Anomalous bias factors of dislocations in bcc iron

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Abstract

Dislocation bias factors in bcc Fe have been calculated based on atomistic interaction energy maps on three kinds of dislocations, namely the $a_0/2\langle 111 \rangle\{110\}$ screw, $a_0/2\langle 111 \rangle\{110\}$ and $a_0\langle 100 \rangle\{001\}$ edge dislocations. The results show that the dislocation bias is higher for the $a_0/2\langle 111 \rangle$ edge dislocation than for the $a_0\langle 100 \rangle$ edge dislocation, even though the latter possesses a larger Burgers vector. This indicates the importance of the dislocation core contribution. For the $a_0/2\langle 111 \rangle\{110\}$ screw dislocation, a negative dislocation bias has been obtained, which implies a more efficient absorption of vacancies than of SIAs. The effect of coexistence of both edge- and screw dislocations are assessed by a total bias. A possible complementary mechanism for explaining the long swelling incubation time in bcc metals is suggested and discussed.

Keywords: Dislocation bias, Atomistic calculation, Interaction energy, bcc

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1. Introduction

Classical radiation damage theory underlines the importance of the dislocation bias, which physically is the preference of absorption of self-interstitial atoms (SIAs) over vacancies by dislocation lines [1]. Such a fundamental radiation effect as void swelling was predicted in 1959 by Greenwood, Foreman and Rimmer (GFR) on the basis of the assumption that radiation damage produces 3-D migrating point defects, SIAs and vacancies, which cluster and contribute to the growth of the dislocation density and of the voids. However, void growth is established due to the growing excess of vacancies in the bulk because SIAs are more effectively absorbed by dislocations. Physically, it is explained by the difference in dilatation volume and related stress-field topology between SIA and vacancy. The dislocation bias factor (B_d) is a quantity that defines the efficiency of absorption of these two defects. Following the GFR theory, the B_d was evaluated on the basis of experimentally measured void swelling on Cu and FeCrNi alloy upon 1 MeV electron irradiation, which produces Frenkel pairs exclusively [2, 3]. The dislocation bias was fitted from the rate theory model with experimental parameters to be in the range of 0.02-0.04. Heavy ion and neutron irradiation, resulting in cascade damage, also suggest the B_d to be of the order of a percent [4]. Importantly, the experimentally deduced value of the B_d was neither essentially dependent on the crystallographic structure of material nor its chemical composition, and swelling rate was typically reported to be of the order of 1%/dpa.

A computational assessment of B_d was done by Wolfer [5] who applied Ham's solution [6] and used isotropic elasticity theory to estimate the interaction of the point defects with a non-split edge dislocation in face centered

26 cubic (fcc) Cu. B_d was found to be 0.25, that is, one order of magnitude
 27 higher than the expected value derived from the experimental observations.
 28 Estimations based on even simpler assumptions, accounting for the relax-
 29 ation volume difference, also provide the values for B_d of the order of 0.1-0.3
 30 for different body centered cubic (bcc) and fcc metals [5]. In the above men-
 31 tioned assessment, Wolfer mentioned that further refinement is necessary to
 32 account for the anisotropy in the long-range interaction and the particular
 33 atomic structure of the dislocation core and point defects for the short-range
 34 interaction. The effect of anisotropy of edge dislocation, as well as of the point
 35 defects, on dislocation bias calculations have recently been studied by Seif
 36 and Ghoniem [7] in different metals, where they found that the anisotropy
 37 plays different roles in fcc Cu and bcc Fe. Moreover, we have computed the
 38 B_d for an edge dislocation in fcc Cu by combining a finite element method
 39 with the interaction energy landscape obtained directly from atomistic calcu-
 40 lations [8]. A discrepancy of 30% for B_d was found if the interaction energy
 41 map is taken from elasticity theory, and the interaction near the dislocation
 42 core also revealed strong deviations, sometimes even the sign of the interac-
 43 tion energy was inverted. Those results proved the usefulness of the atomistic
 44 simulations to assess fine details of defect-dislocation interactions which are
 45 not achievable using an elasticity theory framework only.

