

1 **Using first-principles calculations to predict the mechanical properties of**  
2 **transmuting tungsten under first wall fusion power-plant conditions**

3 Yichen Qian,<sup>1</sup> Mark R. Gilbert,<sup>2</sup> Lucile Dezerald,<sup>3</sup> and David Cereceda<sup>1,\*</sup>

4 <sup>1</sup>*Department of Mechanical Engineering,*  
5 *Villanova University, Villanova, PA 19085, USA*

6 <sup>2</sup>*United Kingdom Atomic Energy Authority, Culham Centre For fusion Energy,*  
7 *Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK*

8 <sup>3</sup>*Department of Materials Science and Engineering,*  
9 *Institut Jean Lamour, Universite de Lorraine, F-54011 Nancy, France*

10 (Dated: March 3, 2021)

11 Tungsten and tungsten alloys are being considered as leading candidates for structural  
12 and functional materials in future fusion energy devices. The most attractive properties of  
13 tungsten for the design of magnetic and inertial fusion energy reactors are its high melt-  
14 ing point, high thermal conductivity, low sputtering yield and low long-term disposal ra-  
15 dioactive footprint. Yet, despite these relevant features, tungsten also presents a very low  
16 fracture toughness, mostly associated with inter-granular failure and bulk plasticity, that  
17 limits its applications. Significant neutron-induced transmutation happens in these tung-  
18 sten components during nuclear fusion reactions, creating transmutant elements including  
19 Re, Os and Ta. Density functional theory (DFT) calculations that allow the calculation of  
20 defect and solute energetics are critical to better understand the behavior and evolution  
21 of tungsten-based materials in a fusion energy environment. In this study, we perform  
22 DFT calculations to predict elastic and plastic mechanical properties (such as bulk modu-  
23 lus, shear modulus, ductility parameter, etc.) on a variety of W-X compositions that result  
24 when pure tungsten is exposed to the EU-DEMO fusion first wall conditions for ten years.

---

\* [david.cereceda@villanova.edu](mailto:david.cereceda@villanova.edu)

## I. INTRODUCTION

25  
26 Tungsten and tungsten alloys are being considered as leading candidates for structural  
27 and functional plasma facing materials (PFMs) in future fusion energy devices. The most  
28 attractive properties of tungsten for the design of magnetic fusion energy reactors are its  
29 high melting point and thermal conductivity, low sputtering yield and low long-term dis-  
30 posal radioactive footprint. These advantages are accompanied unfortunately by a very  
31 low fracture toughness (mostly associated with inter-granular failure and bulk plastic-  
32 ity), low ductility at room temperature, and high ductile-to-brittle transition temperature  
33 (DBTT), that limits its applications [1–5].

34 A deep understanding of both elastic and plastic mechanical properties of tungsten  
35 alloys under first wall fusion power plant conditions is then a necessary step towards  
36 their consolidation as a viable option for this promising technology. Given the difficulty  
37 and the cost to perform experiments in such extreme environments, the use of computa-  
38 tional modeling to provide insights and enrich the experimental knowledge of materials  
39 response has received much attention during the last decades. Among all the available  
40 techniques that allow for the prediction of mechanical properties across different tempo-  
41 ral and spatial scales, density functional theory (DFT) has emerged as one of the most  
42 reliable ones to investigate the electronic structure of condensed matter systems [6].

43 In the elastic region, these first-principles calculations (also called *ab initio* calcula-  
44 tions) have been broadly employed to study the elastic constants and the elastic proper-  
45 ties of pure crystals and multiple alloys, starting in the 1970s and, particularly, in recent  
46 times [7–13].

47 For its part, plastic deformation in body-centered cubic (bcc) metals like tungsten  
48 is peculiar due to the existence of nonplanar dislocations with screw character and  
49 thermally-activated mobility [14–17]. This results in various kinds of complex phenom-  
50 ena such as pencil glide, asymmetry of the critical stress in the twinning and antitwinning  
51 glide directions, asymmetry of the critical stress under tension/compression loading, or

52 anomalous slip [18–28]. Among all the mechanical properties that can be determined in  
53 this plastic regime, ductility of tungsten and tungsten alloys has been the subject of much  
54 research and discussion over the last decades (both experimentally and computationally)  
55 given their well documented brittleness [5, 29]. Despite the scalability limitations of *ab*  
56 *initio* methods to characterize directly dislocation glide, grain boundaries, hardening,  
57 and other mesoscopic phenomena governing the plasticity of body-centered cubic (bcc)  
58 metals, several approaches have proposed measures of ductility based on its relationship  
59 with material parameters that can be determined via DFT simulations. Going back to  
60 the 1950’s, before computational modeling and *ab initio* calculations became effective  
61 methods to study the mechanical properties of materials, Pugh [30] formulated an em-  
62 pirical criterion that characterizes the ductility of materials by the ratio between the bulk  
63 modulus  $B$  and the shear modulus  $G$ . Cauchy pressure, defined in terms of the elastic  
64 constants, has also been employed to evaluate the ductility of metals since it includes  
65 the angular character of atomic bonding [31, 32]. Another criteria for isotropic polycrys-  
66 talline materials is the Poisson’s ratio, which is found to be proportional to the intrinsic  
67 ductility of crystals [33]. During analysis of dislocation nucleation from a crack tip,  
68 Rice [34] proposed that the ductile-brittle behavior of a material can be associated with  
69 the ratio between the surface energy and the so-called unstable stacking fault energy, a  
70 new solid state parameter identified in this analysis that represents the maximum energy  
71 encountered in the block-like sliding of a slip plane.

72 Despite the numerous efforts in the literature to investigate the effects of alloying ele-  
73 ments on various properties of tungsten such as phase stability [10, 35–38], elastic proper-  
74 ties [10, 13, 35–37, 39, 40], ideal tensile strength [10, 41], ductility [42], radiation defects  
75 [36], point defects [35, 43–47], dislocation structure [48, 49], grain boundaries [50], etc.,  
76 to the best of our knowledge there is a lack of understanding on how the expected first  
77 wall fusion power-plant conditions change the mechanical properties of these plasma fac-  
78 ing structural materials over time. In this work, we perform first-principles calculations

79 based on density functional theory to investigate the mechanical response of tungsten ex-  
 80 posed to fusion-like environments. In particular, we focus on how the elastic constants,  
 81 elastic properties, ideal tensile strength, and dislocation-based ductility parameter evolve  
 82 as the composition of tungsten changes during the course of irradiation due to transmu-  
 83 tation.

84 Our paper is organized as follows. After this introduction, we provide an overview  
 85 of tungsten transmutation in a predicted fusion-reactor environment. This is followed  
 86 by Section III, where the first-principles computational methods employed are presented.  
 87 The results are given in Section IV, which includes: (i) the validation exercise, with spe-  
 88 cial focus on the elastic properties of pure tungsten; and (ii) the calculation of the elastic  
 89 constants and elastic properties, the ideal tensile strength, and ductility parameter mea-  
 90 surements for the chemical compositions that appear when pure tungsten transmutes  
 91 during the course of irradiation. We finalize in Section V with a brief discussion and the  
 92 conclusions.

## 93 II. TUNGSTEN TRANSMUTATION

94 To characterize the transmutation properties of W in a fusion-like environment, calcu-  
 95 lations have been carried out using the FISPACT-II inventory code developed and main-  
 96 tained by the United Kingdom Atomic Energy Authority over the last 30 years. FISPACT-  
 97 II [51, 52] solves coupled differential equations describing the rate of change of all pos-  
 98 sible nuclides and thus evolves a nuclide composition in time. In the simplest case, the  
 99 differential equation describing the rate of change for one nuclide is:

$$100 \quad \frac{dN_i}{dt} = \underbrace{-N_i(\lambda_i + \sigma_i\phi)}_{\text{depletion}} + \sum_{j \neq i} \underbrace{N_j(\lambda_{ji} + \sigma_{ji}\phi)}_{\text{creation}} \quad (1)$$

101 where  $N_i$  is the number of atoms of nuclide  $i$  at a given time  $t$ . This differential equation  
 102 is formed from two terms that represent the nuclide depletion (negative contribution) or

103 creation (positive). The loss term,  $-N_i(\lambda_i + \sigma_i\phi)$ , includes  $\lambda_i$  as the decay constant of the  
 104 nuclide (only non-zero if the nuclide is unstable),  $\phi$  as the total neutron flux (in units of  
 105  $\text{n cm}^{-2} \text{ s}^{-1}$ ), and  $\sigma_i$  as the total collapsed cross section for all possible reactions on the  
 106 nuclide (measured in barns and calculated by combining the energy-dependent specified  
 107 neutron field with nuclear reaction cross-section data). For its part, the creation term  
 108 consists of the sum over all other nuclides with the  $ji$  subscripts indicating the production  
 109 of nuclide  $i$  from a reaction or decay on  $j$ . Single-value, total  $\sigma$  cross sections (in  $\text{cm}^{-2}$   
 110 units) in equation (1) are obtained from the sum of the energy dependent cross sections  
 111 values for the reaction weighted by the normalized neutron irradiation spectrum:

$$112 \quad \sigma = \sum_n \sigma_n \frac{\phi_n}{\sum_m \phi_m}, \quad (2)$$

113 where the  $n, m$  sums are performed over the neutron flux vector.

114 For the present work, a  $\underline{\phi}$  vector of fluxes was taken from neutron transport calcula-  
 115 tions performed for a recent conceptual design (see [53, 54] for details) for EU-DEMO; a  
 116 demonstration fusion power plant being researched in Europe [55, 56]. Specifically, the  
 117 spectrum for the outer equatorial first wall of the torus-shaped tokamak has been used,  
 118 which is predicted to be one of the highest flux regions of a fusion reactor (second only  
 119 to the inner equator). The total flux  $\phi$  for this spectrum was  $2.1 \times 10^{14} \text{ n cm}^{-2} \text{ s}^{-1}$ . A  
 120 FISPACT-II calculation evolved initially pure W in this neutron environment for 10 con-  
 121 tinuous full-power years. Figure 1(a) shows the final composition of the material after  
 122 those 10 years in a ‘nuclide map’ [57] tableau.

123 Note that 10 years of continuous operation is longer than that envisaged for first wall or  
 124 divertor armour components in current fusion reactor concepts; for example, EU-DEMO  
 125 operational scenarios consider around 5 years of pulsed operation lifetime for divertors  
 126 - corresponding to  $\sim 2$  full power years (fpy), while in the second, longer phase of EU-  
 127 DEMO operation, blanket and first wall components are expected to experience about 14  
 128 years of pulsed operation ( $\sim 6$  fpy) [58]. In this respect, using the maximum transmuta-  
 129 tion results (at 10 years) presented here to analyze the mechanical impact on transmuta-

130 tion is an upper-bounding case relative to the end-of-life variations that might be expected  
 131 in the next (first) generation of fusion reactors. On the other hand, the lesson from the  
 132 nuclear fission industry is that life extension of components is critical to the commercial  
 133 viability of power plants, and thus 10 fpy may eventually be more representative of the  
 134 lifetime requirements for the first wall armour of commercial reactors.

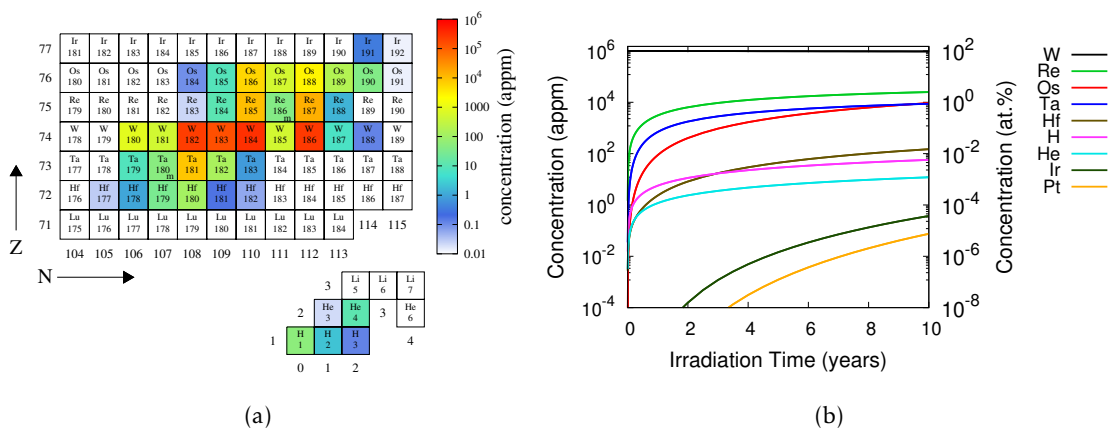


Figure 1. (a) Final nuclide composition of W after 10 years of continuous exposure to EU-DEMO first wall conditions. (b) Transmutation of W during a 10-year irradiation.

135 Figure 1(b) shows how the composition of W changed (transmuted) during the 10-  
 136 year irradiation. The graph shows the concentrations, in atomic parts per million (appm),  
 137 on a logarithmic scale of the elements created during the course of the irradiation. The  
 138 concentrations of each element are the sum over all nuclides of that element (i.e. from one  
 139 row of the nuclide map in figure 1(a)). Table I presents the concentrations of the elements  
 140 produced at 1-year intervals. The table also shows time-averaged concentration error  
 141 estimates for each element, which are derived solely from the nuclear data uncertainties in  
 142 the TENDL-2017 [59] libraries used by FISPACT-II to perform the calculations. FISPACT-  
 143 II obtains errors for a given nuclide/isotope (e.g. <sup>186</sup>W, <sup>185</sup>Re or <sup>2</sup>H) by summing (in  
 144 quadrature) the nuclear data uncertainties on each reaction in the production chains of  
 145 individual nuclides  $N_i$  of the inventory. Production chains are found using a tree search

Table I. Relative concentrations that appear as W transmutes during the course of the 10-year power-plant first wall irradiation. Time-averaged % errors in transmutant concentrations predicted by FISPACT-II are also shown for each element (see main text for details).

