \operatorname{O}_2 \rightarrow \operatorname{Li}_4 \operatorname{SiO}_4 + 2 \operatorname{CO}_2 \uparrow (1)$

In order to obtain relevant composition as in pebbles, powder 2.0 wt% of ultra-disperse SiO_2 powder was added to nano-structured "pure" Li_4SiO_4 . Mixture of both powders was homogenized by ball mills for 3 hours and then annealed at 920 K for 3.5 hours in air (2). Transition of SiO_2 in to the Li_2SiO_3 phase was explained as side effect of formation of Li_2CO_3 on surface of Li_4SiO_4 powder at annealing stage up to 573 K.

 $Li_4SiO_4 + SiO_2 \rightarrow 2 Li_2SiO_3$ (2)

Annealed Li₄SiO₄ pebbles with SiO₂ were encapsulated in quartz tubes in dry argon and air atmosphere. Dry argon and air as irradiation atmosphere was selected to analyze influence of H₂O vapour and CO₂ on radiolysis of Li₄SiO₄ pebbles. Li₄SiO₄ pebbles in quartz tubes were irradiated up to 11 GGy at 570 ± 20 K with accelerated 5 MeV electrons. Temperature of irradiation was selected corresponding to exploitation parameters of HCPB module. Irradiation process was performed by linear electron accelerator ELU-4 (Salaspils, Latvia) up to 120 hours (dose rate 24 kGy h⁻¹), from 4 to 5 hours per day.

To understand influence of air and high temperature ($T_{max} \le 570$ K) on radiolysis of Li_4SiO_4 pebbles, each factor was investigated separately. Three types of nanostructured Li_4SiO_4 powders were irradiated with gamma rays (absorbed dose 56 kGy, dose rate 14 kGy·h⁻¹) at room conditions, to analyze influence of SiO₂ phase on radiolysis at air. Irradiation was performed with gamma rays converted with wolfram plate from accelerated electron flux. Irradiation time ($t_{irr}=4$ h) was selected corresponding to one irradiation step of pebbles. Small absorbed dose and temperature in order to accumulate unstable radiation defects (RD).

To identify accumulated RD and products of radiolysis (RP) of chemisorption products in nano-structured Li_4SiO_4 powders, "pure" Li_2CO_3 and LiOH powders were irradiated (absorbed dose 56 kGy, dose rate 14 kGy·h⁻¹). To investigate thermal stability of accumulated RD, irradiated nano-structured "pure" Li_4SiO_4 powder were thermally treated from 473 to 580±5 K for 30 minutes.

To simulate processes which occurred in Li_4SiO_4 pebbles in irradiation process at high temperature in air, annealed nano-structured Li_4SiO_4 powder with SiO₂, with relevant composition as in pebbles, was selected as investigation material. The powder was thermally treated up to 570 K for 4 hours and irradiated with gamma rays (absorbed dose 56 kGy, dose rate 14 kGy·h⁻¹) at air.

The composition of Li₄SiO₄ pebbles and nano-structured powders before and after each step of preparation was analyzed with powder X-ray diffractometry (p-XRD) and Fourier transform infrared spectroscopy (FT-IR). Amount of accumulated chemisorption products was determined by thermogravimetry and differential thermal analysis (TG-DTA). Specific surface area and grain size of nano-structured powders was investigated with standard BET method and with scanning electron microscopy (SEM), respectively. Formed and accumulated RD and RP were analyzed with electron spin resonance (ESR) and chemical scavenger method.

The p-XRD patterns were obtained by Bruker D8 spectrometer (10-60° 2 θ , source CuK α , λ =0.15418 nm). FTIR spectroscopy was performed by Perkin Elmer FT-IR spectrometer, Spectrum BX (450-4000 cm⁻¹, accuracy ±4 cm⁻¹, pressed in KBr pellets). TG-DTA curves were obtained by Seiko EXTAR 6000 TG/DTA 6300 (290-1070 K, 2 and 10 K min⁻¹, air atmosphere). Grain size of nano-powders was analyzed with SEM Hitachi S-4800 (1.5 and 3 kV, 15 μ A) and specific surface area – by self-made BET method apparatus in the Institute of Inorganic Chemistry of the Riga Technical University. The ESR spectra of the radiation induced free radicals were recorded by a Bruker BioSpin X-band radio spectrometer operating at 100 kHz field modulation (300-400 mT, 30 dB, 9.83 GHz).