46 In this work, we investigate defect-dislocation interactions and perform
 47 calculations of B_d in bcc iron (Fe). In particular, we consider the $a_0/2\langle 111 \rangle\{110\}$
 48 screw, $a_0/2\langle 111 \rangle\{110\}$ and $a_0\langle 100 \rangle\{001\}$ edge dislocations. The screw dis-
 49 locations are the primary defects in non-irradiated bcc metals and alloys
 50 including Fe-based steels [9], while under prolonged irradiation a high den-

sity of dislocation loops is established [10, 11]. The latter are of interstitial nature and two types may be present depending on the chemical composition of the Fe-based alloy and irradiation temperature. In pure Fe at 573 K and above, the $a_0 \langle 100 \rangle$ loops of square shape dominate, while at room temperature mostly $a_0/2 \langle 111 \rangle$ loops are present [12, 10]. In commercial Fe-Cr-based steels both types of loops are present in proportions depending on the Cr content [13, 14]. Here, we provide a computational assessment of the dislocation bias factor for all three possible types of dislocations relevant for bcc Fe and its alloys and discuss the implication of the results.

2. Theory and Methods

The numerical method to obtain the dislocation bias has been explained in our previous work [8]. The basic idea is that the flux induced by the diffusion of point defects is described by Fick’s law with a drift term, and it is solved under steady state by employing the dislocation - point defects interaction energies. The interaction energies are obtained both from atomistic calculations and from elastic calculations. For the aim of completeness, the theoretical equations to obtain the bias, the atomistic calculation details and the calculations of the elastic dislocation-PD interactions are briefly explained in the following sections.

2.1. Bias factor

The dislocation bias factor, sometimes referred to as net bias [15], is defined as:

$$B_d = \frac{Z_{\text{SIA}}}{Z_{\text{vac}}} - 1 \quad (1)$$

73 where Z_{SIA} and Z_{vac} are the dislocation capture efficiencies for the SIA and
74 vacancy, respectively. The dislocation capture efficiency is a measure of en-
75 hanced absorption of a specific point defect by the dislocation due to its inter-
76 action with the point defect. The capture efficiency is determined by various
77 factors such as the dislocation structure and resulting stress field, ambient
78 temperature, dislocation density and others [16]. Previous works, dedicated
79 to assessment of dislocation-mediated creep and swelling [17, 5, 18], provide a
80 framework to compute the capture efficiency Z . In the present work, we fol-
81 low the numerical approach proposed by Wolfer [5], which is briefly explained
82 below:

83 A flux of point defects (of a specific kind) approaching the dislocation
84 core is influenced by both the concentration gradient and the gradient of the
85 defect-dislocation interaction energy. It can be described by Fick's law with
86 a drift term:

$$J = -\nabla(DC) - \beta DC \nabla E \quad (2)$$

87 where D is the diffusion coefficient, C is the concentration of point defects,
88 and β is $1/k_{\text{B}}T$ with k_{B} the Boltzmann constant and T the temperature, E
89 is the defect-dislocation interaction energy and the second term on the right
90 hand side is the drift term.

91 A convenient reformulation is used:

$$J = -e^{-\beta E(r,\theta)} \nabla \Psi \quad (3)$$

92 where $\Psi = DCe^{\beta E(r,\theta)}$ is referred to as the diffusion potential function.

93 Applying the steady state condition $\nabla \cdot J = 0$ in Eq.3:

$$\nabla \cdot (-e^{-\beta E(r,\theta)} \nabla \Psi) = 0. \quad (4)$$

Given the interaction energy $E(r, \theta)$ and boundary conditions, Ψ is numerically solved using FEM. In this work, atomistically calculated interaction energies and elastic interaction models are implemented accordingly in different calculations. Following the conventional approach [5], it is assumed that a point defect is absorbed by the dislocation once it crosses into the core region. Hence, the boundary condition at the dislocation core $r = r_0$, is $\Psi_{r_0} = 0$. At the external boundary, limited by the dislocation capture range, $r = R$, the defect concentration $C(r, \theta)$ is a constant. Naturally, the dislocation capture range corresponds to a distance at which the dislocation-defect interaction is negligible. Hence, $\Psi_R = \bar{D}\bar{C}$ is a non-zero constant.

The total current of defects absorbed by the dislocation is then evaluated as:

$$J_{tot} = r_0 \int_0^{2\pi} J_r(r_0, \theta) d\theta \quad (5)$$

where r_0 is the dislocation core radius vector pointing to the core center and $J_r(r_0, \theta)$ is the current to the core.

The dislocation capture efficiency Z in this case is defined as the ratio of the fluxes for a specific point defect, computed with and without taking into account the dislocation-defect interaction, that is $Z = \frac{J}{J_0}$, where J_0 is the flux excluding the dislocation-defect interaction. The dislocation gliding plane is mounted with a mesh, on each mesh point the flux is obtained by FEM implementing the interaction energy on each specific mesh site. The total flux around the dislocation core is then integrated to obtain the capture efficiency. The latter is used to compute the bias factor.