Year	at%				appm				
	W	Re	Os	Ta	Hf	H	He	Ir	Pt
1	99.61	0.31	0.01	0.07	2.3	5.6	1.2	$4.4 \times 10^{-6}$	$3 \times 10^{-8}$
2	99.14	0.64	0.04	0.18	8.2	11.3	2.4	$1.6 \times 10^{-4}$	$3.6 \times 10^{-6}$
3	98.67	0.95	0.09	0.28	17.3	17.0	3.6	$1.2 \times 10^{-3}$	$5.0 \times 10^{-5}$
4	98.22	1.23	0.17	0.38	29.4	22.6	4.7	$4.9 \times 10^{-3}$	$3.1 \times 10^{-4}$
5	97.77	1.48	0.26	0.48	44.0	28.4	5.9	$1.4 \times 10^{-2}$	$1.2 \times 10^{-3}$
6	97.33	1.72	0.37	0.57	60.9	34.1	7.1	$3.5 \times 10^{-2}$	$3.7 \times 10^{-3}$
7	96.90	1.94	0.49	0.65	80.0	39.8	8.3	$7.2 \times 10^{-2}$	$9.3 \times 10^{-3}$
8	96.49	2.14	0.63	0.73	101.1	45.6	9.5	$1.3 \times 10^{-1}$	$2.1 \times 10^{-2}$
9	96.07	2.33	0.77	0.80	124.1	51.4	10.8	$2.3 \times 10^{-1}$	$4.1 \times 10^{-2}$
10	95.67	2.50	0.93	0.87	148.8	57.1	12.0	$3.7 \times 10^{-1}$	$7.5 \times 10^{-2}$
error (%)	0.13	6.47	7.54	36.14	31.29	12.65	42.44	31.14	37.83

146 algorithm (see [51] for details of the method). The errors shown here for a transmutant  
 147 element are the sums (again, in quadrature) over the predicted errors for each nuclide  
 148 of that element. Errors for Pt and Ir were not calculated for all time steps because the  
 149 concentrations of contributing Pt/Ir nuclides were too numerically insignificant (small)  
 150 for the pathways to be found – the averaged errors in these cases are only over those (later)  
 151 time steps where errors were obtained

152 Even after 10 years and for the (relatively) highly-transmuting W, the material would  
 153 still be more than 95% W. Notice that the profile of growth of each transmutant element  
 154 varies – Os, for example is a secondary transmutant whose rate of production increases as  
 155 the concentration of Re, a primary transmutant, increases.

### III. FIRST-PRINCIPLES COMPUTATIONAL METHODS

156

157 Density Functional Theory (DFT) calculations were performed by using the open-  
158 source software distribution QUANTUM ESPRESSO [60, 61]. The generalized gradient  
159 approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) parametrization [62] was  
160 employed in the formulation of the exchange correlation functional. Optimized Norm-  
161 Conserving Vanderbilt Pseudopotentials [63] compatible with the Virtual Crystal Ap-  
162 proximation (VCA) [64] method were chosen as the most suitable ones to study the variety  
163 of transmuted tungsten compositions that result from the exposure to the first wall con-  
164 ditions described in Section II. By using this VCA approach, the mixed pseudopotential  
165 for any composition at a specific irradiation time in Fig. 1(b) can be generated by defining  
166 “virtual” atoms at concentrations appropriate for the composition.

167 The  $k$ -points were sampled using the Monkhorst-Pack method [65] by a shifted  $30 \times$   
168  $30 \times 30$  grid for the 2-atom bcc supercell used in the calculation of the elastic constants  
169 and the ideal tensile strength. A shifted  $28 \times 28 \times 1$  grid was selected for the 12-atom  
170 bcc supercell employed in the calculation of the stacking fault energies needed to ob-  
171 tain Rice’s ductility parameter. The planewave cutoff energies were  $\sim 2041$  eV (150 Ry)  
172 for the elastic constants and the ideal tensile strength simulations and  $\sim 544$  eV (40 Ry)  
173 for ductility simulations. The convergence tests to choose these values are provided in  
174 Appendix A. Further details on how to extract the elastic and plastic properties of trans-  
175 muting tungsten from the energies calculated via DFT simulations are given below.



176

### A. Elastic constants and elastic properties

177 The change in the total energy per unit volume ( $\Delta U/\Omega$ ) of a system subjected to a  
 178 general deformation can be written, in the contracted *Voigt notation*, as

$$179 \quad \frac{\Delta U}{\Omega} = \frac{1}{2} C_{ij} u_i u_j \quad \text{with} \quad u_i = \begin{cases} \epsilon_i & \text{if } i = 1, 2, 3 \\ 2\epsilon_i & \text{if } i = 4, 5, 6 \end{cases} \quad (3)$$

180 where  $\Omega$  is the volume and  $U$  is the total energy, respectively, of the crystalline unit cell,  
 181  $C_{ij}$  are the components of the stiffness matrix, and  $u_i$  are the engineering strain vectors. In  
 182 the particular case of a cubic crystal such as bcc tungsten, the elastic tensor gets simplified  
 183 due to the symmetries of the lattice [66], *i.e.*:

$$184 \quad C_{ij} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & & & \\ C_{12} & C_{11} & C_{12} & & & \\ C_{12} & C_{12} & C_{11} & & & \\ & & & C_{44} & & \\ & & & & C_{44} & \\ & & & & & C_{44} \end{pmatrix} \quad (4)$$

185 where all the empty entries correspond to  $C_{ij} = 0$ . Then, Eq. 3 can be rewritten as

$$186 \quad \frac{\Delta U}{\Omega} = \frac{1}{2} C_{11} (u_1^2 + u_2^2 + u_3^2) + C_{12} (u_1 u_2 + u_1 u_3 + u_2 u_3) + \frac{1}{2} C_{44} (u_4^2 + u_5^2 + u_6^2) \quad (5)$$

187 Following [67–69], the three non-zero elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  can then be  
 188 obtained by evaluating this Eq. 5 under three deformations: isotropic ( $u_1 = u_2 = u_3 =$   
 189  $\eta, u_4 = u_5 = u_6 = 0$ ), tetragonal ( $u_1 = u_2 = -\eta, u_3 = -2\eta, u_4 = u_5 = u_6 = 0$ ), and trigonal  
 190 ( $u_1 = u_2 = u_3 = 0, u_4 = u_5 = 0, u_6 = \eta$ ), where  $\eta$  denotes the distortion parameter.

191 Since  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$  constitute the entire set of elastic constants for a cubic system,  
 192 other elastic properties of interest for single crystals can be extracted from these energy  
 193 calculations. For example, the Bulk modulus  $B$  and the tetragonal shear elastic constant  
 194  $C'$  can be determined as

$$195 \quad B = \frac{1}{3}(C_{11} + 2C_{12}) \quad (6)$$

$$196 \quad C' = \frac{C_{11} - C_{12}}{2} \quad (7)$$

197 Additionally, mechanical properties of isotropic polycrystalline materials can also be  
 198 determined from the already calculated elastic constants. By applying the Hill average  
 199 [70], the shear modulus  $G$  can be calculated as

$$200 \quad G = \frac{G_V + G_R}{2} \quad (8)$$

201 where  $G_V = \frac{3C_{44} + C_{11} - C_{12}}{5}$  and  $G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})}$  are the Voigt and Reuss bounds, respec-  
 202 tively. Then the Young's modulus  $E$  and the Poisson's ratio  $\nu$  can be obtained as:

$$203 \quad E = \frac{9BG}{3B + G} \quad (9)$$

$$204 \quad \nu = \frac{3B - 2G}{2(3B + G)} \quad (10)$$

## 205 B. Ideal tensile strength

206 The ideal tensile strength of a material  $\sigma_m$ , also called theoretical strength, is defined  
 207 as the maximum stress that the material can sustain. For the uniaxial tensile test, the

208 tensile stress  $\sigma$  relates to the total energy of the system  $U$ , the tensile strain  $\epsilon$ , and the  
 209 volume at a given strain  $\Omega(\epsilon)$  as

$$210 \quad \sigma = \frac{1}{\Omega(\epsilon)} \frac{\partial U}{\partial \epsilon}, \quad (11)$$

211 which allows for the calculation of the ideal tensile strength using first-principles simula-  
 212 tions. To do so, the total energy for the unloaded material is firstly calculated. Second, a  
 213 uniaxial tensile strain  $\epsilon$  is imposed on the system, finding the minimum of the total energy  
 214 by relaxing the atoms at the directions perpendicular to the loading axis. This process is  
 215 repeated for different values of the strain (along the same loading direction) and the total  
 216 energy is obtained as a function of the applied tensile strain. At each strain step (0.02 at  
 217 the beginning and 0.01 as the results approach the region of the ideal strength), the force  
 218 tolerance during the energy minimization was set to a value of  $2.57 \times 10^{-3}$  eV/Å ( $10^{-4}$   
 219 Ry/bohr) for all five components except for the one where the uniaxial tensile strain is  
 220 applied. Eq. 11 is evaluated to calculate the stress  $\sigma$  for each particular strain, and the  
 221 ideal tensile strength  $\sigma_m$  is obtained as the maximum in the stress-strain curve, which  
 222 also relates to the inflection point in the total energy-strain curve [9]. Next, Eq. 11 is eval-  
 223 uated for each value of applied strain to determine the dependence of the stress  $\sigma$  with  
 224 the strain. Finally, the ideal tensile strength  $\sigma_m$  is obtained as the maximum in the stress-  
 225 strain curve, which also relates to the inflection point in the total energy-strain curve [9].

226

### C. Dislocation-based ductility parameter

227 According to the dislocation theory formulated by Rice [34], the brittle-ductile behav-  
 228 ior of a crystalline solid can be characterized by the so-called ductility parameter  $D$  that  
 229 accounts for the competition between the nucleation of dislocations from the crack tip

230 and crack cleavage, *i.e.*:

$$231 \quad D = \frac{\gamma_s}{\gamma_{us}} \quad (12)$$

232 where  $\gamma_s$  is the surface energy and  $\gamma_{us}$  is the unstable stacking fault energy. In the present  
 233 work, we focus on this Rice-criterion of ductility instead of the other three criteria de-  
 234 scribed in Section I since the generalized stacking fault energies (GSFE) that are needed  
 235 in Eq. 12 can be determined directly by using first-principle simulations. Additionally,  
 236 the calculation of the GSFE could also provide physical insights into the movement of  
 237 dislocations, a mechanism that governs plastic deformation in bcc metals like tungsten  
 238 [71–74].

239 The first step in the calculation of the GSFE is the definition of the geometry. A su-  
 240 percell containing twelve surface layers with a unit surface of  $1 \times 1$  and 10 (Å) vacuum  
 241 is created as shown in Fig. 2. This is done for both  $\langle 111 \rangle \{\bar{1}10\}$  and  $\langle 111 \rangle \{11\bar{2}\}$ , the two  
 242 primary slip systems found in these bcc structures [75–78]. Next, a displacement along  
 243 the  $[111]$  direction is imposed on the upper half (7th to 12th layers) of the surface model  
 244 while keeping the lower half (1st to 6th layers) fixed. After introducing the slip, the en-  
 245 tire system is allowed to relaxed along the  $z$  direction. The GSFE (also called  $\gamma$ -surface)  
 246 is then defined as the energy cost per unit area of the cut incurred as a result of the shift,  
 247 *i.e.*:

$$248 \quad \gamma(x) = \frac{E(x) - E_0}{A} \quad (13)$$

249 where  $x$  is the displacement along the shift vector (given as a fraction of the Burgers  
 250 vector  $\mathbf{b} = \frac{1}{2} [111]$ ),  $E(x)$  is the total energy of the system after imposing a slip  $x$ ,  $E_0$  is  
 251 the total energy of the surface model before the slip, and  $A$  is the area of the surface. The  
 252 unstable stacking fault energy  $\gamma_{us}$  is obtained as the maximum value of the GSFE curve

253 and it corresponds to the maximum energy that comes upon sliding the top half along a  
 254 slip plane [34].

255 For its part, the surface energy  $\gamma_s$  is the energy required to create a new surface during  
 256 the cleavage of an infinite crystal in two. Despite its importance to understand surface  
 257 structure, reconstruction, roughening and crystals' equilibrium shape [79], there are some  
 258 challenges to determine it both experimentally [80] and computationally [81]. In this  
 259 work, we use the method proposed by Fiorentini and Methfessel [82] that calculates the  
 260 surface energy as

$$261 \quad \gamma_s \approx \frac{E_{slab}^N - NE_{bulk}}{2} \quad (14)$$

262 where  $E_{slab}^N$  is the total energy of an N-layer slab and  $E_{bulk}$  is the bulk total energy. By  
 263 using this approach, the divergence of the surface energy with the slab thickness is elim-  
 264 inated. Additionally, it does not require the calculation of the bulk energy term on a  
 265 separate system since  $E_{bulk}$  can be taken as the slope of the total energy of the slab over  
 266 the slab thickness.

## 267 IV. RESULTS

268 In this Section, we present results of first-principles calculations to explore the de-  
 269 pendence of the elastic constants, ideal tensile strength, and ductility-parameter on the  
 270 time-dependent composition of transmuted tungsten under first wall fusion power-plant  
 271 conditions.