4.3.2. Formation of radiation defects in lithium orthosilicate

Using chemical scavenger method, it has been determined that under action of accelerated electrons (D_{abs} =11 GGy) at 570±20 K and at dry argon in annealed Li₄SiO₄ pebbles with SiO₂ accumulated both, simple (3.0 10¹⁸ radicals g⁻¹) and multi-electron centres (3.0 10¹⁹ radicals g⁻¹). Multi-electron centres in pebbles mainly consist from aggregates of primary electron type RP, i.e. colloidal lithium (Li_n), but simple centres from localized electrons in oxygen vacancies, so called F⁺ and F^o centres. Both electron type centres possess paramagnetic properties and therefore could be observed in ESR spectra. In ESR spectra Li_n forms characteristic ultra-fine signal with g-factor from 2.001 to 2.004, but F⁺ centers broad multiplex signal with g-factor 2.002.

In obtained ESR spectra of irradiated Li₄SiO₄ pebbles three other signals with contiguously lying values of g-factors: 2.001, 2.011 and 2.016, and different width were observed. It has been suggested that ESR signal of Li_n in obtained spectra was not observed due to aggregation of RP. All three observed signals in ESR spectra were attributed to characteristic RD which accumulates in "pure" Li₄SiO₄ and has been investigated in previous researches. ESR signal with a g-factor 2.002 (Δ H=10 mT) was related to electron type E' centers (ion radical SiO₃³⁻), in contrast to the 2.009 and 2.013 signals, which could be attributed to hole type HC₂ centres (ion-radical SiO₄³⁻).

Both E', and HC₂ centres are primary RD of Li₄SiO₄ (3.-4.) and Li₂SiO₃ phase. However due to high irradiation temperature and recombination processes, concentration of RD is quite small - $4.0 \cdot 10^{15}$ radicals g⁻¹ (99 % E' and 1 % HC₂ centers).

$$\operatorname{SiO_4^{4-}} \leftrightarrow \operatorname{SiO_4^{3-}} + e^- (\operatorname{HC_2 centre}) (3)$$

 $\operatorname{SiO_4^{4-}} + e^- \leftrightarrow \operatorname{SiO_3^{3-}} + \operatorname{O^{2-}} (E^\circ \operatorname{centre}) (4)$

From obtained ESR results it can be suggested that concentration and type of RD in pebbles depends not only on absorbed dose and irradiation temperature, but also on irradiation atmosphere. For example, by replacing dry argon with air, concentration of RD increases several times – up to $5.0 \cdot 10^{17}$ radicals g⁻¹, and amount of HC₂ centres increases from 1 % to 25 %. As well as air atmosphere influence also type of accumulated RD.

In ESR spectra of pebbles were observed not only characteristic signals of E' and HC₂ centres, but also two symmetric lines (g_1 =2.193 and g_2 =1.898) with 50.2 mT splitting. In previous research two symmetric signals were attributed to localized hydrogen (H·), which is characteristic RD of chemisorption products of H₂O (5-6).

 $Li_4SiO_4 + H_2O \rightarrow 2 LiOH + Li_2SiO_3 (5)$

 $\text{Li-OH} \rightarrow \text{Li-O} + \cdot \text{H}$ (6)

Therefore increase of characteristic silicate RD concentration at irradiation process in air could be explained as side effect of radiolysis of chemisorption products of H₂O vapour and CO₂. To understand formation and radiolysis of chemisorption products on surface of Li₄SiO₄ pebbles at these irradiation conditions, influence of temperature ($T_{max} \leq 570$ K) and air were investigated separately.

4.3.3. Influence of air atmosphere and chemical additions

Formation of chemisorption products of H_2O vapour and CO_2 on surface of Li₄SiO₄ pebbles depends not only on irradiation temperature, but also on contact surface area with air. Therefore to increase contact surface area, nano-structured "pure" Li₄SiO₄ powder was selected for investigation.



Fig.4.3.1. p-XRD patterns (A) and FR-IR spectra (B) of obtained nano-structured "pure" Li₄SiO₄ powder

At storage stage from dry air on surface of nano-structured "pure" Li_4SiO_4 powder chemisorbed H₂O vapour and CO₂ (2.2±0.3 wt%). Formation of chemisorption products, i.e. LiOH and Li_2CO_3 , was determined by p-XRD and FT-IR (Fig.4.3.1.). Beside to characteristic signals of lithium silicates in both methods were also observed

signals of impurities, for example, in FT-IR spectra was observed bond vibrations of C-O (ψ =1440 cm⁻¹) and O-H (ψ =2800-3500 cm⁻¹).