116 A similar numerical method has recently been used to calculate the effect
117 of anisotropy, SIA orientation, and one-dimensional migration mechanism
118 on the bias of edge dislocations in bcc Fe and fcc Cu [7]. Different elastic
119 interaction models have been employed in their work. In the present work, in
120 addition to the anisotropic elastic interaction model, a number of atomistic
121 interaction energy maps are calculated from molecular static calculations and
122 we implement them in the FEM numerical method to obtain the dislocation
123 bias on different types and configurations of dislocation in bcc Fe. Details of
124 the atomistic calculation settings are found in the following section.

125 *2.2. Atomistic calculations*

126 To obtain the atomistic information about the defect-dislocation interac-
127 tion, a model treating a periodic array of dislocations by Osetky and Bacon
128 [19] was applied. In the case of edge dislocations, two half crystals, where
129 one has an extra plane of atoms, are strained to have different lattice param-
130 eters in the direction of the Burgers vector. For the screw dislocation, a rigid
131 shift in the periodic boundary conditions perpendicular to the dislocation
132 line was applied, as suggested by Rodney [20]. In order to model an infi-
133 nite straight dislocation, periodic boundary conditions were applied in the
134 direction of the Burgers vector and in the direction of the dislocation line,
135 while fixed boundary condition was applied in the direction that is normal
136 to the glide plane. Typical dimensions of the simulation cells were about
137 $40 \times 40 \times 4$ nm, where 4 nm is the section along the dislocation line. These
138 dimensions are enough to avoid defect-defect self-interaction via the periodic
139 boundary along the dislocation line, as well as dislocation-dislocation image
140 interactions which could possibly affect the equilibrium core structure. The

total number of atoms in these simulation cells system is about $5 \cdot 10^5$, and the dislocation density is of the order of $5 \cdot 10^{14} \text{ m}^{-2}$.

A vacancy is created by removing one atom from the lattice. A SIA is inserted as a dumbbell containing two atoms aligned along $\{110\}$ directions and placed at a distance of $0.4 a_0$ from each other, centered on a lattice site. A combination of conjugate gradient and quasi static relaxation in the microcanonical ensemble was applied to fully relax the crystal to obtain its total energy. The formation energies with and without the dislocation are calculated and the interaction energy is defined as the difference in formation energy with and without the dislocation. The interaction energy with respect to the dislocation core-defect position provides the interaction energy map for a particular dislocation-defect combination. Note that for a SIA, being a $\langle 110 \rangle$ dumbbell in bcc Fe [21, 22], the particular orientations of the dumbbells also play a role, meaning that all non-equivalent configurations must be assessed.

Most of the calculations were performed using the embedded atom method (EAM) potential derived by Dudarev and Derlet [23]. The potential was developed to account for the specific properties of SIAs and ensures a correct stability of the $\langle 110 \rangle$ dumbbell configuration over the $\langle 111 \rangle$ crowdion, which is of fundamental importance in the present investigation. Despite the fact that the potential was fitted to a number of important properties of bcc Fe, the core of the screw dislocation relaxes to a degenerate three-fold structure. To validate the effect of the core structure, we also employed the EAM potential developed by Mendelev et al. [24], which correctly reproduces both properties of point defects and screw dislocation core structure [25]. The

166 results show that the Z and B_d values computed for the screw dislocation
167 by both potentials are qualitatively in agreement. We therefore choose to
168 use the potential of Dudarev and Derlet, which has one obvious advantage
169 over the Mendelev potential, namely the shorter cut-off range. This cut-off
170 range is crucial for the present study due to the significant computational
171 resources required to assess the interaction energy landscapes in crystals con-
172 taining $5 \cdot 10^5$ atoms while considering six variants of the SIA and three types
173 of dislocations.

174 *2.3. Analytical screw dislocation-defect interaction*

175 In this work we compare the analytical dislocation-defect interactions
176 derived from elasticity theory with the results from atomistic calculations.
177 Given that the Zener anisotropy factor of bcc Fe is 2.3, it is not appropriate to
178 treat it as an isotropic bulk. Therefore, only the anisotropic dislocation model
179 is used in this work to compare with the atomistically calculated dislocation.
180 Our treatment of the anisotropic interaction between edge dislocation and
181 PDs is explained in [8]. All elastic constants C_{ij} used in the elastic interaction
182 models are calculated from molecular static calculations using the same EAM
183 potential as we used in the atomistic interaction energy calculations. In this
184 section the anisotropic interaction model is explained for the interaction of
185 the point defects with a screw dislocation, as briefly described below.