### 272 A. Benchmarking - pure tungsten

273 As a preliminary step in our calculations, the elastic and plastic properties of pure  
 274 tungsten were obtained and compared with previous works in the literature. Table II  
 275 summarizes the lattice parameter, elastic constants and elastic properties from this work

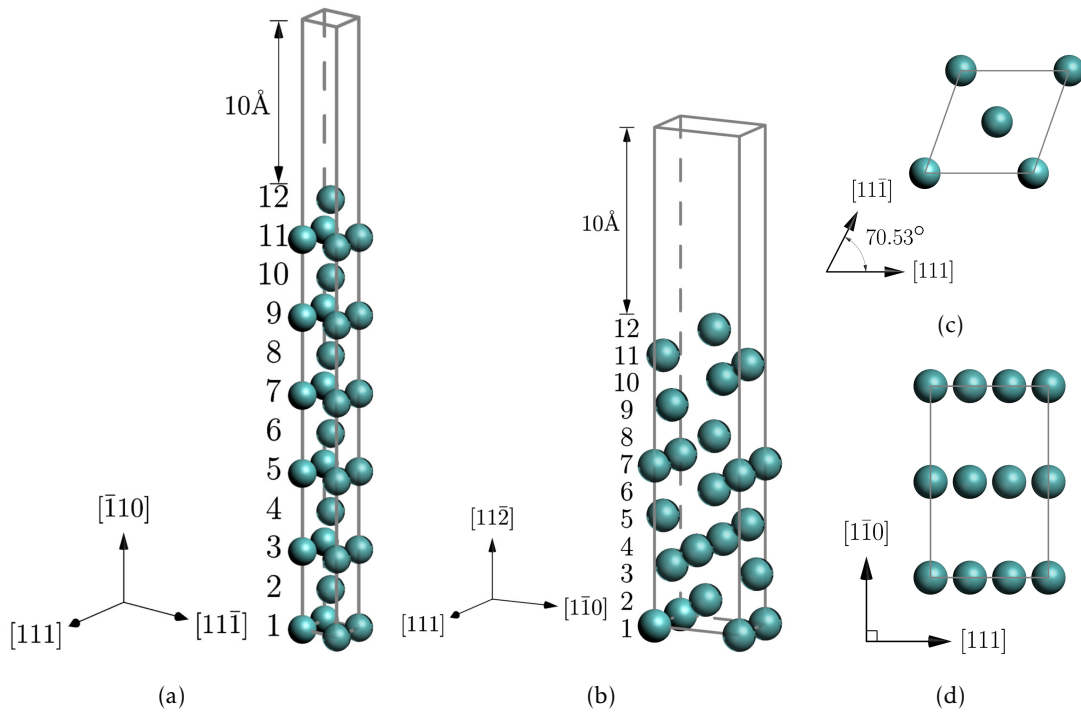


Figure 2. Atomic arrangement of the surface models used to calculate  $\gamma_{us}$  of transmuting tungsten on both (a)  $\langle 111 \rangle \{ \bar{1}10 \}$  and (b)  $\langle 111 \rangle \{ 11\bar{2} \}$  slip systems.

276 and previous studies. For their part, the values of the ideal tensile strength  $\sigma_m$ , the surface  
 277 energy  $\gamma_s$  and unstable stacking fault energy  $\gamma_{us}$  are shown in Table III. These results are  
 278 consistent with their counterparts from previous works (the relative differences are less  
 279 than 15% in Table II and less than 12% in Table III). Additionally, given the variety of  
 280 methods compared, convergence studies were also performed on several properties of  
 281 interest. The reader is referred to appendix A for more details about these convergence  
 282 tests.

283

Table II. Theoretical and experimental equilibrium lattice parameters  $a_0$ , bulk modulus  $B$ , elastic constants  $C_{ij}$ , tetragonal shear modulus  $C'$ , shear modulus (G) and Young's modulus (E) of pure tungsten from our calculations and previous works.

Software package, Pseudopotential <sup>†</sup>	$a_0$ (Å)	$C_{11}$ (GPa)	$C_{12}$ (GPa)	$C_{44}$ (GPa)	B (GPa)	$C'$ (GPa)	G (GPa)	E (GPa)
EMTO, PAW [83]	3.195	536.7	179.9	168.6	298.8	178.4	172.5	434.0
QE, NCPP [84]	3.187	499 <sup>‡</sup>	201 <sup>‡</sup>	149	300	160	154 <sup>‡</sup>	394 <sup>‡</sup>
VASP, PAW [85]	3.1755	529.94	211.19	140.59	317.44	159.38	148.11	384.52
VASP, PAW [86]	3.17	536.3	202.2	138.7	313.6 <sup>‡</sup>	167.1 <sup>‡</sup>	149.4 <sup>‡</sup>	386.8 <sup>‡</sup>
QE, USPP [87]	3.1903	518	197	141	304	160	160 <sup>‡</sup>	408 <sup>‡</sup>
Exp. (0 K) [88]	3.165	532.55	204.95	163.13	314.15	163.80	163.40	417.76
Exp. (300 K)	-	530.25	201.9	160.92	311.35	164.18	160.18	410.09
QE, NCPP [This work]	3.1835	512.501	197.906	142.461	302.771	157.298	148.22	382.669
	[6%]	[5%]	[6%]	[15%]	[5%]	[12%]	[14%]	[12%]

<sup>†</sup> Acronyms used for software packages and pseudopotentials: Exact Muffin-Tin Orbitals (EMTO) formalism [89], Projector Augmented Wave(PAW), Norm Conserving pseudopotentials(NCPP), Ultra-Soft pseudopotentials(USPP).

<sup>‡</sup> Values are obtained by substituting the elastic constants calculated via first-principles calculations into Eq. 6 – 9.

284

## B. Elastic behavior of transmuted tungsten

285

286

287

288

289

With the confidence conferred by the benchmarking exercise of pure tungsten, next we proceed to calculate the elastic and plastic properties for a number of tungsten compositions that result during the first ten years of continuous exposure to EU-DEMO first wall conditions. The chemical compositions of transmuted tungsten shown in Fig. 1(b) and Table I were used to generate the required pseudopotentials via the VCA method

Table III. Theoretical ideal tensile strength  $\sigma_m$ , corresponding strain  $\epsilon_m$ , surface energy  $\gamma_s$ , and unstable stacking fault energy  $\gamma_{us}$  of pure W from our calculations and previous works.

Software package, Pseudopotential <sup>†</sup>	$\sigma_m$ (GPa)	$\epsilon_m$ (%)	$\{\bar{1}10\}$ slip system		$\langle 111 \rangle \{11\bar{2}\}$ slip system	
			$\gamma_s$ (J/m <sup>2</sup> )	$\gamma_{us}$ (J/m <sup>2</sup> )	$\gamma_s$ (J/m <sup>2</sup> )	$\gamma_{us}$ (J/m <sup>2</sup> )
CPMD, GTH [9]	26.7	11.7	-	-	-	-
QE, PAW [10]	29.6	14	-	-	-	-
VASP, PAW	29.1 [86]	14 [86]	3.181[42]	1.633 [42] 1.6983[90]	3.367[42]	1.830[42] 1.7464[90]
VASP, PAW[91]	-	-	3.197	~1.680	~3.377	~1.764
QE, NCPP [this work]	27.763[6%]	14[19%]	3.3083[4%]	1.6870[3%]	3.7620[12%]	1.8755[7%]

<sup>†</sup> Acronyms used for software packages and pseudopotentials: Car–Parrinello Molecular Dynamic (CPMD) code [92], Goedecker-Teter-Hutter pseudopotentials [93].

290 [64]. In addition to studying the current composition (i.e. all transmutants in table I) at  
 291 each irradiation time, two other scenarios were considered: (i) chemical composition at  
 292 each irradiation time with tungsten and the primary transmutant (Re); (ii) chemical com-  
 293 position at each irradiation time with the top 3 transmutants (Re, Os, Ta). The purpose  
 294 of investigating these two supplementary scenarios is to understand how the mechanical  
 295 properties change as specific transmutants are added.

296 Figure 3 shows the time dependence of the lattice parameter and the elastic constants  
 297 as the chemical composition of the tungsten-based materials change due to irradiation.  
 298 This linear behavior has been confirmed in previous experimental [94] and computational  
 299 [10, 48] measurements of W-Re alloys.

300 In Figure 4 we provide detailed results on the evolution of elastic properties such as  
 301 the Bulk modulus  $B$ , the tetragonal shear elastic constant  $C'$  and mechanical properties  
 302 of polycrystalline materials like the shear modulus  $G$  and the Young's modulus  $E$ . As  
 303 described in Section III A, the above properties can be obtained directly from relations  
 304 between elastic constants, by applying the Hill average, or by imposing Voigt and Reuss



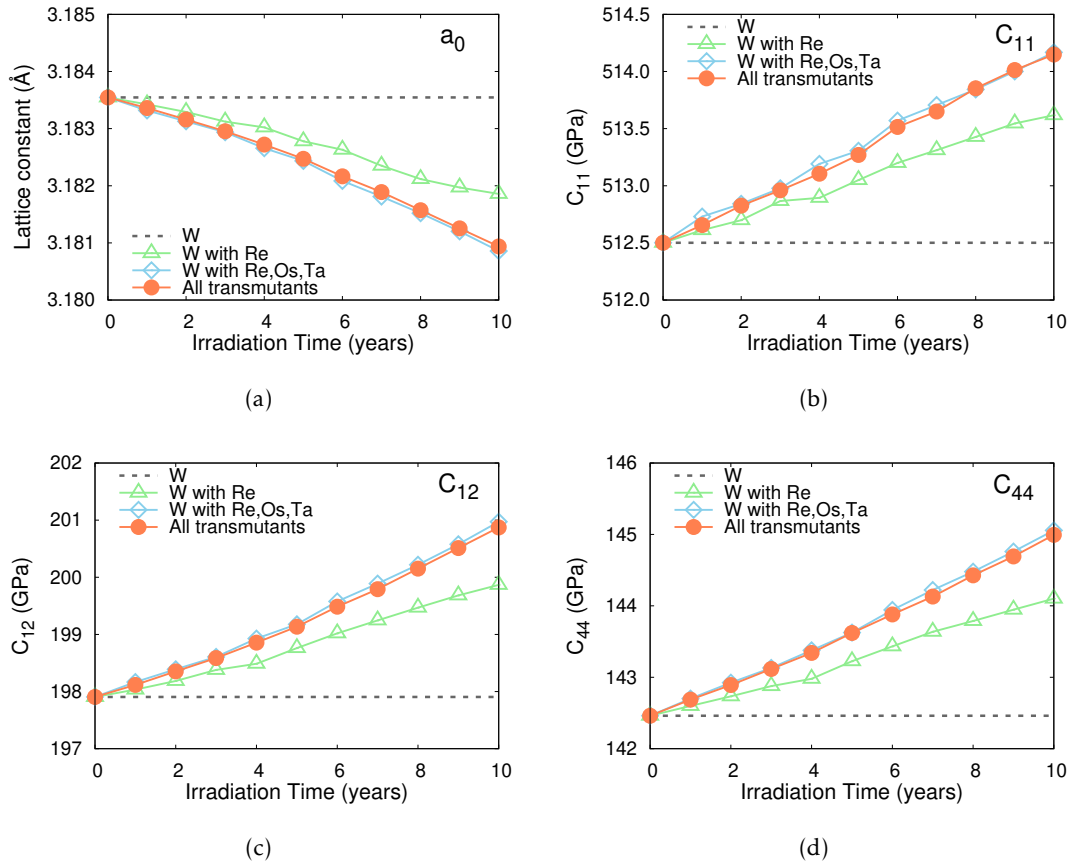


Figure 3. Evolution of the equilibrium lattice parameter  $a_0$  and the elastic constants  $C_{ij}$  of transmuting tungsten during the first ten years of continuous exposure to EU-DEMO first wall conditions.

305 bounds. The monotonic behavior observed in our calculations is also in agreement with  
 306 previous computational works that studied W-Re alloys [10].

307 In advance of discussing these results and their implications in detail in the following  
 308 section, we note the following features from the figures: (i) the lattice constant and  $C'$  are  
 309 the only measurements decreasing as irradiation time (and therefore the relative concen-  
 310 tration of transmutants) increases. All other properties monotonically increase with irra-  
 311 diation time; (ii) the magnitude of the slope when only the primary transmutant (Re) is

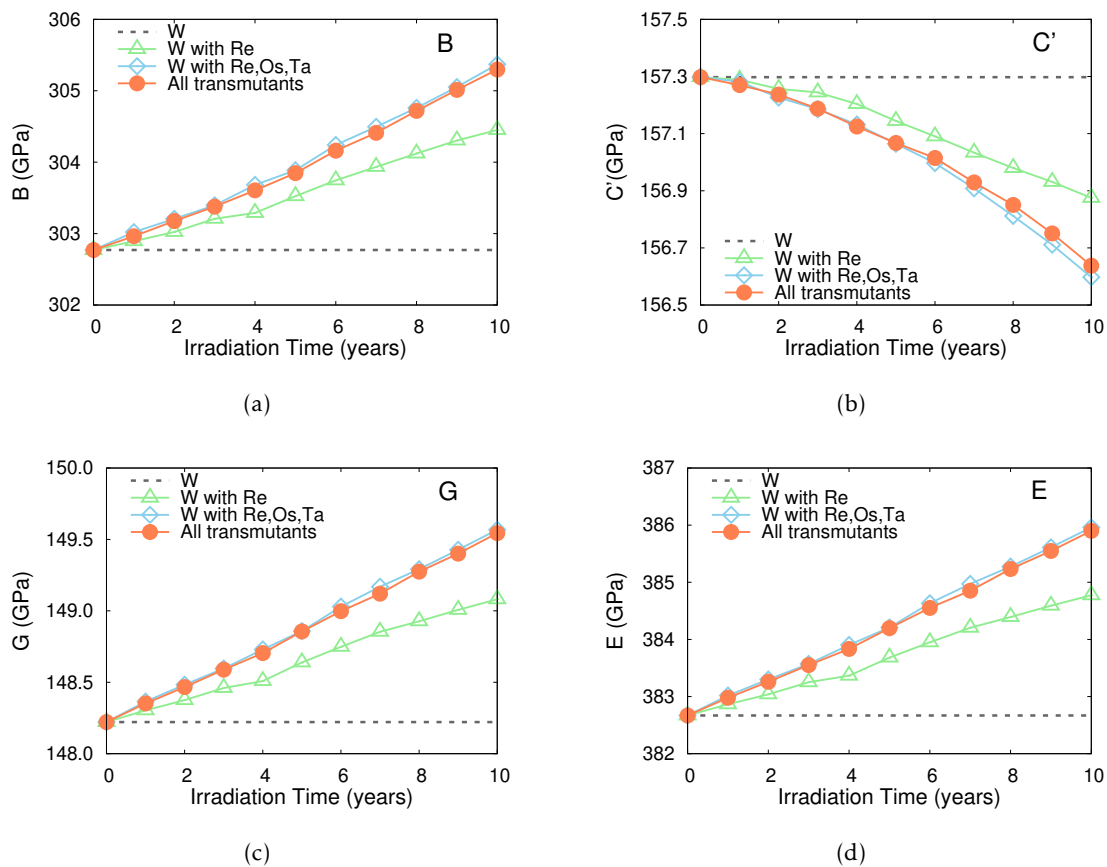


Figure 4. Evolution of the bulk modulus  $B$ , tetragonal shear modulus  $C'$ , shear modulus ( $G$ ), and Young's modulus ( $E$ ) of transmuting tungsten during the first ten years of continuous exposure to EU-DEMO first wall conditions.