Under action of gamma rays (D_{abs} =56 kGy, P_{abs} =14 kGy h⁻¹) at room conditions in air, changes of p-XRD patterns (Fig. 2, A) were not observed. This effect could be explained with small absorbed dose of gamma rays. Under action of 56 kGy absorbed dose decomposition degree of Li₄SiO₄ (7) is too small to be detected ($\alpha_{56 kGy} \approx 0.01 \text{ mol}\%$).

$$Li_4SiO_4 \rightarrow 2Li + Li_2SiO_3 + \frac{1}{2}O_2(7)$$

In ESR spectra (Fig.4.3.2, B) of irradiated nano-structured "pure" Li₄SiO₄ powder seven signals with g-factor 1.898, 2.002, 2.010, 2.015, 2.026, 2.036 and 2.193 were observed. Five signals are identical to ESR signals which were observed at air irradiated Li₄SiO₄ pebbles and were identified as E' and HC₂ centers and H. However interpretation of two last ESR signals (g_1 =2.036 and g_2 =2.026) in spectra was more complicated.



Fig.4.3.2. p-XRD patterns (A) and ESR spectra (B) of nano-structured "pure" Li_4SiO_4 powder after irradiation with gamma rays ($D_{abs.}=56 \text{ kGy}$, P=14 kGy h⁻¹) in air.

Mostly in irradiated Li_4SiO_4 containing ceramics these two quite small signals could be attributed to hole type RD - peroxide radical (\equiv Si-O-O·). For all that in ESR spectra of irradiated "pure" LiOH and Li_2CO_3 powders from 338 to 348 mT were also observed similar signals. Thus it has been suggested that formation of signals in ESR spectra of "pure" Li_4SiO_4 powders could be related not only to peroxide radical, but also to accumulated RD or RP of chemisorption products.

On basis of obtained results it was concluded that air essentially influence radiolysis of ceramic of nano-structured "pure" Li_4SiO_4 powder. From obtained ESR results it was suggested that formation and type of RD in nano-structured powder is linked not only to irradiation atmosphere, but also on additions of SiO₂.

For example, adding 2.0 wt% of SiO₂ to Li₄SiO₄ powder, concentration of accumulated RD decreases up to 40% - from $4.6 \cdot 10^{18}$ to $2.7 \cdot 10^{18}$ radicals g⁻¹. Addition of SiO₂ practically does not change ratio of RD of silicates: 79 % E' and 20 % HC₂ centres, but amount of RD which could be linked to chemisorption products changes significantly. Atomic hydrogen practically does not accumulate, but intensity of un-identified two ESR signals decreases up to 10 times – from $1.2 \cdot 10^{17}$ to $1.0 \cdot 10^{16}$ radicals g⁻¹.

Additions of SiO₂ to nano-structured Li₄SiO₄ powder practically do not influence specific surface area, and therefore decrease of concentration of RD most likely could

be related to chemical properties of SiO₂. It has been suggested that SiO₂ on surface of Li_4SiO_4 powder particles forms layer which could disturb and prevent chemisorption process of H₂O vapour and CO₂. Using TG-DTA it has been determined that 2.0 wt% of SiO₂ in Li_4SiO_4 decreases sorption of gases from air up to 7 times - from 14.0 to 2.0±0.3 wt%.

Annealing of Li₄SiO₄ powder with 2.0 wt% SiO₂ at air also decreases concentration of RD up to 25 % - from 2.7 10^{18} to 2.0 10^{18} radical g⁻¹, yet signals of H· in ESR spectra forms again. It has been suggested that SiO₂ on surface of particles, at high temperature in air, transforms in Li₂SiO₃ phase and due to angulations of particles decreases specific surface - from 22 to 17 ± 2 m² g⁻¹. Therefore decrease of RD was attributed to change of contact surface with air, but formation of H· was explained by chemical properties of Li₂SiO₃ (8).

 $Li_2SiO_3 + 2H_2O \rightarrow 2LiOH + H_2SiO_3(8)$

Beside of radiolysis of chemisorption products of H₂O vapour and CO₂, radiolysis of Li₄SiO₄ pebbles is affected also by temperature (T_{max} =570±20 K). To understand influence of irradiation temperature on radiolysis, "pure" Li₄SiO₄ powder was selected as investigation material, due to high concentration of RD.