186 Within the framework of linear elasticity theory, the interaction energy
187 between the point defect and a dislocation separated by a distance r is given
188 by

$$E(r) = -\epsilon_{ij}P_{ij}, \quad (6)$$

189 where ϵ is the strain field of the dislocation and P_{ij} are components of the
 190 dipole force tensor P .

191 The anisotropic strain field of a screw dislocation was calculated from
 192 the anisotropic stress field given by [26]. A dipole force tensor describes the
 193 influence that a point defect has on its neighbours. It is calculated following
 194 the standard method by obtaining the Kanzaki force [27, 22, 28]

$$P_{ij} = \sum_{k=1}^N R_i^{(k)} F_j^{(k)}, \quad (7)$$

195 where the summation is over N neighbours of the defect, i and j are the
 196 directions, R is the i th component of the vector joining atom k and the
 197 central atom, and F is the Kanzaki force.

198 The Kanzaki force for our EAM potential is directly calculated from
 199 molecular statics following the detailed descriptions in [27, 28]. The dipole
 200 tensor of the vacancy and of the six different configurations of $\langle 110 \rangle$ dumb-
 201 bells are calculated and then used individually in the interaction calculation
 202 of Eq.6. The interaction energy of a screw dislocation with a SIA is pre-
 203 sented by the average interaction energies of the screw dislocation with the
 204 six dumbbell orientations.

205 **3. Results and discussions**

206 *3.1. Dislocation core radius*

207 A standard way to define the dislocation core is to assign a cylinder with
 208 a radius (henceforth core radius) within which a spontaneous absorption of a
 209 point defect is expected. The core radius is therefore defined by the strength

210 and topology of the dislocation-defect interaction. In the analytical expres-
 211 sion, the capture efficiency is predicted to be core radius dependent [29].
 212 In our case, the interaction energy is obtained from atomistic calculations,
 213 therefore the core radii must be chosen carefully. To begin, we analysed the
 214 sensitivity of the capture efficiency with regard to the dislocation core radius,
 215 assuming that the core is represented by a cylinder. Fig.1 shows Z_{SIA} and
 216 Z_{vac} calculated using the energy landscape from isotropic elasticity theory
 217 and atomistic simulations, for the $\langle 100 \rangle$ edge dislocation as a function of
 218 r_0 . The integration was performed by taking 873 K as ambient temperature
 219 and assigning the dislocation density to 10^{14} m^{-2} . As one sees, the capture
 220 efficiency Z values are strongly dependent on the choice of r_0 , especially in
 221 the case of the SIA. When r_0 is larger than around 24 Å, the interaction
 222 energy becomes too weak to overcome the influence of the thermal diffusion.
 223 To assign some physical meaning to the dislocation core radius, we used an
 224 interaction energy gradient threshold [7], resulting in different dislocation
 225 radii for different species. Inside the radius all defects of that species are
 226 absorbed by the dislocation. The dislocation core radius is thus determined
 227 as where the gradient of the interaction energy, scaled by the Burgers vector,
 228 is comparable to the thermal energy:

$$b\nabla|E| = k_{\text{B}}T. \quad (8)$$

229 This criterion is applied to obtain the capture radii on each individual
 230 combination of defects and dislocation, in the atomistic interaction maps
 231 and in the elastic interaction maps. The average interaction gradient on
 232 the radius is used. However, in the here used temperature range, the $\nabla|E|$
 233 difference is not significant, and we therefore use the radii corresponding to

234 $T=873$ K for all temperatures. This results in core radii as shown in Tab.1.

235 3.2. Bias factor for edge dislocations

236 While in most of the bcc metals SIAs typically occupy $\langle 111 \rangle$ crowdion
237 configurations [30], a $\langle 110 \rangle$ dumbbell is the most energetically favourable
238 configuration in bcc Fe due to its magnetism [22]. Occupying such a configu-
239 ration, the SIA performs 3D migration by translation-rotation jumps [21, 31].
240 While the SIA migrates towards the dislocation core it will undergo constant
241 change of the particular orientation of its $\langle 110 \rangle$ axis. It is therefore impor-
242 tant to assess the interaction energy landscape for all possible variants of
243 SIA-dislocation orientations. For the $\langle 100 \rangle$ dislocation, the high symmetry
244 results in three orientations of the $\langle 110 \rangle$ dumbbells. However, the $1/2\langle 111 \rangle$
245 dislocations retain a high asymmetry. This has been taken into account in
246 our calculations. In order to represent the interaction energy for the constant
247 change of the particular orientation of a $\langle 110 \rangle$ dumbbell, the average interac-
248 tion energy on each lattice site is calculated from each individual interaction
249 energy map of a given orientation. The near core interaction fields are plot-
250 ted for both types of edge dislocation, including the atomistic calculation
251 and elastic anisotropic models. The profile of anisotropic interactions of the
252 $\langle 100 \rangle$ type with the point defects, shown in Fig.2 as C and D, resemble the
253 atomistic interactions, shown in Fig.2 as A and B, very well, with weaker
254 interactions on each individual site. On the other hand, the atomistic inter-
255 action profiles for the $1/2\langle 111 \rangle$ type, shown in Fig.3 as A and B, do not have
256 high similarity to either of the analytical interaction models.