312 considered, (no matter whether it is positive for some properties and negative for others)  
 313 is always smaller than the one for the current composition with all transmutants or the  
 314 scenario that includes the top 3 transmutants; and (iii) the effect of adding all remaining  
 315 transmutants is negligible when compared with the impact of the chemical compositions  
 316 that includes the top 3 transmutants (Re, Os, Ta).

### C. Ideal tensile strength of transmuting tungsten

The stress-strain curve is one of the most fundamental tools to understand the mechanical behavior of materials. It reveals many of the elastic and plastic properties of interest, including but not limited to Young's modulus, yield strength, ultimate tensile strength, etc. Here we perform a systematic study of the ideal tensile strength of pure W, transmuting W (with all transmutants), W with primary transmutant (Re), and W with top 3 transmutants (Re, Os, Ta) as a function of the chemical compositions that result when pure tungsten is exposed to the EU-DEMO first wall conditions for ten years. While studying the effect of temperature on the stress-strain curve is outside the scope of this paper, it is still of interest to calculate the theoretical ideal tensile strength of transmuting tungsten in its ground state and relate our findings to the larger mechanical behavior of these candidate materials if possible.

First, we study the stress-strain relations of these materials as we increase the irradiation time. By way of example, the results for the chemical composition of transmuting tungsten that appears by the sixth year of irradiation are presented in Fig. 5(a). These reveal that the overall stress-strain curve drops as the number (and amount) of transmuting elements increases. Next, we analyze the impact on the ideal tensile strength  $\sigma_m$ , defined as the maximum in the stress-strain curve. The inset of Fig. 5(a) shows that while  $\sigma_m$  also decreases with the presence of transmuting elements, the related strain  $\epsilon_m$  for which  $\sigma_m$  is achieved remains constant and  $\sim 14\%$  for all the chemical compositions studied. Figure 5(b) summarizes the evolution of  $\sigma_m$  during the first ten years of irradiation in increments of one year. As the figure shows,  $\sigma_m$  monotonically decreases with the irradiation time for all the scenarios considered. This is consistent with previous works that studied the ideal tensile strength of tungsten and tungsten alloys by first-principles calculations [10, 41]. Furthermore, adding all transmutants results only in a slight deviation from the chemical compositions that includes the top 3 transmutants (Re, Os, Ta). The observed higher values of  $\sigma_m$  for W including primary transmutant (Re) with respect

344 to all-transmutants composition also aligns with the results obtained when studying the  
 345 elastic behavior of transmuting tungsten, where the magnitude of the slope for W with  
 346 primary transmutant was always smaller than the one for the current composition with  
 347 all transmutants.

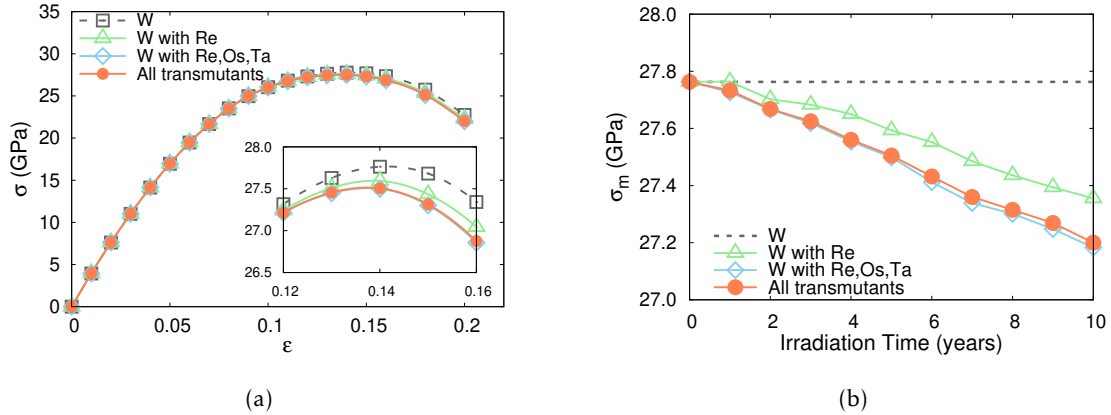


Figure 5. (a) The stress-strain curves under [001] tensile strain after six years of irradiation. (b) Evolution of the ideal tensile strength of transmuting tungsten during the first ten years of continuous exposure to EU-DEMO first wall conditions. These calculations are performed in their ground state and therefore they can not be compared directly to experimental stress-strain curves.

348

#### D. Dislocation-based ductility parameter of transmuted tungsten

349 In this section, we investigate the effect of transmuting elements on the ductility pa-  
 350 rameter of tungsten for  $\langle 111 \rangle \{ \bar{1}10 \}$  and  $\langle 111 \rangle \{ 11\bar{2} \}$  slip systems. We decided to focus  
 351 here on pure W, the chemical composition that includes only the primary transmutant  
 352 (Re), and the chemical composition that includes all transmutants. This choice is jus-  
 353 tified by (i) the increased computational cost to calculate  $\gamma_{us}$  (the reader is referred to  
 354 appendix A for more details about the convergence tests shown there), and (ii) the small  
 355 variations observed when studying the elastic properties and the ideal tensile strength

356 of the chemical composition including top 3 transmutants (Re, Os, Ta) and the chemical  
357 composition with all the transmutants.

358 As noted in Section III C, the dislocation-based ductility parameter  $D$  formulated by  
359 Rice [34] can be obtained in terms of the surface energy  $\gamma_s$  and the unstable stacking  
360 fault energy  $\gamma_{us}$ . Next, we describe the results obtained when calculating each of these  
361 measurements, as well as the resultant ductility parameter.

362  $\gamma_{us}$  is defined as the maximum value of the generalized stacking fault energy(GSFE)  
363 curve. As such, we need to calculate the GSFE curve for each of the chemical compositions  
364 and irradiation times considered. Figures 6(a) and 6(b) show the obtained GSFE curves of  
365 both  $\langle 111 \rangle \{\bar{1}10\}$  and  $\langle 111 \rangle \{11\bar{2}\}$  slip systems for the chemical compositions that results  
366 after irradiating pure tungsten at fifth year. The figures reveal several interesting trends  
367 that are consistent with previous works in the field. Firstly,  $\gamma_{us}$  is always in the middle  
368 of the energy path from one equilibrium position to another on a  $\{\bar{1}10\}$  plane while there  
369 is certain asymmetry towards the first equilibrium position on a  $\{11\bar{2}\}$  plane [42, 78, 91,  
370 95]. Secondly, adding transmuted elements lowers  $\gamma_{us}$  of both slip systems [13, 37, 96].  
371 Thirdly,  $\gamma_{us}$  is higher for the  $\langle 111 \rangle \{11\bar{2}\}$  slip system [36, 42, 87, 91, 95]. The evolution of  
372  $\gamma_{us}$  for both slip systems during the first ten years of irradiation is summarized in Fig. 6(c)  
373 and 6(d). These results show higher values of  $\gamma_{us}$  of the  $\langle 111 \rangle \{11\bar{2}\}$  slip system over the  
374 entire time domain, and a monotonic decrease of  $\gamma_{us}$  as the irradiation time (and therefore  
375 the amount of transmuted elements) increases.

376 For its part, the calculation of  $\gamma_s$  in terms of the chemical composition and the ir-  
377 radiation time requires a preliminary step: the confirmation that  $\gamma_s$  does not diverge  
378 with increasing slab thickness [82, 97]. Following the method proposed by Fiorentini and  
379 Methfessel [82], Fig. 7(a) shows the calculated surface energies as a function of the slab  
380 thickness for the chemical compositions (all transmutants) that appear after 4 years of ir-  
381 radiation in tungsten. It can be seen from these results that convergence of  $\gamma_s$  is achieved  
382 with increasing the number of layers and a slab thickness of 12 layers assures a relative

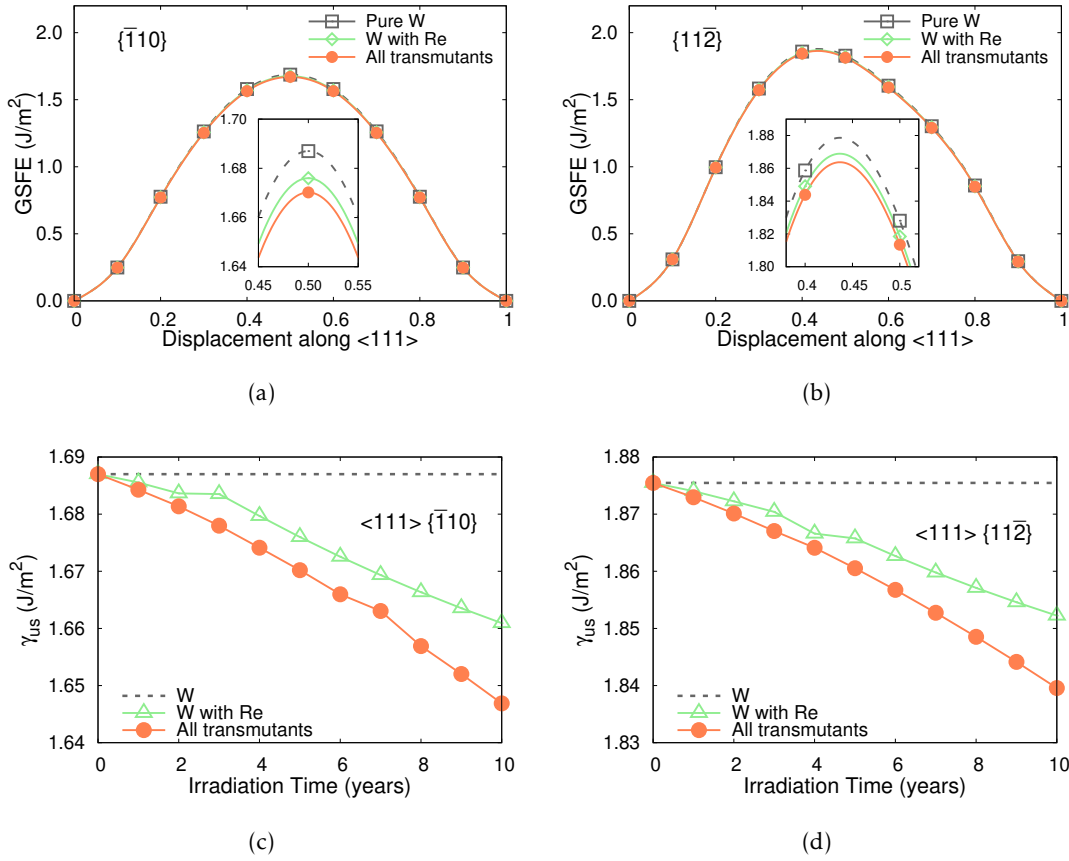


Figure 6. The general stacking faults energy for the slip along  $\langle 111 \rangle$  direction in (a)  $\{\bar{1}10\}$  and (b)  $\{11\bar{2}\}$  plane after 5 years of irradiation. Evolution of the unstable stacking fault energy  $\gamma_{us}$  for pure tungsten and transmuting tungsten during the first ten years of irradiation under EU-DEMO first wall conditions for both (c)  $\langle 111 \rangle \{\bar{1}10\}$  and (d)  $\langle 111 \rangle \{11\bar{2}\}$  slip systems.

383 difference of less than 0.02%. With the confidence conferred on our approach by the con-  
 384 vergence tests, next we proceed to calculate the surface energy for a number of chemical  
 385 compositions, irradiation times, and both slip systems. The results are summarized in  
 386 Fig. 7(b). Despite the higher values of  $\gamma_s$  for the  $\langle 111 \rangle \{11\bar{2}\}$  slip system, there is a small  
 387 variation in terms of the chemical composition and the irradiation time studied, specially  
 388 when compared with the evolution of  $\gamma_{us}$  shown in Fig. 6(c) and 6(d).

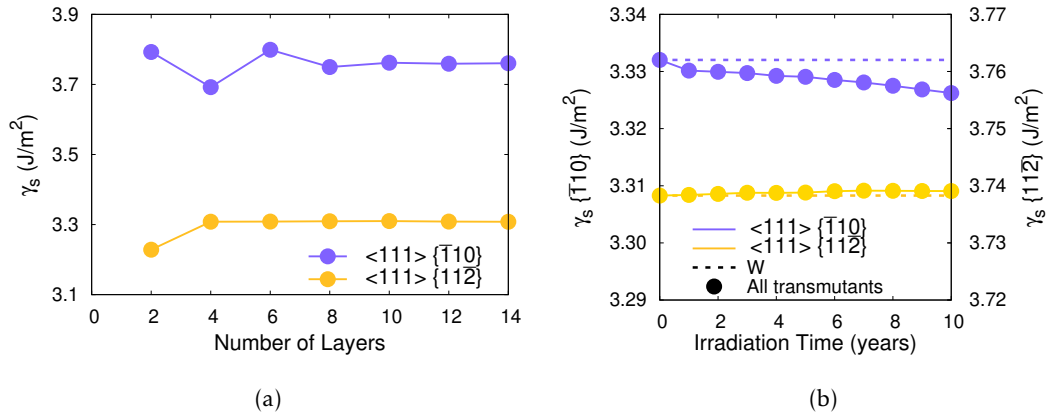


Figure 7. (a) Calculated surface energies for transmuting tungsten (all transmutants) as a function of the slab thickness after four years of irradiation; (b) Evolution of the surface energy for pure tungsten and transmuting tungsten during the first ten years of irradiation under EU-DEMO first wall conditions for both  $\langle 111 \rangle \{\bar{1}10\}$  and  $\langle 111 \rangle \{11\bar{2}\}$  slip systems.