Using chemical scavenger method, it has been determined that under action of gamma rays in "pure" nano-structured Li₄SiO₄ powder mostly forms multi-electron centres. Obtained results correlate with ESR results, and therefore it has been suggested that multi-electron centres in "pure" nano-structured Li₄SiO₄ powder mainly consists from E' centres, due to small absorbed dose. Electron type E' centres are thermally un-stable and mainly recombine from 450 to 620 K (Fig. 4.3.3). Previously with thermally stimulated luminescence method it was showed that E' centres in recombination process formed exited states of SiO₄⁴⁻ ions or L-centres.



Fig.4.3.3 Concentration of electron type centres in irradiated "pure" Li₄SiO₄ powder before and after influence of thermal treatment up to 620 K for 30 minutes in air

Using ESR method it has been observed that up to 650 K accumulated HC₂ centres, un-identified signals and atomic hydrogen, in nanostructured powders also were unstable and recombine. H· and hole type HC₂ centres recombine up to 470 K, but unidentified RD recombine at temperature range from 460 to 590 K. Therefore at 570 K in radiolysis of Li₄SiO₄ pebbles should accumulate only E' centres. However at air irradiated pebbles not only E' centres, but also HC₂ centres and H· accumulates. It has been suggested that this effect may be related to chemisorption process of CO₂ and H₂O vapour on surface of Li₄SiO₄ pebbles at high temperature. To understand influence of irradiation temperature and air on radiolysis of Li_4SiO_4 pebbles, annealed Li_4SiO_4 powder with SiO_2 was selected as investigation material. The nanostructured powder was deselected due to relevant composition as in pebbles.

Using TG-DTA it has been observed that up to 570 K from air on surface of annealed nano-structured Li_4SiO_4 powder with SiO₂ accumulates up to 12.0±0.3 wt% of H₂O and CO₂. In thermal treatment process both, H₂O vapour and CO₂, in the Li₄SiO₄ powder form Li_2CO_3 and LiOH, respectively. However in obtained p-XRD characteristic patters of chemisorption products are quite small.

It has been suggested that this effect could be related to X-ray amorphous of Li_2CO_3 and LiOH. In same time, after irradiation ($D_{abs.}=56 \text{ kGy}$) at air, intensity of chemisorption products patterns increases essentially. It has been assumed that increase of intensity is related with radiation induced crystallization of chemisorption products. Radiation induced crystallization of amorphous compounds has been previously reported.

In ESR spectra of thermally treated and in air irradiated Li₄SiO₄ powder signals with gfactor 1.898, 1.998, 1.999, 2.002, 2.010, 2.015, 2.026, 2.036 and 2.193 were observed. Most intensive three signals were attributed to E' and HC₂ centres, but other to chemisorption products of LiOH and Li₂CO₃. It has been observed that radiolysis of chemisorption products essentially affects the radiation stability of the Li₄SiO₄ powder and increases the concentration of RD up to 50% - from $2.0 \cdot 10^{18}$ to $3.0 \cdot 10^{18}$ radicals g⁻¹. Summarizing obtained results it has been concluded that radiolysis of annealed Li₄SiO₄ pebbles with SiO₂ at high temperature (T_{max}=570±20 K) is affected by air, i.e. chemisorption products of H₂O vapour and CO₂. First, under action of high temperature on surface of pebbles form X-ray amorphous chemisorption products of H₂O vapour and CO₂, i.e. LiOH and Li₂CO₃. Second, under action of accelerated electrons chemisorption products form RD, which are radiation and thermally unstable. However, radiolysis of chemisorption products essentially decreases radiation stability of Li₄SiO₄ pebbles and increase concentration of RD up to several times.

Therefore it can be concluded that Li_2CO_3 layer which forms after annealing $(T_{max}=1243 \text{ K}, t_{max}=168 \text{ h}, \text{ air})$ on surface of Li_4SiO_4 pebbles can reduce the radiation stability of tritium breeder. As well as under long term exploitation condition in HCPB module on surface of Li_4SiO_4 pebbles may increases concentration of Li_n and so could be affected tritium diffusion and caused tritium accumulation.

One of options to resolve this problem is annealing of HCPB module before tritium breeder exploitation above 973 K at inert atmosphere to desorb chemisorbed gases from surface of pebbles. Second option is a change of the ceramic composition. Pebbles with Li_4SiO_4 as main phase have appropriate tritium breeder parameters, i.e. high lithium density, high melting point and good tritium release behaviour. Therefore it may be favourable to change the secondary phase and to replace Li_2SiO_3 with a less reactive and more mechanically stable lithium metatitanate (Li_2TiO_3) phase. The Li_2TiO_3 also has smaller decomposition degree, and thus it could increase radiation stability of Li_4SiO_4 pebbles.