257 The bias calculated from those interaction maps are shown in Fig.4 under
258 different temperatures with a fixed dislocation density of 10^{13} m^{-2} . Compar-

259 ing the bias obtained from the two types of dislocation using the atomistically
 260 calculated interaction maps, a larger bias factor is observed for the $1/2\langle 111 \rangle$
 261 type than for the $\langle 100 \rangle$ type. However, the opposite result is obtained from
 262 the elastic anisotropic models. That is, the bias factors for the $\langle 100 \rangle$ type
 263 are larger than those for the $1/2\langle 111 \rangle$ type. This follows the argument based
 264 on the conventional estimation of B_d , that the larger the Burgers vector,
 265 the higher the bias factor should be [32]. However, such a view neglects
 266 particular details of the defect-dislocation interaction in the vicinity of the
 267 dislocation core, and the argument was not in agreement with the exper-
 268 iment carried out by Katoh [33] under neutron irradiation. By comparing
 269 Fig.2 A, B and Fig.3 A, B, the attractive regions (negative interaction energy
 270 region) in the SIA-dislocation interaction maps, which are marked as subplot
 271 B in both figures, are much more significant than the attractive regions in
 272 the vacancy-dislocation interaction maps, which are marked as subplot A.
 273 This difference ensures a stronger sink capture efficiency for SIAs than for
 274 vacancies in both cases. However, the repulsive region of the SIA-dislocation
 275 interaction is more pronounced for the $\langle 110 \rangle$ (Fig.2) compared to that for the
 276 $1/2\langle 111 \rangle$ (Fig.3) dislocations. The large repulsive region screens out SIAs ap-
 277 proaching from that side, resulting in a relatively small dislocation bias for
 278 the $\langle 100 \rangle$ type. As the sink capture efficiency values show in Fig.6, it is the
 279 diffusion of SIAs to the dislocation that dominates the difference in the dislo-
 280 cation bias factors for the two edge dislocations. It is worth mentioning that
 281 even though the atomistic- and anisotropic elastic B_d values for the $1/2\langle 111 \rangle$
 282 are similar, this is coincidental considering the significant differences in the
 283 individual capture efficiencies.

284 3.3. Bias factor for the screw dislocation

285 The screw dislocation is of primary interest since it is the basic extended
286 lattice defect in non-irradiated bcc metals. The interaction energies obtained
287 from the atomistic calculations and the anisotropic analytical models are
288 shown in Fig.5. Three-fold interaction symmetries are obtained. The main
289 difference between the atomistic calculated interaction energy and the analytical
290 interaction energy is in the core region. For both vacancy and SIA cases,
291 the interactions obtained from the atomistic calculations are much stronger
292 and longer in range than the analytical ones. Comparing Fig.5 with Fig.2 and
293 Fig.3, the interaction energy of the screw dislocation is much weaker than
294 that of the edge dislocations. The capture efficiencies have been computed
295 for the screw dislocation as a function of temperature and dislocation density,
296 as shown in Fig.6 and Fig.7. The results show that Z_{vac} are larger than
297 Z_{SIA} in all conditions tested. That is to say, the B_d of a screw dislocation
298 calculated using atomistic interactions are all negative. In the SIA case the
299 reason for this is that the flux approaching the core is partly repelled by the
300 strong compressive fields around it, while in the vacancy case there are no
301 such strong repelling fields and the attractive interaction energies between
302 the two cases are comparable. This results in a larger net flux into the core
303 for the vacancy than for the SIA. The same pattern of the interaction energy
304 and the same trend for the dislocation bias are observed using the Mendelev
305 potential, with even stronger repulsion zones and therefore even larger negative
306 capture efficiency and bias values. The negative bias implies that more
307 vacancies than SIAs are absorbed in the dislocations. The supersaturation
308 of the SIAs left in the bulk should help to build up edge dislocation loops or

309 help the growth of existing loops.