389 Once both  $\gamma_s$  and  $\gamma_{us}$  are calculated in terms of the chemical composition and the  
 390 irradiation time, the ductility parameter  $D$  is obtained by substituting these terms into  
 391 Eq. 12. We present results for the two slip systems of interest in Figure 8, where the  
 392 linear dependency with irradiation time is clearly distinguished. It can also be observed  
 393 that  $D$  is higher on the  $\langle 111 \rangle \{11\bar{2}\}$  slip system and the positive impact of adding more  
 394 transmuting elements for a given irradiation time. This is in agreement with the well  
 395 accepted improvement of the ductility of W when adding Re [36, 42, 87, 91, 95, 98].

396

## V. DISCUSSION

397

### A. Nuclear transmutation

398 Section II presented typical transmutation results for pure W in a fusion reactor first  
 399 wall (plasma-exposed) environment. While tungsten is a relatively highly transmuting  
 400 element (for example, compare the relative burn-up of W to other elements in figure 6

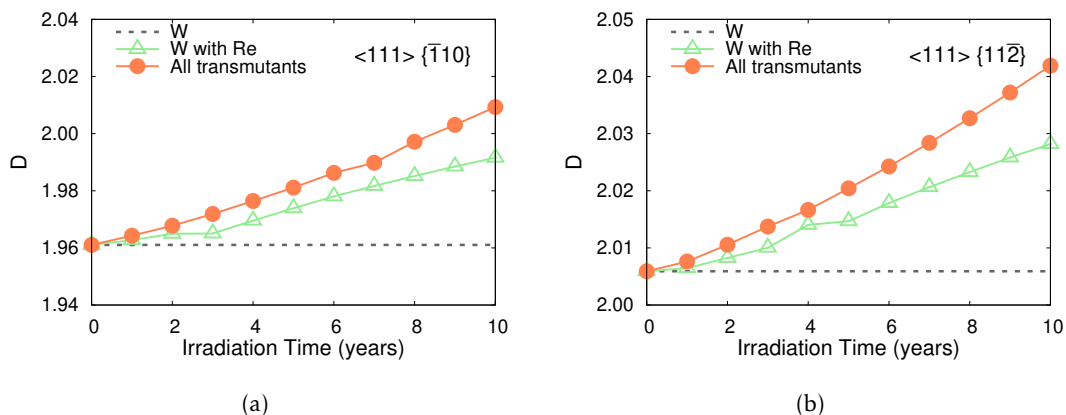


Figure 8. Evolution of the ductility parameter  $D$  for transmuted tungsten along the (a)  $\langle 111 \rangle \{ \bar{1}10 \}$  and (b)  $\langle 111 \rangle \{ 11\bar{2} \}$  slip systems during the first ten years of continuous exposure to EU-DEMO first wall conditions.

of [99]), figure 1(b) and table I showed that W will remain relatively pure even after 10 years of exposure, with only 4-5 atomic % of transmutation impurities. However, even at such low concentrations, transmutants such as Re, Os, and Ta could still have significant impact on the engineering performance of W-based components in fusion systems. For example, 5 % Re in tungsten can cause a 10-20% reduction in the thermal diffusivity (and hence thermal conductivity) [100]. In a first wall fusion reactor having such a large variation of thermal performance in armour (where W is the preferred choice) would pose an engineering design challenge.

Even more problematic for the engineering of fusion components is uncertainties in predictions associated with nuclear response. In the present work, we have shown a rare attempt to quantify uncertainties in transmutation predictions – in codes such as FISPACT-II [51] uncertainty quantification (UQ) is typically focused on radiological responses, which is clearly important as safety margins must be well understood to plan maintenance, handling, and dismantling operations where human workers may be involved. However, where mechanical, structural, and thermal behaviour may be impacted



416 by the complete burn-up (transmutation) response (i.e. not merely from the typically  
417 small concentrations of radioactive products of nuclear reactions) it will be vital to pro-  
418 vide UQ for the complete inventory evolution response.

419 The calculations performed in this work showed errors on the main transmutation  
420 products (Re and Os) of less than 10 %, which is reasonable and typical of errors originat-  
421 ing purely from nuclear data – see, for example, [101, 102], where decay-heat predictions  
422 by FISPACT-II for important fusion materials show good agreement with experimental  
423 measurements and where the computational errors generally encompass the  
424 experimental values. However, the errors shown in table I, are not the complete picture  
425 - full UQ for the results would require, in addition to the errors originating from the nu-  
426 clear data used in the inventory simulations, assessment of the errors associated with the  
427 neutron transport simulations used to generate the neutron spectrum.

428 In the present, the spectrum comes from a neutron transport simulation (performed  
429 using MCNP [103]) of highly conceptualized model for EU-DEMO [55, 56]. As well as  
430 the errors inherent in the neutron transport simulations, which originates from the same  
431 nuclear data used for the inventory simulations with FISPACT-II, there is the unquantified  
432 – and likely quite large – uncertainty in the fusion reactor model itself.

433 A key challenge for the future development of fusion, which will never have the wealth  
434 of experimental devices afforded the fission industry during its development, is to assess  
435 these engineering uncertainties, perhaps using Monte-Carlo-based sensitivity studies on  
436 the reactor design parameters or otherwise.

## 437 **B. Effects of transmutant elements on the mechanical properties**

438 In Sections III A - III C we have provided calculations of the lattice parameter, elastic  
439 behavior, ideal tensile strength, and ductility parameter as new transmutant elements  
440 are added to the initial composition of pure tungsten due to irradiation. Furthermore,  
441 to better understand the effect of the most predominant elements produced in W under

442 fusion-neutron irradiation, we also studied chemical compositions corresponding W with  
443 transmutant Re (W-Re) and also with Re, Os, and Ta (W-Re-Os-Ta) for each irradiation  
444 time. Here we consider the most important implications of the above calculations.

445 The results shown in Fig. 3 and Fig. 4 reveal that the lattice constant  $a_0$  and the tetrag-  
446 onal shear modulus  $C'$  are the only two elastic measurements decreasing with increasing  
447 the amount of transmutant elements. These effects are closely related to the variation of  
448 the number of valence electrons per atom. For example, the reduction of the lattice con-  
449 stant (for a given irradiation time) with increasing the amount of transmutant elements is  
450 in agreement with experimental measurements and  $d$ -band filling predictions [94]. The  
451 decrease of  $C'$  with increasing impurity elements also suggests how transmuting tungsten  
452 becomes structurally unstable as the number of valence electrons increases. If we analyze  
453 the effect on other elastic constants and properties such as  $C_{11}$ ,  $C_{44}$ , and  $E$ , their growth  
454 with increasing the solid solute concentrations and the number of valence electrons is in  
455 agreement with previous experimental [94] and computational works [10, 13, 87, 104].  
456 When evaluating the quantitative effects of the chemical composition on the elastic be-  
457 havior, the small amounts of impurity elements that appear due to transmutation (cf. Ta-  
458 ble I) justify the smooth change of all these elastic parameters (the maximum difference  
459 observed is 1.8% for  $C_{44}$  after 10 years of irradiation). Still, it is noticeable the major  
460 qualitative role that Re plays in the evolution of the elastic behavior, compensating the  
461 effect of other transmutant elements like Ta that decrease the number of valence electrons  
462 [10, 104]. Finally, it can be observed from these figures that the effect of burn-up creating  
463 impurity elements with a relative concentration  $\leq 0.87$  at.% is negligible. This has compu-  
464 tational consequences as adding extra elements significantly increases the computational  
465 cost of the simulations.

466 For its part, the variability of the ideal tensile strength shown in Fig. 5(a) can be ex-  
467 plained by investigating the electronic structures of the chemical compositions compared.  
468 When Group-VI transition metals like tungsten are deliberately alloyed with elements

469 with more valence electrons like Re or if those elements grow-in due to transmutation,  
 470 the elastic shear instability is hindered by the Jahn-Teller distortion [105]. The result is a  
 471 material that presents a slightly lower ideal tensile strength when compared to the pure  
 472 element, as it is shown in the aforementioned figure. This is in fact consistent with previ-  
 473 ous experimental and computational works that describe how the peak stress of W-Re al-  
 474 loys are lower than the corresponding values of pure W [10, 104, 106–108]. Furthermore,  
 475 similarly to the observations when studying the elastic behavior of transmuted tungsten,  
 476 the small variations of the ideal tensile strength for a given irradiation time when adding  
 477 Hf, H, He, Ir, and Pt can be explained by the small relative concentrations of these ele-  
 478 ments (always  $\leq 0.87$  at.%) that appear during the course of the 10-year power-plant first  
 479 wall irradiation.

480 Another important physical aspect of mechanical deformation in bcc crystals is their  
 481 ductility. As described in Section III C, the Rice criterion [34] was chosen to estimate the  
 482 ductility of transmuted tungsten. As such, the dependence of both  $\gamma_{us}$  and  $\gamma_s$  with re-  
 483 spect to the chemical composition needs to be investigated prior to the calculation of the  
 484 dislocation-based ductility parameter  $D$  (cf. Eq. 12). Several features can be discussed  
 485 from these results, shown in Figs. 6 and 7. Firstly, the value of  $\gamma_{us}$  for each chemical  
 486 composition on the  $\langle 111 \rangle \{\bar{1}10\}$  slip system is always smaller than its counterpart on the  
 487  $\langle 111 \rangle \{11\bar{2}\}$  slip system (cf. Fig. 6(a) and 6(b)). This suggests, confirming the findings  
 488 in previous works [77, 109], that slip should predominantly occur on  $\{\bar{1}10\}$  planes. Sec-  
 489 ondly, the addition of transmuted elements decreases  $\gamma_{us}$ . Previous works have shown  
 490 a different behavior depending on the number of valence electrons of the add-elements.  
 491 Adding elements with more valence electrons than W (such as Re, Os, Ir, Pt) have con-  
 492 sistently reduced  $\gamma_{us}$  [42, 107] while adding elements with less valence electrons than W  
 493 (such as Ta, Ti, Nb, Hf) tend to slightly increase it [42, 107]. However, when comparing  
 494 the value of  $\gamma_{us}$  in pure W, W-Re and the chemical composition with all transmutants, we  
 495 observe that the addition of elements always make  $\gamma_{us}$  to shrink. On this basis, we find

496 that the higher relative concentration of Re with respect to other transmutants (cf. Table  
 497 I) plays a crucial role here, hindering the effect that other transmutant elements with less  
 498 valence electrons than W should have.

499 Additionally, the results shown in Fig. 7(b) reveal that  $\gamma_s$  on the  $\langle 111 \rangle \{\bar{1}10\}$  slip system  
 500 is also smaller than its counterpart on the  $\langle 111 \rangle \{11\bar{2}\}$  slip system. Still, the limited vari-  
 501 ability of  $\gamma_s$  with the chemical composition as irradiation time increases implies that the  
 502 main factor governing the dependence of  $D$  with the chemical composition is  $\gamma_{us}$ . Con-  
 503 necting the above observations regarding  $\gamma_{us}$  and  $\gamma_s$ , the results shown in Fig. 8 indicate  
 504 that, for a given chemical composition, the ductility parameter is higher as the amount  
 505 of transmutants is increased. This suggests that the addition of Re (which significantly  
 506 decreases  $\gamma_{us}$  for a relatively constant  $\gamma_s$ ) is the main factor responsible for this increment  
 507 in the ductility.

### 508 C. Evolution of the mechanical properties with irradiation time

509 Previous works in the literature have extensively studied the effects of alloying ele-  
 510 ments on various properties of tungsten such as phase stability [10, 35–38], elastic prop-  
 511 erties [10, 13, 35–37, 39, 40], ideal tensile strength [10, 41], ductility [42], radiation de-  
 512 fects [36], point defects [35, 43–47], dislocation structure [48, 49], grain boundaries [50],  
 513 etc. However, to the best of our knowledge, there is a lack of understanding on how  
 514 the expected first wall fusion power-plant conditions change the mechanical properties  
 515 of these structural materials over time. Furthermore, most of these works have studied  
 516 the effects when adding single or a reduce number of alloying elements to tungsten. In  
 517 this work we address this gap by investigating not only the time dependence of the me-  
 518 chanical properties but also the effect of adding a combination of all the elements that  
 519 appear due to transmutation. Our primary observation from the results shown in Figs. 3,  
 520 4, 5(b), 7(b), and 8 is that the time evolution of the mechanical properties is governed  
 521 by the characteristics of the transmutant element with the highest relative concentration.

522 As described in Table I, this corresponds to Re, an element with more valence electrons  
523 than W. The mechanical properties that monotonically increase when Re is added also in-  
524 crease as the exposure to first wall conditions continues, and vice versa. This effect (either  
525 increasing or decreasing the specific property) is slightly augmented when all the trans-  
526 mutants are considered, but the trend is governed by the primary transmutant element,  
527 no matter whether the other transmutants actually increase or decrease the number of  
528 valence electrons. However, we issue this conclusion with caution, as the relative concen-  
529 trations of the deliberately added alloying elements in other candidate materials such as  
530 tungsten-based high-entropy alloys [110] are more similar and their mechanical behavior  
531 is expected to be different.

## 532 VI. CONCLUSIONS

533 To summarize, we have used the FISPACT-II inventory code to calculate how the chem-  
534 ical composition of pure W changed when exposed to the EU-DEMO fusion first wall con-  
535 ditions for ten years. We have also performed first-principles calculations to characterize  
536 how the elastic constants, elastic properties, ideal tensile strength, unstable stacking fault  
537 energy, surface energy, and ductility parameter evolve as new transmutant elements are  
538 added to pure W due to transmutation.

539 Our first conclusion from these investigations is that W will remain relatively pure  
540 even after 10 years of exposure to first wall fusion conditions, with only 4-5 at.% of trans-  
541 mutant elements. Secondly, we have observed that the effects of these transmutant ele-  
542 ments on the mechanical properties of transmuting tungsten is closely related to the rel-  
543 ative variation of the number of valence electrons per atom as the composition changes.  
544 In particular, we find that the relative difference of these valence electrons created by the  
545 most predominant transmutant element (Re), has an important influence all the prop-  
546 erties calculated. Furthermore, the impact of minor transmutants (those with a relative  
547 concentration  $\leq 0.87$  at.%) seems negligible. Finally, our analysis of the mechanical prop-

548 erties as exposure to first wall fusion conditions continues over time also suggests that  
 549 Re plays an important role in the evolution of the mechanical properties, increasing for  
 550 example the Young’s modulus, shear modulus, bulk modulus, and the ductility param-  
 551 eter; and decreasing the lattice constant, tetragonal shear elastic constant, ideal tensile  
 552 strength, and the unstable stacking fault energy.

