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Assessment of the dislocation bias in fcc metals and extrapolation to austenitic steels

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Abstract

A systematic study of dislocation bias has been performed using a method that combines atomistic and elastic dislocation-point defect interaction models with a numerical solution of the diffusion equation with a drift term. Copper, nickel and aluminium model lattices are used in this study, covering a wide range of shear moduli and stacking fault energies. It is found that the dominant parameter for the dislocation bias in fcc metals is the width of the stacking fault ribbon. The variation in elastic constants does not strongly impact the dislocation bias value. As a result of this analysis and its extrapolation, the dislocation bias of the widely applied austenitic stainless steels of 316 type is predicted to be about 0.1 at temperature close to the swelling peak (815 K) and typical dislocation density of 10^{14} m^{-2} . This is in line with the bias calculated using the elastic interaction model, which

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implies that the prediction method can be used readily in other fcc systems even without EAM potentials. By comparing the bias values obtained using atomistic- and elastic interaction energies, about 20% discrepancy is found, therefore a more realistic bias value for the 316 type alloy is 0.08 in these conditions.

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

1. Introduction

Irradiation of metals can significantly alter their properties such as dimensional stability. Since void swelling was first discovered under neutron irradiation in 1967 [1], intensive efforts have been applied to characterize and understand the mechanisms behind its emergence. The preferential absorption of self interstitials (SIA) at dislocations, first suggested by Greenwood, Foreman and Rimmer [2], has been incorporated in rate theory models for swelling as a possible driving force for radiation induced dimensional change. As the SIAs are absorbed more efficiently at dislocations than vacancies, a net excess number of vacancies is accumulated in the bulk and either condense as new voids or increase the volume of existing voids by flowing into them. The higher absorption rate is caused by the stronger attraction of an SIA to a dislocation as compared with a vacancy. The parameter that characterizes the difference in the absorption efficiency is the bias factor.

Various swelling models have been constructed based on the micro structure evolution under irradiation. The first and probably still the most pop-

17 ular model is so-called the standard rate theory (SRT) model, based on the
 18 concept of sink bias [3, 4, 5]. It is formulated within the framework of the
 19 mean field type chemical reaction rate theory. The model implies that the
 20 irradiation produces only Frenkel pairs created evenly in space and time, and
 21 voids are neutral sinks absorbing both vacancies and SIAs equally. The main
 22 driving force for swelling, therefore, is the dislocation bias. A more system-
 23 atic and detailed model, the Bullough, Eyre and Krishan (BEK) model [6],
 24 was formulated on the extension of the SRT model. It took into account the
 25 vacancy loops produced by vacancy emission and biased interstitial absorp-
 26 tions. In this model, the dislocation bias (B_d) is still the dominant driving
 27 force for the irradiation-induced void swelling [4]. To model the effects of
 28 high energetic neutron irradiation, the more sophisticated production bias
 29 model [7, 8, 9] has been proposed. It characterises the damage production
 30 and annihilation more accurately than the previous two models because it
 31 incorporates generation of mobile SIA clusters known to be produced directly
 32 in displacement cascades. The 1D migrating SIA clusters play an important
 33 role in this model, and the dislocation are biased in absorption of both SIAs
 34 and mobile SIA clusters.

35 The dislocation bias factor is thus an essential parameter for the present
 36 computational models for void swelling. The study of the bias factor is mo-
 37 tivated by both the fundamental scientific interest and technological need
 38 to tailor candidate materials for the high swelling resistance as required for
 39 the next generation of nuclear reactors. To assess the propensity in regards

40 to void swelling of those candidate structural materials, the computational
41 evaluation of dislocation bias is one of the first steps to be done before the
42 actual irradiation testing. However, the dislocation bias factors vary signifi-
43 cantly with crystalline structure, material composition, irradiation tempera-
44 ture and dislocation density. Therefore an efficient and repeatable approach
45 is required to evaluate the dislocation bias since the conditions change con-
46 tinuously under irradiation. Various analytical studies based on elasticity
47 theory have been carried out [10, 11, 12, 13] to evaluate the dislocation bias,
48 however as Wolfer pointed out [14], the frequently used isotropic elastic the-
49 ory is not enough to describe the elastic interactions between dislocation and
50 migrating defects, and the near-dislocation-core interaction from continuum
51 elasticity theory is insufficient. Furthermore, the dislocation bias of an alloy
52 is not available from a purely analytical approach.