310 Furthermore, the B_d calculated using the analytical interactions are zero
311 within the precision limits. Given the fact that there is no displacements on
312 the plane perpendicular to the dislocation line in a screw dislocation, only a
313 very weak stress field from the anisotropy on this plane exert an influence on
314 any point defects. It is hence reasonable for the analytical interactions not
315 to have any impact on the preferential absorption rate. On the other hand,
316 the linear elastic description breaks down in the core region and hence the
317 atomistic interaction is more realistic. The negative bias implies that a screw
318 dislocation preferentially absorbs vacancies. Nonetheless, in a real irradiated
319 material, the screw dislocations and edge dislocations usually coexist [9].
320 More discussions are presented in the next subsection.

321 *3.4. Comparison of screw- and edge dislocations*

322 Fig.6 and Fig.7 show capture efficiencies Z as a function of temperature
323 and dislocation density, respectively. Fig.6 shows data produced by taking
324 the dislocation density to be 10^{13} m^{-2} , while the data in Fig.7 corresponds to
325 773 K. The results reveal that Z grows as dislocation density increases and
326 temperature decreases. Such trends are consistent with common expecta-
327 tions, since temperature effectively 'weakens' the interaction energy gradient,
328 while the dislocation density controls the available sink volume. The same
329 trends were found in our recent study dedicated to the calculation of B_d in
330 fcc Cu[8].

331 For the edge dislocations, Z_{SIA} are larger than Z_{vac} , while it is the opposite
332 for the screw dislocation: Z_{SIA} are smaller than Z_{vac} . As we mentioned before,
333 the coexistence of edge- and screw dislocations contribute to macroscopic

334 effects such as swelling. Therefore it is more reasonable to look at the total
 335 effect of the Z values. In order to estimate the joined influence from them,
 336 we define a total dislocation bias. It is assumed that the densities of the
 337 three different types of dislocations, namely $1/2\langle 111 \rangle$ screw, $1/2\langle 111 \rangle$ edge
 338 and $\langle 100 \rangle$ edge, are a , b and c respectively, and that the point defects can be
 339 absorbed by any of them, then the total bias is defined as

$$B_d = \frac{aZ_{\text{SIA}}^{SD} + bZ_{\text{SIA}}^{\langle 111 \rangle} + cZ_{\text{SIA}}^{\langle 100 \rangle}}{aZ_{\text{vac}}^{SD} + bZ_{\text{vac}}^{\langle 111 \rangle} + cZ_{\text{vac}}^{\langle 100 \rangle}} - 1 \quad (9)$$

340 where SD represents the screw dislocation, $\langle 111 \rangle$ is the $1/2\langle 111 \rangle$ type
 341 edge dislocation and $\langle 100 \rangle$ represents the $\langle 100 \rangle$ type edge dislocation.

342 The fact that $Z_{\text{vac}} > Z_{\text{SIA}}$ in the screw dislocation case counteracts the bias
 343 from the edge dislocation. This balancing of the total dislocation bias could
 344 indicate a contributing mechanism for the swelling incubation in bcc metals,
 345 as explained briefly below.

346 Following the analysis of bias factors for different types of dislocations, we
 347 suggest that the microstructure-driven interplay balancing the sinks of point
 348 defects could be the feature defining the onset of stable (i.e. steady-state)
 349 void swelling in bcc metals. The above mentioned interplay with progress-
 350 ing irradiation is expressed qualitatively in the following. The unirradiated
 351 material contains predominantly screw dislocations. During irradiation, the
 352 edge dislocation population will be built up in the form of dislocation loops,
 353 whose properties will approach that of straight edge dislocations when large
 354 enough. With increasing irradiation dose, the total length of edge disloca-
 355 tions will keep increasing. Thus, at a certain dose, the positive bias of edge
 356 dislocations will outbalance the negative bias of screw dislocations and a bias

driven swelling sets in, according to Eq.9. Further investigation is needed to put this scenario on a firm quantitative ground, specifically the bias of 2D dislocation loops would need to be quantified, and the irradiation-induced microstructure evolution would need to be explicitly modelled. However, it has been previously noted that the transition from an incubation region to swelling is linked to a qualitative change in the microstructure as well as the absolute swelling correlates with the density of radiation-induced dislocation loops [34, 35, 33], and the above suggested scenario is well in line with those findings.

4. Conclusions

In this work we have performed a computational assessments of capture efficiencies and bias factors for screw- and edge dislocations in bcc Fe. B_d was computed by combining information from atomistic simulations and the finite element calculation approach. Atomistic calculations were used to obtain the interaction energy landscape for SIA/vacancy-dislocation interactions.