### 553 ACKNOWLEDGMENTS

554 This work used the Extreme Science and Engineering Discovery Environment (XSEDE),  
 555 which is supported by National Science Foundation grant number ACI-1548562. Specifi-  
 556 cally, YQ and DC acknowledge support from XSEDE allocations MSS190015 and MAT200015.  
 557 YQ and DC also acknowledge computer time allocations at Villanova’s HPC-CoE clus-  
 558 ter. MRG acknowledges funding from the RCUK Energy Programme [grant number  
 559 EP/T012250/1].

### 560 Appendix A: Convergence of the DFT calculations

561 Figures 9 and 10 show the convergence of the lattice parameter, elastic constants, and  
 562 elastic properties with respect to the plane-wave energy cutoff and the  $k$  mesh. These  
 563 results suggest that an energy cutoff of 150 Ry and a  $30 \times 30 \times 30$   $k$ -point mesh are sufficient  
 564 to perform our first-principles calculations of the elastic behavior.

565 The convergence of the unstable stacking fault energy  $\gamma_{us}$  with respect to the energy  
 566 cutoff,  $k$  mesh and slab size is shown in Fig. A.11. First, we studied the convergence of  $\gamma_{us}$   
 567 with respect to the energy cutoff and  $k$  points, keeping a fixed slab structure of 8 layers.  
 568 In Fig. A.11(a) the  $k$ -points were sampled using a fixed  $16 \times 16 \times 1$  grid, being the energy  
 569 cutoff the only parameter allowed to change. The results show that an energy cutoff of 40  
 570 Ry turns out to be sufficient, specially considering the computational cost and the number  
 571 of GSFE calculations needed. In Fig. A.11(b) we did the opposite, fixing the energy cutoff

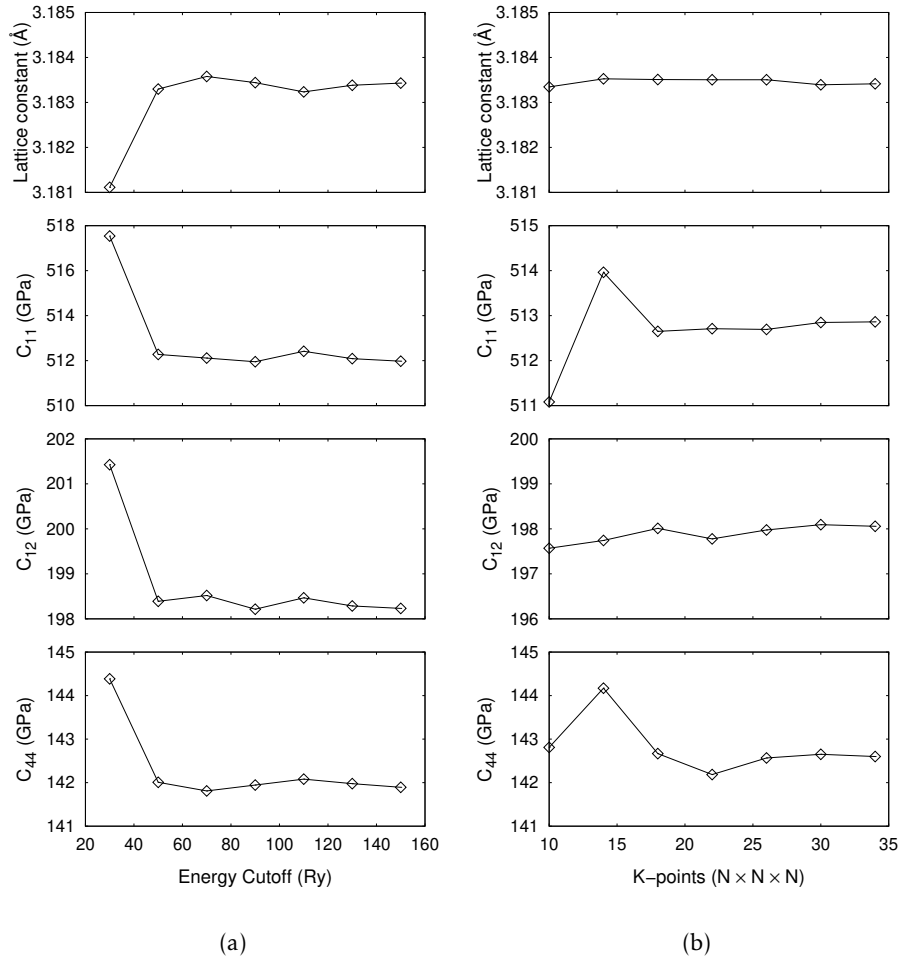


Figure 9. Convergence of the lattice constant and elastic constants  $C_{11}$ ,  $C_{12}$  and  $C_{44}$  as a function of the plane-wave energy cutoff (a) and  $k$  mesh (b). The energy cutoff convergence (left) is studied keeping the  $k$ -points fixed to  $20 \times 20 \times 20$ . The  $k$  mesh convergence (right) is studied keeping an energy cutoff of 80 Ry.

572 to 60 Ry and allowing the  $k$ -points sample to change. Only small variations of less than  
 573 0.03% (for  $\langle 111 \rangle \{ \bar{1}10 \}$ ) and 0.01% (for  $\langle 111 \rangle \{ 11\bar{2} \}$ ) were found when comparing the re-  
 574 sults between a  $28 \times 28 \times 1$  and a  $30 \times 30 \times 1$  grid. As such, we chose the  $28 \times 28 \times 1$   $k$ -point  
 575 mesh as a good compromise between computational accuracy and computational cost for

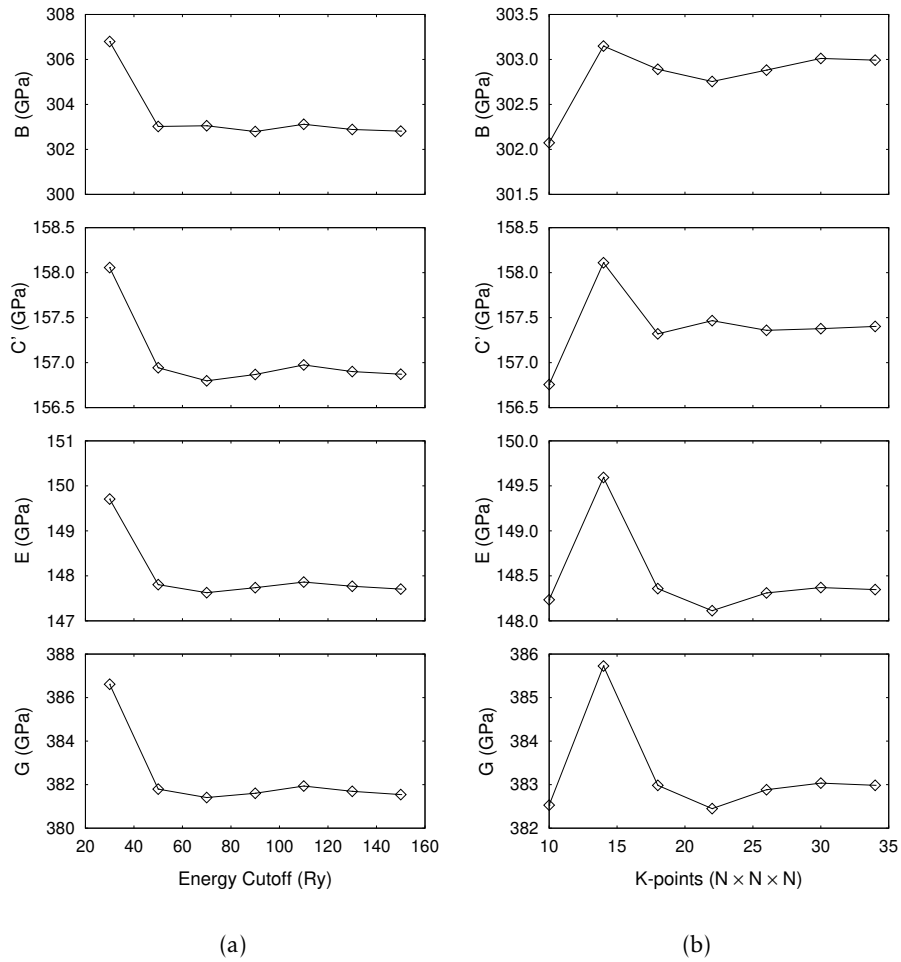


Figure 10. Convergence of the bulk modulus  $B$ , the tetragonal shear elastic constant  $C'$ , the shear modulus  $G$ , and the Young's modulus  $E$  as a function of the plane-wave energy cutoff (a) and  $k$  mesh (b). The energy cutoff convergence (left) is studied keeping the  $k$ -points fixed to  $20 \times 20 \times 20$ . The  $k$  mesh convergence (right) is studied keeping an energy cutoff of 80 Ry.

576 both slip systems. Then we fixed the energy cutoff to 40 Ry and the  $k$  points sampling  
 577 to a  $28 \times 28 \times 1$  grid, allowing the slab size to change. Previous works in the literature (cf.  
 578 Table III) have shown that  $\gamma_{us}$  for the  $\langle 111 \rangle \{11\bar{2}\}$  slip system is higher than its counter-  
 579 part for the  $\langle 111 \rangle \{\bar{1}10\}$  slip system. This trend appears at 12 layers in Fig. A.11(c). Given



580 the significant computational increase of choosing 14 layers instead of 12 layers shown in  
581 Fig. A.11(d), we decided to chose a slab size of 12 layers in our simulations.

582 These convergence tests and the selection of accurate but reasonable DFT parame-  
583 ters are relevant to our approach given the significant computational cost of the first-  
584 principles simulations performed to obtain the GSFE along the entire  $\langle 111 \rangle$  path for each  
585 of chemical compositions at each the irradiation time.

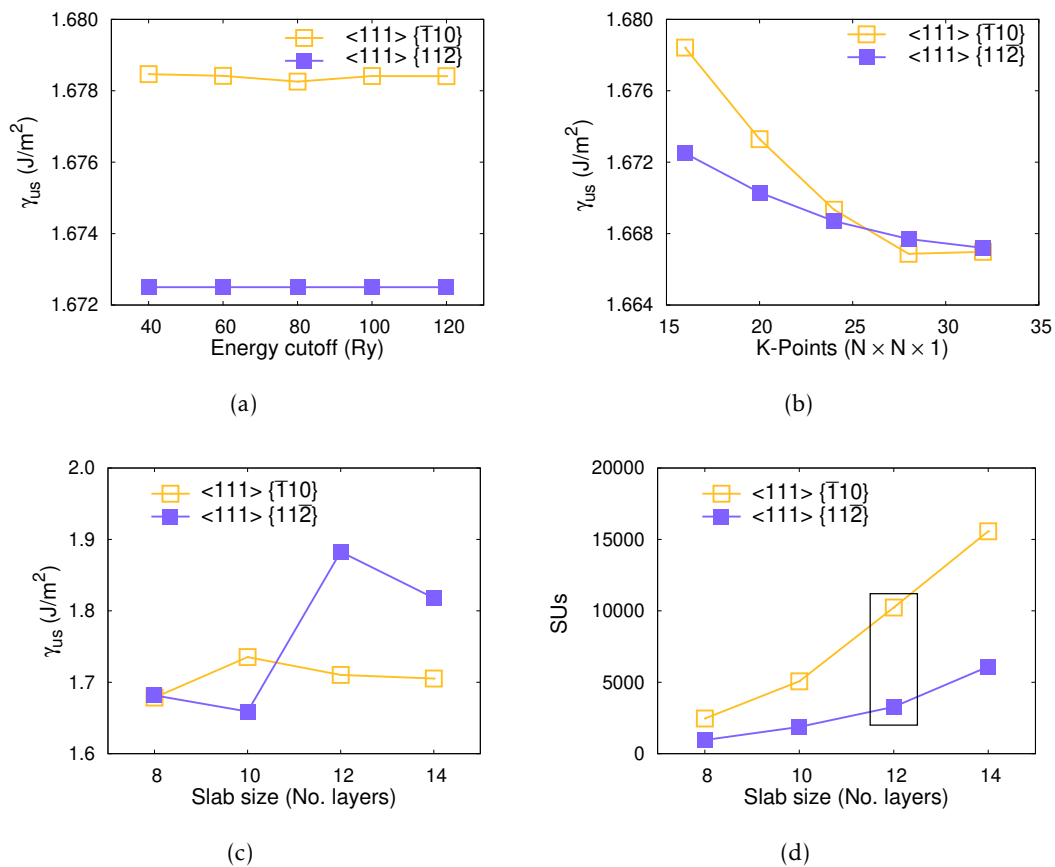


Figure 11. Benchmarking to identify the set of parameters that guarantee accurate and efficient DFT calculations of the unstable stacking fault energy  $\gamma_{us}$  for transmuted tungsten. Fig. 11(a), 11(b), and 11(c) show the convergence with the energy cutoff, k-points sampling, and slab size, respectively. Fig. 11(d) shows the total number of SUUs needed to complete each simulation. The highlighted region in Fig. 11(d) indicates the total number of SUUs for the final set of parameters.