Collaboration

- 1. KIT, Germany Dr. A. Möslang, Dr. V. Chakin
 - on the investigations of the irradiated Be HIDOBE-I pebbles;
 - in the frame of EFDA Goal Oriented Training Programme "EUROBREED"

- 2. KIT, Germany –Dr. R. Knitter common investigations of lithium orthosilicate pebbles blanket breeder materials, 1 joint publication prepared;
- 3. NRG, the Netherlands Dr. L. Magielsen, MSc. S.van Til- in the frame of the PIE experiments on HIDOBE-I beryllium pebbles;
- 4. TEKES, Finland Dr. Jari Likonen, on analysis of tritium in carbon based samples.
- 5. MDeC, Romania Dr. C.atalin Stansion, on analysis of tritium in carbon based samples.
- 6. Tarty University Dr. Madis Kiisk -on analysis of tritium in carbon based samples.

5. STAFF MOBILITY ACTIONS

5.1. STAFF MOBILITY VISITS

Gunta Kizane took part in:

• Discussion on the results of the JT tasks "JW11-FT-1.19", JW12-FT-1.20" at the Progress Meeting in Horia Hulubei National Institute R&D in Physics and Nuclear Engineering, Bucharest, Romania, 07-09 Mai, 2012.

• General Technical Meeting of the JET Task Force – Fusion Technology work under tasks "JW11-FT-1.19", JW12-FT-1.20" and present an explanation of the background, purpose and objectives of the task "JW13-FT-1.23" at the Kick-off Technical meeting, 11–14 Dec, 2012, the JET, Culham Science Centre, Abingdon, UK. Oral presentation

Elina Pajuste	took part in:		
	KIT, Karlsruhe, Got EUROBREEED, mobility 58 days Feb		
	Apr 2012 Training in methods for analysis of tritium release of		
	fusion reactor materials		
Olgerts Dumbrajs	IPP Garching (Fusion Roadmap), 24 July -27 July, 2012.		
	IPP Garching, 1 September – 31 October, 2012.		
Jurijs Zhukovskis	KIT Karlsruhe, 29 May – 12 June, 2011		
	KIT Karlsruhe, 5 October – 20 October, 2011		
Olgerts Lielausis	IPP Garching, 12 April -16 April, 2011		
	IPP Garching, 28 July – 30 July, 2011		
	IPP Garching, 4 October – 6 October, 2011		
	IPP Garching, 26 October – 29 October, 2011		

6. OTHER ACTIVITIES

6.1. Conferences, Workshops and Meetings

Results of fusion research were presented at the conferences:

- 1. The 28th Scientific Conference of Institute of Solid State Physics. University of Latvia, Riga, February 14-16, 2012.
- 2. The 70th Scientific Conference of University of Latvia, Riga, February 11-13, 2012.
- 3. International Baltic Sea Region Conference "Functional Materials and Nanotechnologies 2012" (FM&NT-2012) Riga, April 2012. Institute of Solid State Physics, University of Latvia.
- 4. I Semi-annual monitoring meeting JET Fusion Technology on the tasks JW12-FT-1.20 on the 5th June 2012.
- 5. 17th Joint Workshop on Electron Cyclotron Emission and Electron Cyclotron Resonance Heating, 7-11 May 2012, Deurne, The Netherlands.
- 6. 17th International Conference on Mathematical Modelling and Analysis (MMA2012) 6-9 June 2012, Tallinn, Estonia.