An unexpected result was obtained for the $1/2\langle 111 \rangle$ edge dislocation, whose B_d was found to be higher than that for the $\langle 100 \rangle$ edge dislocation. At first glance this result contradicts the general perception that B_d is proportional to the dislocation stress-field and hence proportional to the absolute value of the Burgers vector. The atomistic calculations of the interaction landscapes show that the near core region is essentially different for the two edge dislocations. The stronger and broader repulsive region in the $\langle 100 \rangle$ edge-SIA interaction map plays an important role in screening out SIAs approaching from that side and thus explains the unexpectedly low B_d for the

381 $\langle 100 \rangle$ edge dislocation.

382 For the screw dislocation, negative bias values ($Z_{\text{vac}} > Z_{\text{SIA}}$) were obtained
383 using atomistic interaction energies and negligible bias was obtained using
384 the analytical models. These results can be readily understood by comparing
385 the interaction energy landscapes that the atomistic and analytical models
386 predict. For the atomistic case, three repulsion zones drive away SIAs but
387 not vacancies. For the analytical case, the interaction energies are almost
388 negligible.

389 The effect of dislocation density on Z was assessed for the temperature
390 range 623-823 K, which is typical for the application of Fe-based ferric steels
391 (e.g. high Cr steels) in the nuclear industry where the swelling phenomenon
392 is a practical issue. It is found that while a temperature increase leads to the
393 reduction of Z , the increase of dislocation density causes an increase of Z .
394 A combination of the Z values from edge- and screw dislocations is used to
395 assess the joint influence. A possible supplementary mechanisms of the long
396 incubation time in the bcc material has been suggested from the point of the
397 view of the joint dislocation bias.

398 **Acknowledgements**

399 This work is supported by the national project on Generation IV reactor
400 research and development (GENIUS) in Sweden, by the Göran Gustafsson
401 Stiftelse and by the European Atomic Energy Community's (Euratom) Sev-
402 enth Framework Programme FP7/2007-2013 under grant agreement No.604862
403 (MatISSE project). This work contributes to the Joint Program on Nuclear
404 Materials (JPNM) of the European Energy Research Alliance (EERA). The

405 Swedish National Infrastructure for Computing (SNIC) sources are used for
406 part of this work.

407 [1] G. Greenwood, A. Foreman, D. Rimmer, J. Nucl. Mater. 1 (1959) 305–
408 324.

409 [2] S. Golubov, B. Singh, H. Trinkaus, Philos. Mag. A 81 (2001) 2533–2552.

410 [3] G. Walters, J. Nucl. Mater. 136 (1985) 263–279.

411 [4] F. Garner, M. Toloczko, B. Sencer, J. Nucl. Mater. 276 (2000) 123–142.

412 [5] W. Wolfer, J. Comput. Aided Mater. Des. 14 (2007) 403–417.

413 [6] F. S. Ham, J. Appl. Phys. 30 (1959) 915–926.

414 [7] D. Seif, N. Ghoniem, J. Nucl. Mater. 442 (2013) S633 – S638.

415 [8] Z. Chang, P. Olsson, D. Terentyev, N. Sandberg, J. Nucl. Mater. 441
416 (2013) 357–363.

417 [9] J. Nagakawa, A. Sato, M. Meshii, Philos. Mag. 32 (1975) 1107–1128.

418 [10] S. J. Zinkle, B. N. Singh, J. Nucl. Mater. 351 (2006) 269–284.

419 [11] N. Yoshida, M. Kiritani, F. Eiichi Fujita, J. Phys. Soc. Jpn. 39 (1975)
420 170–179.

421 [12] M. Jenkins, C. English, B. Eyre, Philos. Mag. A 38 (1978) 97–114.

422 [13] S. Porollo, A. Dvoriashin, A. Vorobyev, Y. V. Konobeev, J. Nucl. Mater.
423 256 (1998) 247–253.