- 
- 586 [1] E. Lassner and S. Wolf-Dieter, Tungsten: Properties, Chemistry, Technology of the Element, Alloys, and Chemicals  
587 (Springer US, 1999).
- 588 [2] H. Bolt, V. Barabash, W. Krauss, J. Linke, R. Neu, S. Suzuki, N. Yoshida, and A. U. Team,  
589 Materials for the plasma-facing components of fusion reactors, *Journal of nuclear materials*  
590 **329**, 66 (2004).
- 591 [3] A. Giannattasio and S. G. Roberts, Strain-rate dependence of the brittle-to-ductile transition  
592 temperature in tungsten, *Philosophical Magazine* **87**, 2589 (2007).
- 593 [4] S. J. Zinkle and N. M. Ghoniem, Prospects for accelerated development of high performance  
594 structural materials, *Journal of Nuclear Materials* **417**, 2 (2011).
- 595 [5] M. Rieth, S. Dudarev, S. Gonzalez de Vicente, J. Aktaa, T. Ahlgren, S. Antusch, D. Arm-  
596 strong, M. Balden, N. Baluc, M.-F. Barthe, et al., Recent progress in research on tungsten  
597 materials for nuclear fusion applications in europe, *Journal of Nuclear Materials* **432**, 482  
598 (2013).
- 599 [6] J. F. Dobson, G. Vignale, and M. P. Das, Electronic density functional theory: recent progress and new directions  
600 (Springer Science & Business Media, 2013).
- 601 [7] W. A. Counts, M. Friak, D. Raabe, and J. Neugebauer, Using ab initio calculations in design-  
602 ing bcc mgli-x alloys for ultra-lightweight applications, *Advanced Engineering Materials*  
603 **12**, 1198 (2010).
- 604 [8] D. Roundy, C. Krenn, M. L. Cohen, and J. Morris Jr, The ideal strength of tungsten, *Philo-  
605 sophical magazine A* **81**, 1725 (2001).
- 606 [9] S. Giusepponi and M. Celino, The ideal tensile strength of tungsten and tungsten alloys by  
607 first-principles calculations, *Journal of nuclear materials* **435**, 52 (2013).
- 608 [10] C. Yang and L. Qi, Ab initio calculations of ideal strength and lattice instability in w-ta and  
609 w-re alloys, *Physical Review B* **97**, 014107 (2018).
- 610 [11] N. Nagasako, M. Jahnátek, R. Asahi, and J. Hafner, Anomalies in the response of v, nb, and  
611 ta to tensile and shear loading: Ab initio density functional theory calculations, *Physical*  
612 *Review B* **81**, 094108 (2010).
- 613 [12] Y. Ma, Q.-F. Han, Z.-Y. Zhou, and Y.-L. Liu, First-principles investigation on mechanical  
614 behaviors of w-cr/ti binary alloys, *Journal of Nuclear Materials* **468**, 105 (2016).

- 615 [13] X. Li, S. Schönecker, R. Li, X. Li, Y. Wang, J. Zhao, B. Johansson, and L. Vitos, Ab initio cal-  
616 culations of mechanical properties of bcc w-re-os random alloys: effects of transmutation  
617 of w, *Journal of Physics: Condensed Matter* **28**, 295501 (2016).
- 618 [14] V. Vitek, Core structure of screw dislocations in body-centred cubic metals: relation to  
619 symmetry and interatomic bonding, *Philosophical Magazine* **84**, 415 (2004).
- 620 [15] S. Wurster, B. Gludovatz, and R. Pippan, High temperature fracture experiments on  
621 tungsten-rhenium alloys, *International Journal of Refractory Metals and Hard Materials*  
622 **28**, 692 (2010).
- 623 [16] H. Li, S. Wurster, C. Motz, L. Romaner, C. Ambrosch-Draxl, and R. Pippan, Dislocation-core  
624 symmetry and slip planes in tungsten alloys: Ab initio calculations and microcantilever  
625 bending experiments, *Acta Materialia* **60**, 748 (2012).
- 626 [17] G. D. Samolyuk, Y. Osetsky, and R. Stoller, The influence of transition metal solutes on the  
627 dislocation core structure and values of the peierls stress and barrier in tungsten, *Journal of*  
628 *Physics: Condensed Matter* **25**, 025403 (2013).
- 629 [18] M. a.-S. Duesbery and V. Vitek, Plastic anisotropy in bcc transition metals, *Acta Materialia*  
630 **46**, 1481 (1998).
- 631 [19] K. Ito and V. Vitek, Atomistic study of non-schmid effects in the plastic yielding of bcc  
632 metals, *Philosophical Magazine A* **81**, 1387 (2001).
- 633 [20] V. Bulatov, O. Richmond, and M. Glazov, An atomistic dislocation mechanism of pressure-  
634 dependent plastic flow in aluminum, *Acta materialia* **47**, 3507 (1999).
- 635 [21] C. Woodward and S. Rao, Ab-initio simulation of isolated screw dislocations in bcc mo and  
636 ta, *Philosophical Magazine A* **81**, 1305 (2001).
- 637 [22] R. Gröger and V. Vitek, Breakdown of the schmid law in bcc molybdenum related to the  
638 effect of shear stress perpendicular to the slip direction, in *Materials Science Forum*, Vol.  
639 **482** (Trans Tech Publ, 2005) pp. 123–126.
- 640 [23] J. Chaussidon, M. Fivel, and D. Rodney, The glide of screw dislocations in bcc fe: atomistic  
641 static and dynamic simulations, *Acta materialia* **54**, 3407 (2006).
- 642 [24] M. Gilbert, S. Queyreau, and J. Marian, Stress and temperature dependence of screw dislo-  
643 cation mobility in  $\alpha$ -fe by molecular dynamics, *Physical Review B* **84**, 174103 (2011).
- 644 [25] D. Cereceda, M. Diehl, F. Roters, D. Raabe, J. M. Perlado, and J. Marian, Unraveling the tem-  
645 perature dependence of the yield strength in single-crystal tungsten using atomistically-

- 646 informed crystal plasticity calculations, *International Journal of Plasticity* **78**, 242 (2016).
- 647 [26] C. Marichal, K. Srivastava, D. Weygand, S. Van Petegem, D. Grolimund, P. Gumbsch, and  
648 H. Van Swygenhoven, Origin of anomalous slip in tungsten, *Physical review letters* **113**,  
649 025501 (2014).
- 650 [27] L. Dezerald, D. Rodney, E. Clouet, L. Ventelon, and F. Willaime, Plastic anisotropy and  
651 dislocation trajectory in bcc metals, *Nature communications* **7**, 1 (2016).
- 652 [28] A. Krach, E. Clouet, L. Dezerald, L. Ventelon, F. Willaime, and D. Rodney, Non-glide effects  
653 and dislocation core fields in bcc metals, *npj Computational Materials* **5**, 1 (2019).
- 654 [29] J. Marian, C. S. Becquart, C. Domain, S. L. Dudarev, M. R. Gilbert, R. J. Kurtz, D. R. Mason,  
655 K. Nordlund, A. E. Sand, L. L. Snead, *et al.*, Recent advances in modeling and simulation  
656 of the exposure and response of tungsten to fusion energy conditions, *Nuclear Fusion* **57**,  
657 092008 (2017).
- 658 [30] S. Pugh, Xcii. relations between the elastic moduli and the plastic properties of polycrys-  
659 talline pure metals, *The London, Edinburgh, and Dublin Philosophical Magazine and Jour-*  
660 *nal of Science* **45**, 823 (1954).
- 661 [31] D. Pettifor, Theoretical predictions of structure and related properties of intermetallics,  
662 *Materials science and technology* **8**, 345 (1992).
- 663 [32] D. Suetin, I. Shein, and A. Ivanovskii, Structural, elastic, electronic and magnetic properties  
664 of perovskite-like  $\text{Co}_3\text{Wc}$ ,  $\text{Rh}_3\text{Wc}$  and  $\text{Ir}_3\text{Wc}$  from first principles calculations, *Solid state*  
665 *sciences* **12**, 814 (2010).
- 666 [33] G. N. Greaves, A. Greer, R. S. Lakes, and T. Rouxel, Poisson's ratio and modern materials,  
667 *Nature materials* **10**, 823 (2011).
- 668 [34] J. R. Rice, Dislocation nucleation from a crack tip: an analysis based on the peierls concept,  
669 *Journal of the Mechanics and Physics of Solids* **40**, 239 (1992).
- 670 [35] M. Muzyk, D. Nguyen-Manh, K. J. Kurzydłowski, N. L. Baluc, and S. L. Dudarev, Phase  
671 stability, point defects, and elastic properties of w-v and w-ta alloys, *Phys. Rev. B* **84**, 104115  
672 (2011).
- 673 [36] M. Muzyk, D. Nguyen-Manh, J. Wróbel, K. Kurzydłowski, N. Baluc, and S. Dudarev, First-  
674 principles model for phase stability, radiation defects and elastic properties of w-ta and  
675 w-v alloys, *Journal of Nuclear Materials* **442**, S680 (2013).
- 676 [37] N. Wei, T. Jia, X. Zhang, T. Liu, Z. Zeng, and X. Yang, First-principles study of the phase

- 677 stability and the mechanical properties of w-ta and w-re alloys, *AIP Advances* **4**, 057103  
678 (2014).
- 679 [38] C.-H. Huang, L. Gharaee, Y. Zhao, P. Erhart, and J. Marian, Mechanism of nucleation and in-  
680 cipient growth of re clusters in irradiated w-re alloys from kinetic monte carlo simulations,  
681 *Physical Review B* **96**, 094108 (2017).
- 682 [39] D. Jiang, C. Ouyang, and S. Liu, Mechanical properties of w-ti alloys from first-principles  
683 calculations, *Fusion Engineering and Design* **106**, 34 (2016).
- 684 [40] Y.-J. Hu, S.-L. Shang, Y. Wang, K. A. Darling, B. G. Butler, L. J. Kecskes, and Z.-K. Liu,  
685 Effects of alloying elements and temperature on the elastic properties of w-based alloys by  
686 first-principles calculations, *Journal of Alloys and Compounds* **671**, 267 (2016).
- 687 [41] S. Giusepponi and M. Celino, The ideal tensile strength of tungsten and tungsten alloys by  
688 first-principles calculations, *Journal of nuclear materials* **435**, 52 (2013).
- 689 [42] J. Qian, C. Wu, J. Fan, and H. Gong, Effect of alloying elements on stacking fault energy and  
690 ductility of tungsten, *Journal of Alloys and Compounds* **737**, 372 (2018).
- 691 [43] T. Suzudo, M. Yamaguchi, and A. Hasegawa, Stability and mobility of rhenium and osmium  
692 in tungsten: first principles study, *Modelling and Simulation in Materials Science and En-  
693 gineering* **22**, 075006 (2014).
- 694 [44] M. Hossain and J. Marian, Stress-dependent solute energetics in w-re alloys from first-  
695 principles calculations, *Acta materialia* **80**, 107 (2014).
- 696 [45] L. Gharaee, J. Marian, and P. Erhart, The role of interstitial binding in radiation induced  
697 segregation in w-re alloys, *Journal of Applied Physics* **120**, 025901 (2016).
- 698 [46] S. Giusepponi and M. Celino, The effects of vacancies in the mechanical properties of tung-  
699 sten: A first-principles study, *Nuclear Instruments and Methods in Physics Research Section*  
700 *B: Beam Interactions with Materials and Atoms* **342**, 70 (2015).
- 701 [47] W. Setyawan, G. Nandipati, and R. J. Kurtz, Ab initio study of interstitial cluster interaction  
702 with re, os, and ta in w, *Journal of Nuclear Materials* **484**, 30 (2017).
- 703 [48] L. Romaner, C. Ambrosch-Draxl, and R. Pippin, Effect of rhenium on the dislocation core  
704 structure in tungsten, *Physical review letters* **104**, 195503 (2010).
- 705 [49] H. Li, S. Wurster, C. Motz, L. Romaner, C. Ambrosch-Draxl, and R. Pippin, Dislocation-core  
706 symmetry and slip planes in tungsten alloys: Ab initio calculations and microcantilever  
707 bending experiments, *Acta materialia* **60**, 748 (2012).

- 708 [50] X. Wu, Y.-W. You, X.-S. Kong, J.-L. Chen, G.-N. Luo, G.-H. Lu, C. Liu, and Z. Wang, First-  
709 principles determination of grain boundary strengthening in tungsten: dependence on  
710 grain boundary structure and metallic radius of solute, *Acta Materialia* **120**, 315 (2016).
- 711 [51] J. -Ch. Sublet, J. W. Eastwood, J. G. Morgan, M. R. Gilbert, M. Fleming, and W. Arter,  
712 FISPACT-II: An advanced simulation system for activation, transmutation and material  
713 modelling, *Nucl. Data Sheets* **139**, 77 (2017), [http://dx.doi.org/10.1016/j.nds.2017.](http://dx.doi.org/10.1016/j.nds.2017.01.002)  
714 [01.002](http://dx.doi.org/10.1016/j.nds.2017.01.002).
- 715 [52] M. Fleming, T. Stainer, and M. R. Gilbert, The FISPACT-II User Manual, Tech. Rep. UKAEA-  
716 R(18)001 (UKAEA, 2018) available from <http://fispact.ukaea.uk>.
- 717 [53] U. Fischer, C. Bachmann, J. P. Catalan, T. Eade, D. Flammini, M. Gilbert, J. Jaboulay,  
718 A. Konobeev, D. Leichtle, L. Lu, F. Malouch, F. Moro, P. Pereslavitsev, Y. Qiu, J. Sanz,  
719 P. Sauvan, G. Stankunas, , A. Travleev, A. Turner, F. Ogando, I. Palermo, and R. Villari.,  
720 Methodological approach for DEMO neutronics in the European PPPT programme: Tools,  
721 data and analyses, *Fus. Eng. Des.* **123**, 26 (2017).
- 722 [54] M. R. Gilbert, T. Eade, C. Bachmann, U. Fischer, and N. P. Taylor, Waste assessment of eu-  
723 ropean demo fusion reactor designs, *Fus. Eng. Des.* **136**, 42 (2018), [https://doi.org/10.](https://doi.org/10.1016/j.fusengdes.2017.12.019)  
724 [1016/j.fusengdes.2017.12.019](https://doi.org/10.1016/j.fusengdes.2017.12.019).
- 725 [55] G. Federici, R. Kemp, D. Ward, C. Bachmann, T. Franke, S. Gonzalez, C. Lowry, M. Gado-  
726 ska, J. Harman, B. Meszaros, C. Morlock, F. Romanelli, and R. Wenninger, Overview of eu  
727 demo design and r&d activities, *Fus. Eng. Des.* **89**, 882 (2014), proceedings of the 11th  
728 International Symposium on Fusion Nuclear Technology-11 (ISFNT-11) Barcelona, Spain,  
729 15-20 September, 2013.
- 730 [56] G. Federici, C. Bachmann, L. Barucca, W. Biel, L. Boccaccini, R. Brown, C. Bustreo,  
731 S. Ciattaglia, F. Cismondi, M. Coleman, V. Corato, C. Day, E. Diegele, U. Fischer, T. Franke,  
732 C. Gliss, A. Ibarra, R. Kembleton, A. Loving, F. Maviglia, B. Meszaros, G. Pintsuk, N. Taylor,  
733 M. Tran, C. Vorpahl, R. Wenninger, and J. You, Demo design activity in europe: Progress  
734 and updates, *Fus. Eng. Des.* **136**, 729 (2018), special Issue: Proceedings of the 13th Inter-  
735 national Symposium on Fusion Nuclear Technology (ISFNT-13).
- 736 [57] M. R. Gilbert, L. W. Packer, J.-C. Sublet, and R. A. Forrest, Inventory simulations under  
737 neutron irradiation: Visualization techniques as an aid to materials design, *Nuclear Science*  
738 *and Engineering* **177**, 291 (2014), <https://doi.org/10.13182/NSE13-76>.