7. PUBLICATIONS 2012

7.1. FUSION PHYSICS AND PLASMA ENGINEERING

- 7.1.1. Publications in scientific journals
- 1. J. Cepitis, O. Dumbrajs, H. Kalis, A. Reinfelds, and U. Strautins "Analysis of equations arising in gyrotron theory" Nonlinear Analysis: Modelling and Control **17**, 139 (2012).
- 2. A. Reinfelds, O. Dumbrajs, H. Kalis, J. Cepitis, and D. Constantinescu, *"Numerical experiments with single mode gyrotron equations"* Mathematical Modelling and Analysis **17**, 251 (2012).
- 3. O. Dumbrajs, G.S. Nusinovich, and T.M. Antonsen, Jr., "*Regions of azimuthal instability in gyrotrons*" Phys. Plasmas **19**, 063103 (2012).
- 4. O. Dumbrajs and T. Idehara "*Analysis of aftercavity interaction in European ITER gyrotrons and in the compact sub-THz gyrotron FU CW-CI*" J. Infrared Milli. Terahz. Waves **33**, 1171 (2012).
- 5. O. Dumbrajs, T. Idehara, T. Saito, and Y. Tatematsu "Calculations of starting currents and frequencies in frequency tunable gyrotrons" Japanese Journal of Applied Physics **51**, 126601 (2012).
- 6. O. Dumbrajs and G.S. Nusinovich "On optimization of sub-THz gyrotron parameters" Phys. Plasmas **19**, 103112 (2012).
- A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, Modeling of yttrium, oxygen atoms and vacancies in γ-iron lattice. - *J. Nucl. Mater.* (2011) 416, p. 40-44.
- 8. 2. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, Interaction between oxygen and yttrium impurity atoms as well as vacancies in *fcc* iron lattice: *Ab initio* modeling. *Proc. NATO ARW "Nanodevices and Nanomaterials for Ecological Security"* (Eds. Yuri N. Shunin and Arnold E. Kiv; Springer: Dordrecht, 2012), p. 149-160.
- 9. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, and A. Möslang, *Ab initio* modelling of the yttrium and oxygen nanoparticle formation inside *fcc* iron lattice for ODS steels development. *J. Phys.: Conf. Ser.*, accepted.

7.1.2. Conference articles

- Klyukin A., Experimental investigations of flows of liquid metal's films and jets in application toward Tokamak's facilities. Abstracts of the Russian Conference on MHD -Perm, Institute of Continuous Media Mechanics, Ural Branch of Russian Academy of Sciences June 18-22, 2012, Perm, (URL) http://mhd.icmm.ru/RMHD-2012-ThesisBook.pdf.
- K.A. Avramides, A.K. Ram, O. Dumbrajs, S. Alberti, T.M. Tran, and S. Kern, *"On the numerical scheme employed in gyrotron interaction simulations,"* 17th Joint Workshop on Electron Cyclotron Emission and Electron Cyclotron Resonance Heating, 7-11 May 2012, Deurne, The Netherlands.
- 3. O. Dumbrajs and A. Reinfelds, *"Qualitative investigation of dynamical system arising in plasma physics,"* 17th International Conference on Mathematical Modelling and Analysis (MMA2012) 6-9 June 2012, Tallinn, Estonia.
- 4. A. Gopejenko, Yu.F. Zhukovskii, P. Vladimirov, E.A. Kotomin, Yu. Mastrikov, and A. Möslang, "Ab initio modeling of the yttrium and oxygen nanoparticle formation inside fcc iron latice for ODS steels development". First Baltic School on Application of Neutron and Synchrotron Radiation in Solid State Physics and Material Science, BSANS-2012 (Riga, Latvia, October, 2012).- Abstract: p. 30.
- Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, Yu.F. Zhukovskii, E.A. Kotomin, and A. Möslang, "*Ab initio* simulation of growth of vacancies formed clusters in α-Fe lattice". *Annual Monitory Meeting of European Fusion Development Agreement, EFDA 2012* (Ljubljana, Slovenia, June, 2012).
- A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Quantum chemical simulations on binding energies of pair and tripe-wise defects in *fcc*-Fe lattice for ODS steels". 8th International conference "Functional materials and nanotechnologies", FMNT-8 (Riga, Latvia, April, 2012).– Abstract: p. 306.
- 6. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, and A. Möslang, "Quantum chemical calculations of binding energies between Y and O impurity atoms and Fe vacancies inside iron lattice for ODS steels". 10th International Conference "Information Technologies and Management", IT&M'2012 (Riga, Latvia, April, 2012).Abstract: p. 19.
- A. Gopejenko, Yu.F. Zhukovskii, P.N. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, and A. Möslang. "*Ab initio* calculations of binding energies between defects in *fcc* Fe lattice for further kinetic Monte-Carlo simulation on ODS steel". 28th ISSP Conference (Riga, Latvia, February, 2012).– Abstracts: p. 19.

7.2. FUSION TECHNOLOGY

7.2.1. Publications in scientific journals

- 1. A. Zarins, A. Supe, G. Kizane, R. Knitter, L. Baumane. Accumulation of radiation defects and products of radiolysis in lithium orthosilicate pebbles with silicon dioxide additions under action of high absorbed doses and high temperature in air and inert atmosphere, Journal of Nuclear Materials, 429, 2012, p. 34-39
- 2. A. Vitins, G. Kizane, A. Matiss, E. Pajuste, V. Zubkovs. Tritium release from the pebble bed assemblies neutron irradiated beryllium pebbles under action of temperature. Journal of nuclear materials, reviewed on October, 2012.