- 424 [14] D. Gelles, J. Nucl. Mater. 108 (1982) 515–526.
- 425 [15] W. Wolfer, R. Konings, Comprehensive nuclear materials. Oxford: El-
426 sevier (2012) 1–45.
- 427 [16] L. Mansur, A. Brailsford, W. Wolfer, J. Nucl. Mater. 105 (1982) 36–38.
- 428 [17] P. Heald, Philos. Mag. 31 (1975) 551–558.
- 429 [18] W. Wolfer, M. Ashkin, J. Appl. Phys. 47 (1976) 791–800.
- 430 [19] Y. N. Osetsky, D. J. Bacon, Modell. Simul. Mater. Sci. Eng. 11 (2003)
431 427.
- 432 [20] D. Rodney, Acta Mater. 52 (2004) 607–614.
- 433 [21] R. Johnson, Phys. Rev. 134 (1964) A1329.
- 434 [22] C. Domain, C. Becquart, Phys. Rev. B 65 (2001) 024103.
- 435 [23] S. Dudarev, P. Derlet, J. Phys.: Condens. Matter 17 (2005) 7097.
- 436 [24] M. Mendelev, S. Han, D. Srolovitz, G. Ackland, D. Sun, M. Asta, Philos.
437 Mag. 83 (2003) 3977–3994.
- 438 [25] J. Chaussidon, M. Fivel, D. Rodney, Acta Mater. 54 (2006) 3407–3416.
- 439 [26] Y. Chou, T. Mitchell, J. Appl. Phys. 38 (1967) 1535–1540.
- 440 [27] G. Simonelli, R. Pasianot, E. Savino, Phys. Rev. B 50 (1994) 727.
- 441 [28] E. Hayward, C. Deo, B. P. Uberuaga, C. N. Tomé, Philos. Mag. 92
442 (2012) 2759–2778.

- 443 [29] L. K. Mansur, Nucl. Technol. 40 (1978) 5–34.
- 444 [30] D. Nguyen-Manh, A. Horsfield, S. Dudarev, Phys. Rev. B 73 (2006)
445 020101.
- 446 [31] F. Willaime, C. Fu, M. Marinica, J. Dalla Torre, Nucl. Instr. Meth.
447 Phys. Res. B 228 (2005) 92–99.
- 448 [32] R. Bullough, M. Wood, E. Little, ASTM special technical publication
449 (1981) 593–609.
- 450 [33] Y. Katoh, A. Kohyama, D. S. Gelles, J. Nucl. Mater. 225 (1995) 154–
451 162.
- 452 [34] E. Little, R. Bullough, M. Wood, Proceedings of the Royal Society of
453 London. Series A, Mathematical and Physical Sciences (1980) 565–579.
- 454 [35] Y. V. Konobeev, A. Dvoriashin, S. Porollo, F. A. Garner, J. Nucl. Mater.
455 355 (2006) 124–130.

Table 1: Dislocation core radii that are used in this work.

	Atomistic		Elastic model	
	vacancy	SIA	vacancy	SIA
Edge $\langle 100 \rangle$	9 Å	12.5 Å	5 Å	8 Å
Edge $1/2\langle 111 \rangle$	8 Å	13 Å	5 Å	8 Å
Screw $1/2\langle 111 \rangle$	6.5 Å	8 Å	5 Å	7 Å

Figure 1: The effect of the dislocation core radii on the capture efficiencies of edge dislocation $\langle 100 \rangle \{001\}$ type. Atomistic and analytical represent the atomistic and analytical interaction energy.

Figure 2: Interaction energies with the edge dislocation of $\langle 100 \rangle \{001\}$ type. A. the atomistically calculated interaction between the dislocation and a vacancy; B. the atomistically calculated average interaction between the dislocation and all the nonequivalent $\langle 110 \rangle$ SIAs; C. the anisotropic interaction energies between the dislocation and a vacancy; D. the anisotropic interaction energies between the dislocation and a $\langle 110 \rangle$ SIA.

Figure 3: Interaction energies with the edge dislocation of $1/2\langle 111 \rangle$ $\{110\}$ type. A. the atomistically calculated interaction between the dislocation and a vacancy; B. the atomistically calculated average interaction between the dislocation and all the nonequivalent $\langle 110 \rangle$ SIAs; C. the anisotropic interaction energies between the dislocation and a vacancy; D. the anisotropic interaction energies between the dislocation and a $\langle 110 \rangle$ SIA.

Figure 4: The dislocation bias of both types edge dislocations. $\langle 100 \rangle$ and $\langle 111 \rangle$ represent $\langle 100 \rangle \{001\}$ type and $1/2\langle 111 \rangle \{110\}$ type, respectively.

Figure 5: Interaction energies with the screw dislocation of $1/2\langle 111 \rangle$ $\{110\}$ type. A. the atomistically calculated interaction between the dislocation and a vacancy; B. the atomistically calculated average interaction between the dislocation and all the nonequivalent $\langle 110 \rangle$ SIAs; C. the anisotropic interaction energies between the dislocation and a vacancy; D. the anisotropic interaction energies between the dislocation and a $\langle 110 \rangle$ SIA.

Figure 6: Comparison of capture efficiencies of the three kinds of dislocations as a function of temperature. SD and ED represent screw dislocation and edge dislocation respectively.

Figure 7: Comparison of the capture efficiencies of the three kinds of dislocations as a function of temperature. SD and ED represent screw dislocation and edge dislocation respectively.