- 739 [58] M. R. Gilbert, T. Eade, C. Bachmann, U. Fischer, and N. P. Taylor, Activation, decay heat, and  
740 waste classification studies of the European DEMO concept, *Nucl. Fus.* **57**, 046015 (2017),  
741 <https://doi.org/10.1088/1741-4326/aa5bd7>.
- 742 [59] A. J. Koning and D. Rochman, TENDL-2017 (2017), release Date: April 25, 2018. Available  
743 from [https://tendl.web.psi.ch/tendl\\_2017/tendl2017.html](https://tendl.web.psi.ch/tendl_2017/tendl2017.html).
- 744 [60] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L.  
745 Chiarotti, M. Cococcioni, I. Dabo, et al., Quantum espresso: a modular and open-source  
746 software project for quantum simulations of materials, *Journal of physics: Condensed mat-*  
747 *ter* **21**, 395502 (2009).
- 748 [61] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car,  
749 C. Cavazzoni, D. Ceresoli, M. Cococcioni, et al., Advanced capabilities for materials mod-  
750 elling with quantum espresso, *Journal of Physics: Condensed Matter* **29**, 465901 (2017).
- 751 [62] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple,  
752 *Physical review letters* **77**, 3865 (1996).
- 753 [63] D. Hamann, Optimized norm-conserving vanderbilt pseudopotentials, *Physical Review B*  
754 **88**, 085117 (2013).
- 755 [64] L. Bellaiche and D. Vanderbilt, Virtual crystal approximation revisited: Application to di-  
756 electric and piezoelectric properties of perovskites, *Physical Review B* **61**, 7877 (2000).
- 757 [65] H. J. Monkhorst and J. D. Pack, Special points for brillouin-zone integrations, *Physical re-*  
758 *view B* **13**, 5188 (1976).
- 759 [66] J. F. Nye et al., Physical properties of crystals: their representation by tensors and matrices  
760 (Oxford university press, 1985).
- 761 [67] M. Mehl, J. Osburn, D. Papaconstantopoulos, and B. Klein, Structural properties of ordered  
762 high-melting-temperature intermetallic alloys from first-principles total-energy calcula-  
763 tions, *Physical Review B* **41**, 10311 (1990).
- 764 [68] K. Chen, L. Zhao, and J. S. Tse, Ab initio study of elastic properties of ir and ir 3 x com-  
765 pounds, *Journal of applied physics* **93**, 2414 (2003).
- 766 [69] F. Giustino, Materials modelling using density functional theory: properties and predictions  
767 (Oxford University Press, 2014).
- 768 [70] R. Hill, The elastic behaviour of a crystalline aggregate, *Proceedings of the Physical Society.*  
769 *Section A* **65**, 349 (1952).



- 770 [71] R. Peierls, The size of a dislocation, *Proceedings of the Physical Society* **52**, 34 (1940).
- 771 [72] F. Nabarro, Dislocations in a simple cubic lattice, *Proceedings of the Physical Society* **59**,  
772 256 (1947).
- 773 [73] M.-C. Marinica, L. Ventelon, M. Gilbert, L. Proville, S. Dudarev, J. Marian, G. Bencteux,  
774 and F. Willaime, Interatomic potentials for modelling radiation defects and dislocations in  
775 tungsten, *Journal of Physics: Condensed Matter* **25**, 395502 (2013).
- 776 [74] A. Stukowski, D. Cereceda, T. D. Swinburne, and J. Marian, Thermally-activated non-  
777 schmid glide of screw dislocations in w using atomistically-informed kinetic monte carlo  
778 simulations, *International Journal of Plasticity* **65**, 108 (2015).
- 779 [75] D. Caillard, Kinetics of dislocations in pure fe. part i. in situ straining experiments at room  
780 temperature, *Acta Materialia* **58**, 3493 (2010).
- 781 [76] D. Caillard, Kinetics of dislocations in pure fe. part ii. in situ straining experiments at low  
782 temperature, *Acta Materialia* **58**, 3504 (2010).
- 783 [77] C. Marichal, H. Van Swygenhoven, S. Van Petegem, and C. Borca, {110} slip with {112} slip  
784 traces in bcc tungsten, *Scientific reports* **3** (2013).
- 785 [78] D. Cereceda, A. Stukowski, M. Gilbert, S. Queyreau, L. Ventelon, M. Marinica, J. Perlado,  
786 and J. Marian, Assessment of interatomic potentials for atomistic analysis of static and  
787 dynamic properties of screw dislocations in w, *Journal of Physics: Condensed Matter* **25**,  
788 085702 (2013).
- 789 [79] C. Carter, R. Balluffi, and S. Allen, *Kinetics of materials* (2005).
- 790 [80] W. Tyson and W. Miller, Surface free energies of solid metals: Estimation from liquid surface  
791 tension measurements, *Surface Science* **62**, 267 (1977).
- 792 [81] J. Boettger, Nonconvergence of surface energies obtained from thin-film calculations, *Phys-  
793 ical Review B* **49**, 16798 (1994).
- 794 [82] V. Fiorentini and M. Methfessel, Extracting convergent surface energies from slab calcula-  
795 tions, *Journal of Physics: Condensed Matter* **8**, 6525 (1996).
- 796 [83] X. Li, S. Schönecker, R. Li, X. Li, Y. Wang, J. Zhao, B. Johansson, and L. Vitos, Ab initio cal-  
797 culations of mechanical properties of bcc w–re–os random alloys: effects of transmutation  
798 of w, *Journal of Physics: Condensed Matter* **28**, 295501 (2016).
- 799 [84] L. Romaner, C. Ambrosch-Draxl, and R. Pippan, Effect of rhenium on the dislocation core  
800 structure in tungsten, *Phys. Rev. Lett.* **104**, 195503 (2010).

- 801 [85] D. Jiang, Q. Zhou, L. Xue, T. Wang, and J. Hu, First-principles study the phase stability  
802 and mechanical properties of binary w-mo alloys, *Fusion Engineering and Design* **130**, 56  
803 (2018).
- 804 [86] Y.-L. Liu, H.-B. Zhou, Y. Zhang, S. Jin, and G.-H. Lu, The ideal tensile strength and defor-  
805 mation behavior of a tungsten single crystal, *Nuclear Instruments and Methods in Physics*  
806 *Research Section B: Beam Interactions with Materials and Atoms* **267**, 3282 (2009), pro-  
807 ceedings of the Ninth International Conference on Computer Simulation of Radiation Ef-  
808 fects in Solids.
- 809 [87] G. D. Samolyuk, Y. N. Osetsky, and R. E. Stoller, The influence of transition metal solutes  
810 on the dislocation core structure and values of the peierls stress and barrier in tungsten,  
811 *Journal of Physics: Condensed Matter* **25**, 025403 (2012).
- 812 [88] F. H. Featherston and J. Neighbours, Elastic constants of tantalum, tungsten, and molybde-  
813 num, *Physical Review* **130**, 1324 (1963).
- 814 [89] L. Vitos, I. Abrikosov, and B. Johansson, Anisotropic lattice distortions in random alloys  
815 from first-principles theory-art. no. 156401, *PHYSICAL REVIEW LETTERS* **8715**, 6401  
816 (2001).
- 817 [90] Y.-H. Li, H.-B. Zhou, L. Liang, N. Gao, H. Deng, F. Gao, G. Lu, and G.-H. Lu, Transition  
818 from ductilizing to hardening in tungsten: The dependence on rhenium distribution, *Acta*  
819 *Materialia* **181**, 110 (2019).
- 820 [91] G. Bonny, D. Terentyev, A. Bakaev, P. Grigorev, and D. Van Neck, Many-body central force  
821 potentials for tungsten, *Modelling and Simulation in Materials Science and Engineering* **22**,  
822 053001 (2014).
- 823 [92] W. Andreoni and A. Curioni, New advances in chemistry and materials science with cpmd  
824 and parallel computing, *Parallel Computing* **26**, 819 (2000).
- 825 [93] S. Goedecker, M. Teter, and J. Hutter, Separable dual-space gaussian pseudopotentials,  
826 *Phys. Rev. B* **54**, 1703 (1996).
- 827 [94] R. Ayres, G. Shannette, and D. Stein, Elastic constants of tungsten- rhenium alloys from 77  
828 to 298 k, *Journal of Applied Physics* **46**, 1526 (1975).
- 829 [95] Y.-H. Li, H.-B. Zhou, L. Liang, N. Gao, H. Deng, F. Gao, G. Lu, and G.-H. Lu, Transition  
830 from ductilizing to hardening in tungsten: The dependence on rhenium distribution, *Acta*  
831 *Materialia* **181**, 110 (2019).

- 832 [96] S. Wurster, N. Baluc, M. Battabyal, T. Crosby, J. Du, C. García-Rosales, A. Hasegawa, A. Hoff-  
833 mann, A. Kimura, H. Kurishita, et al., Recent progress in r&d on tungsten alloys for divertor  
834 structural and plasma facing materials, *Journal of Nuclear Materials* **442**, S181 (2013).
- 835 [97] N. E. Singh-Miller and N. Marzari, Surface energies, work functions, and surface relaxations  
836 of low-index metallic surfaces from first principles, *Physical Review B* **80**, 235407 (2009).
- 837 [98] M. Gilbert and J.-C. Sublet, Neutron-induced transmutation effects in w and w-alloys in a  
838 fusion environment, *Nuclear Fusion* **51**, 043005 (2011).
- 839 [99] M. R. Gilbert and J. -Ch. Sublet, Scoping of material response under DEMO neutron irra-  
840 diation: Comparison with fission and influence of nuclear library selection, *Fus. Eng. Des.*  
841 **125**, 299 (2017), <https://doi.org/10.1016/j.fusengdes.2017.06.016>.
- 842 [100] F. Hofmann, D. R. Mason, J. K. Eliason, A. A. Maznev, K. A. Nelson, and S. L. Dudarev, Non-  
843 contact measurement of thermal diffusivity in ion-implanted nuclear materials, *Scientific*  
844 *Reports* **5**, 16042 (2015).
- 845 [101] M. R. Gilbert, O. Vilkhivskaya, and J. -Ch. Sublet,  
846 Fusion decay heat validation, FISPACT-II & TENDL-2019, ENDF/B-VIII.0, JEFF-3.3, EAF2010, and IRDFF-II nu  
847 Tech. Rep. UKAEA-CCFE-RE(20)04 (UKAEA, 2020) available from [http://fispact.](http://fispact.ukaea.uk)  
848 [ukaea.uk](http://fispact.ukaea.uk).
- 849 [102] M. R. Gilbert and J. Sublet, Experimental decay-heat simulation-benchmark for 14 MeV  
850 neutrons & complex inventory analysis with FISPACT-II, *Nucl. Fus.* **59**, 086045 (2019).
- 851 [103] MCNP6 user manual, version 2.0 (2017), edited by C.J. Werner, Los Alamos document num-  
852 ber: LA-UR-17-29981, Rev. 0. Further details at <http://mcnp.lanl.gov/>.
- 853 [104] H. Li, C. Draxl, S. Wurster, R. Pippan, and L. Romaner, Impact of *d*-band filling on the  
854 dislocation properties of bcc transition metals: The case of tantalum-tungsten alloys inves-  
855 tigated by density-functional theory, *Phys. Rev. B* **95**, 094114 (2017).
- 856 [105] H. A. Jahn and E. Teller, Stability of polyatomic molecules in degenerate electronic states i  
857 orbital degeneracy, *Proceedings of the Royal Society of London. Series A-Mathematical and*  
858 *Physical Sciences* **161**, 220 (1937).
- 859 [106] A. Luo, D. Jacobson, and K. Shin, Solution softening mechanism of iridium and rhenium in  
860 tungsten at room temperature, *International Journal of Refractory Metals and Hard Mate-*  
861 *rials* **10**, 107 (1991).
- 862 [107] L. Qi and D. Chrzan, Tuning ideal tensile strengths and intrinsic ductility of bcc refractory

- 863 alloys, Physical review letters **112**, 115503 (2014).
- 864 [108] Q. Wang, G. Du, N. Chen, C. Jiang, and L. Chen, Ideal strengths and thermodynamic prop-  
865 erties of w and w-re alloys from first-principles calculation, Fusion Engineering and Design  
866 **155**, 111579 (2020).
- 867 [109] D. Ali, N. Mushtaq, and M. Butt, Investigation of active slip-systems in some body-centered  
868 cubic metals, Journal of materials science **46**, 3812 (2011).
- 869 [110] O. El-Atwani, N. Li, M. Li, A. Devaraj, J. Baldwin, M. M. Schneider, D. Sobieraj, J. S. Wróbel,  
870 D. Nguyen-Manh, S. A. Maloy, et al., Outstanding radiation resistance of tungsten-based  
871 high-entropy alloys, Science advances **5**, eaav2002 (2019).