7.2.2. Conference articles

1. Liga Avotina, Gunta Kizane, Janis Kalnacs, Larisa Baumane, Linda Ansone, Analysis of Fullerene C₆₀ Possible Formed in the Divertor Area of a Tokamak Like Devices. International conference "*Functional Materials and Nanotechnologies 2013*" (FM&NT 2013), Tartu, Estonia, April 21-24, 2013. Book of abstracts, 2013, PO-116.

2. A. Zarins, G. Kizane, A. Supe, R. Knitter, M. Kolb, O. Leys. Influence of Li₂TiO₃ on chemical reactivity of Li₄SiO₄ pebbles. *International conference "Functional Materials and Nanotechnologies 2013" (FM&NT 2013)*, Tartu, Estonia, April 21-24, 2013. Book of abstracts, 2013, PO-154.

3. Mihails Halitovs, Gunta Kizane, Liga Avotina, Jari Likonen, Nicolas Bekris, Catalin Stan-Sion and EFDA JET contributors. Tritium retention studies in W coated JET divertor CFC tiles. *International conference "Functional Materials and Nanotechnologies 2013" (FM&NT 2013)*, Tartu, Estonia, April 21-24, 2013. Book of abstracts, 2013, PO-105.

4. M. Halitovs, G.Kizane, A.Vitins, E.Pajuste, L.Avotina, J.Jansons. Comparison of Tritium Accumulation in Varios Divertor Tiles Depending on the Geometrical Positioning in the Divertor Structure. *Functional materials and nanotechnologies* 2012, Institute of Solid State Physics, University of Latvia, Riga, Latvia, April 17-20, 2012. Book of abstracts, Riga, 2012, 308.

5. A. Zarins, G. Kizane, A. Supe, L. Baumane, A. Berzins, Dz. Rasmane, I. Steins. Influence of SiO₂ admixes on radiolysis of powders of Li₄SiO₄. *International conference "Functional materials and nanotechnologies 2012" (FM&NT 2012)*, Institute of Solid State Physics, University of Latvia, Riga, Latvia, April 17-20, 2012. Book of abstracts, 2012, p. 307.

6. E. Pajuste, G. Kizane, A. Vitins, V. Zubkovs, A. Zarins. Tritium behavior in neutron irradiated beryllium pebbles regarding their microstructure. 10th IEA International Workshop on Beryllium technology (BeWS-10), Karlsruhe Institute of Technology, Karlsruhe, Germany, September 19-21, 2012. Book of abstracts, Karlsruhe, Germany, S2-0005.

7. ElinaPajuste, GuntaKizane, Sander van Til, AigarsVitins, VitalijsZubkovs, Olga Paskova, Aleksandrs Matiko. Tritium bulk distribution and chemical state in beryllium pebbles irradiated in experiment HIDOBE01, In *27th International Sypmphosium on Fusion Technology (SOFT-26)*. September 24 – 28, 2012: Liege, Belgium

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1. A.Zarins, G. Kizane, R. Knitter, A. Supe. Influence of chemisorption products of carbon dioxide on radiolysis of tritium breeding ceramic. *11th International Symposium on Fusion Nuclear Technology (ISFNT-11)*, Barcelona, Spain, 16-20 September, 2013. Accepted.

Local conferences

1. L. Avotiņa, G.Ķizāne, S.Romanelli, J.Kalnačs and EFDA JET contributors. Thermal analysis of plazma unaffected JET divertor powders in inert and air atmosphere. *71th Conference of University of Latvia*, Section of Analytical Chemistry, Riga, Latvia, February 22, 2013 (in Latvian).

2. A. Zariņš, G. Ķizāne, A. Supe, R. Knitter, L. Ansone. Simulation of thermal treatment process to relevant tritium breeding ceramic in air atmosphere. 71th *Conference of University of Latvia*, Section of Analytical Chemistry, Riga, Latvia, February 22, 2013(in Latvian)..

3. M. Haļitovs, G. Ķizāne, L. Avotiņa, Br. Leščinskis, JET-EFDA contributors. Accumulation of tritium in various JET divertors. 71th Conference of University of Latvia, Section of Analytical Chemistry, Riga, Latvia, February 22, 2013(in Latvian)..

4. L. Avotiņa, G. Ķizāne, A. Zariņš, J. Kalnačs, S. Gruenhagen S. Romanelli and EFDA JET contributors. Thermal analysis of dust and flakes and long-chain hydrocarbon compounds probably formed in the JET vacuum vessel. 29th Scientific Conference of Institute of Solid State Physics, Riga, Latvia, February 20. - 22., 2013. Abstracts, UL Institute of Solid State Physics, Riga, 2013, p. 56.

