|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **WPPWIE Deliverables Status Report** | | | | | **Date:** | | | 01-Sep-2022 | | |
| **Subproject:** | SP D / PSI and SOL Modelling | | | | **Deliverable ID** | | | PWIE-SP D.2.T-T002-D002/D003 | | |
| **Deliverable owner:** | M. Probst / F.Aumayr (OEAW) | | | | **Deliverable due date** | | | 31-12-2022 | | |
| **WP Leader:**  **SP Coordinator:** | S. Brezinsek (FZJ)  A. Kirschner (FZJ) | | | |  | | |  | | |
| **Task title:** | SP D.2 Production of Atomic/Molecular and Surface Data | | | | | | | | | |
| **Deliverable title:** | D3.1: Effect of seeding projectiles (e.g. Ar, Kr) on tungsten sputtering / D3.1; Electron impact cross sections (ionization, excitation), D3.3 Combine BCA and MD at transition from low energies to BCA limit (OAEW)  Erosion information of surfaces including morphology, roughness, fuzz (OAEW) | | | | | | | | | |
| **Status:** |  | **Completed** |  | **Partially completed** | |  | **Delayed** | |  | **Cancelled** |
| Please write a short status report (max. ½ pages) here.  Please check the status of the deliverable(s) with a “x” in the row above.  If the deliverable(s) are delayed, please also indicate an estimated completion date in the report text.  If the deliverable(s) include machine time, please indicate the number of days that have been used for the deliverable(s) in the report text.  For reference, the specification of this task from the PMP is given below. | | | | | | | | | | |
| **Reference from PMP:** | | | | | | | | | | |
| This subproject contains the calculation of rate coefficients for ionization, dissociation, recombination and excitation of atoms and molecules under fusion-relevant plasma conditions. This includes atomic and molecular species of H, D, T as well as helium and seeding gases and also elements as result of wall erosion (W, Be, steel). Moreover, molecules containing Be/H and W/H are considered.  The generation of surface data includes erosion yields and reflection coefficients, also considering morphology effects, mixing of materials and redeposited layers. The output also should provide angular and energy information of the eroded and reflected species. The study of dust formation (e.g. via arcing or melting mechanisms, clustering) is also envisaged. Possible tools are based for instance on Molecular Dynamics or the Binary Collision Approximation. | | | | | | | | | | |
| **Inputs required:**  Experimental data for comparison if applicable (e.g. data from SP A, SP B, SP E, SP X) | | | | | | | | | | |
| **Tasks to be performed:**   * Development of dust formation models (CEA) * Calculation of rate coefficients for ionization/excitation, MD simulations (ÖAW) * SDTrimSP related modelling of erosion including morphology, roughness, fuzz (ÖAW) * Model development for production mechanisms for dust formation from melting (VR) * Production of erosion yields for redeposited W in comparison to bulk W (VTT) * Development of machine learning for interatomic W potentials (VTT) * Production of erosion yields and reflection coefficients for rough W surfaces (VTT) * Upgrade of AM database and CRM for molecules (VTT)   SDTrimSP-3D based erosion modelling considering roughness, morphology (MPG) | | | | | | | | | | |
| **Deliverables:**   |  |  | | --- | --- | | **Deliverable ID** | **Deliverable Title** | | D001 | Dust production model for anomalous events and detached conditions (CEA) | | D002 | D3.1: Effect of seeding projectiles (e.g. Ar, Kr) on tungsten sputtering / D3.1; Electron impact cross sections (ionization, excitation), D3.3 Combine BCA and MD at transition from low energies to BCA limit (OAEW) | | D003 | Erosion information of surfaces including morphology, roughness, fuzz (OAEW) | | D004 | Model for dust production from melting; prediction of dust formation from molten metal, droplet ejection (VR) | | D005 | D5.1 Erosion and retention properties of redeposited tungsten, D5.2 Interaction potential of tungsten to be used for sputtering/reflection modelling / D5.3 Sputtering and reflection yields for various kinds of tungsten morphologies (VTT) | | D006 | Upgraded atomic/molecular database and CRM for molecules (VTT) | | D007 | Erosion information of 2D surfaces (various morphologies) in comparison to experiments (MPG) | | | | | | | | | | | |
| **Management Information**  **Human Resources (2022)**:   |  |  |  |  | | --- | --- | --- | --- | | **Deliverable Owner** | **Beneficiary** | **PM** | **Deliverable (Team)** | | A. Michau | CEA | 2 | D001 (A. Michau, K. Hassouni) | | M. Probst | ÖAW | 3 | D002 (M. Probst, S. Huber, J. Romero, D. Süß) | | F. Aumayr | ÖAW | 2 | D003 (F. Aumayr, P.S. Szabo, Ch. Cupak) | | S. Ratynskaia | VR | 7 | D004 (S. Ratynskaia, L. Vignitchouk, L. Brandt, M. Crialesi Esposito, N. Scapin) | | K. Nordlund | VTT | 5 | D005 (K. Nordlund, F. Granberg, N. Ghazemi, A. Lopez Cazalilla) | | M. Groth | VTT | 1 | D006 (M. Groth, A. Holm) | | U. von Toussaint | MPG | 2 | D007 (U. von Toussaint, R. Preuss) | | **Total** |  | 22 |  |   **Machine Resources (2022):**   |  |  |  |  | | --- | --- | --- | --- | | **Device** | **Beneficiary** | **Days** | **Related Deliverable** | | n.a. |  |  |  |   **Other resources:**   * HPC requests   **Collaborations:**   * WPTE   **Other information:**   * Connected to TSVVs associated with WPPWIE   IO and ITPA | | | | | | | | | | |