5. A. Zariņš, G. Ķizāne, A. Supe, R. Knitter, L. Ansone. Reasons of formation of Li₂CO₃ layer on sub-surface of tritium breeding ceramic: Thermal treatment in air atmosphere. *29th Scientific Conference of Institute of Solid State Physics*, Riga, Latvia, February 20. - 22., 2013. Abstracts, UL Institute of Solid State Physics, Riga, 2013, p. 57.

6. A. Zariņš, G. Ķizāne, A. Supe, L. Baumane, A. Bērziņš, Dz. Rašmane, I. Šteins. Influence of thermal treatment on radiation stability and radiolysis on nanopowders of lithium orthosilicate in air atmosphere. 28th Scientific Conference of Institute of Solid State Physics, Riga, Latvia, February 8. - 10., 2012. Abstracts, UL Institute of Solid State Physics, Riga, 2012, p. 43.

7. A. Zariņš, G. Ķizāne, A. Supe, L. Baumane, A. Bērziņš, Dz. Rašmane, I. Šteins. Influence of air on radiolysis of lithium orthosilicate nanopowder at high temperature. 70th Conference of University of Latvia, Section of Analytical and Physical Chemistry, Riga, Latvia, February 9, 2012 (in Latvian)..

8. A. Jeršova, D. Grossin, K.-A. Gross, A. Vīksna, A. Zariņš, L. Bauermeistere. Investigation of thermal stability of amorphous phase hydroxyl-apatite with strontium replaces. 70th Conference of University of Latvia, Section of Analytical and Physical Chemistry, Riga, Latvia, February 9, 2012, (in Latvian)..

9. M. Haļitovs, G.Ķizāne, L.Avotiņa, A.Vītiņš, E.Pajuste, J.Jansons. Extraction of tritium accumulated in fusion divertor tiles under various external conditions. 28th Scientific Conference of Institute of Solid State Physics, Riga, Latvia, February 8. - 10., 2012. Abstracts, UL Institute of Solid State Physics, Riga, 2012, p. 44;

10. L.Avotiņa, G.Ķizāne, M.Haļitovs, J.Gabrusenoks, A.Bērziņš. Differencies of structure into bulk of the jet divertor tile 14bwg4b against plasma facing surface. 28th Scientific Conference of Institute of Solid State Physics, Riga, Latvia, February 8.-10., 2012. Abstracts, UL Institute of Solid State Physics, Riga, 2012, p. 45.

11. E. Pajuste, G. Ķizāne, A. Vītiņš, V. Zubkovs. Structural changes of the neutron irradiated beryllium pebbles during tritium thermodesorption. 28th Scientific Conference of Institute of Solid State Physics, Riga, Latvia, February 8. - 10., 2012. Abstracts, UL Institute of Solid State Physics, Riga, 2012, p. 6

12. M. Haļitovs, G. Ķizāne, L. Avotiņa, A. Vītiņš, E. Pajuste, J. Jansons. Investigation of tritium accumulated in laser-cleaned composite material divertor tiles. 70^{th}

Conference of University of Latvia, Section of Analytical and Physical Chemistry, Riga, Latvia, February 9, 2012, (in Latvian)..

7.4. Doctoral and Graduate Theses Defenced in the 11th October, 2012 Elina Pajuste "Tritium behavior in fusion reactor materials"

Defenced Master course thesis in the June, 2012

- 1. Līga Avotiņa "The estimation of interaction between structure and tritium distribution in materials of various divertors"
- 2. Mihails Halitovs "The evaluation of tritium distribution in plasma facing materials of various divertors"
- 3. Artūrs Zariņš "Influence of silicon dioxide and heat treatment on physicochemical processes of lithium containing ceramic in inert and air atmosphere"
- 4. Vitālijs Zubkovs "Tritium accumulation in beryllium pebbles under the exposure to fast neutron flux"

1st course PhD students in the field of fusion science since the 1st October, 2012:

- 1. Līga Avotiņa "Influence of accumulated tritium on plasma exposed ITER like wall divertor materials"
- 2. Mihails Halitovs "The evaluation of tritium distribution in plasma facing materials of various divertors"
- 3. Andris Lescinskis "Sorption desorption process of tritium in liquid lithium under action of various external conditions"
- 4. Artūrs Zariņš "Radiolysis in inert and air atmosphere of variously synthesized and pre-treated tritium breeding ceramics"