53 In our previous work [15], a method that combines the interaction en-
54 ergy from atomistic calculations and the bias calculation from a numerical
55 finite element method (FEM) was shown to be an improvement of the an-
56 alytical method, and it gives a reasonable prediction of the dislocation bias
57 in fcc Cu. A similar method has been also used recently to study the effect
58 of anisotropy, SIA orientation, and one-dimensional migration mechanism
59 on the bias of edge dislocations in bcc Fe and fcc Cu [16]. However, the
60 calculation of atomistic interaction energy in an alloy are hindered by the
61 development of the alloy semi-empirical embedded atom method (EAM) po-
62 tential and by the complexity of local chemical composition. In the present

work, three representative face centered cubic (fcc) model lattices are chosen for a systematic study of the dislocation bias in fcc crystals. Atomistic simulations with empirical potentials are applied to map the dislocation-point defect (PD) interaction energy and a numerical solution using the finite element method is obtained for the diffusion equation in order to estimate capture efficiencies and the dislocation biases in Cu, Ni and Al. By manipulating the anisotropic elastic interaction models (The elastic interaction models are always assumed to be anisotropic in this paper, unless otherwise stated), a systematic study is performed in order to evaluate the impacts of the stacking fault energy (SFE) and elastic constants on the dislocation bias. The dislocation bias of a typical austenitic steel is then predicted by extrapolating the results obtained for pure fcc metals and taking the experimentally known elastic properties and SFE.

2. Theory and Methods

A detailed description of the methods employed in this work is presented in [15]. The main idea is to solve the diffusion equation with a drift term numerically using an interaction map which describes the interaction profile of dislocation and PDs. The diffusion equations are solved by applying the finite element method. The capture efficiency is defined as the ratio of PD fluxes with and without interaction with the dislocation, i.e. $Z = \frac{J}{J_0}$. J is the flux of PDs including the interaction with the dislocation and J_0 is the flux excluding the interaction. The dislocation bias is defined as $B_d = \frac{Z_{SIA}}{Z_{vac}} - 1$.

85 By using atomistic simulations we obtained the interaction energy be-
 86 tween a dislocation and PDs in an fcc metal without suffering from the lim-
 87 itations imposed by elasticity theory. Comparison of atomistic and elastic
 88 interactions shows about the reliability of the elastic description. The elastic
 89 interaction model is built following the detailed description in our previous
 90 work [15]. All elastic constants used in the models are determined by the
 91 EAM potentials via molecular static calculations. The elastic interaction en-
 92 ergies are then used to obtain the dislocation bias following the same method-
 93 ology as used for the atomistic interaction energies. It worth noticing that
 94 for the analytical solution in the framework of linear elasticity theory, a dis-
 95 location in a fcc crystal is usually treated as a single core line with $a_0/2\langle 110 \rangle$
 96 Burgers vector, even though the dislocations in fcc metals are characterized
 97 by splitting into two partials. To mitigate this problem, a two partial dislo-
 98 cation model is constructed by superimposing the interaction energy of two
 99 individual dislocation cores each with a Burgers vector of $a_0/4\langle 110 \rangle$, sepa-
 100 rated by a distance which is the same as in the atomistic interaction energy
 101 profiles. This ignores the screw component of each partial [17], but since that
 102 component mainly induces shear deformations in the lattice, it is expected
 103 to interact only weakly with the PDs.

104 In the atomistic simulations, the computational model containing an edge
 105 dislocation is set up by misfitting two half crystal lattices so that the upper
 106 one contains an extra half plane, as described in detail in [18]. They join along
 107 the dislocation slip plane and thus an edge dislocation with $b = a_0/2\langle 110 \rangle$ is

108 generated in the center. The simulation boxes in Cu, Ni and Al are about
 109 $70a_0 * 7a_0 * 76a_0$ in the $[110]$, $[-11-2]$ and $[-111]$ directions respectively. In
 110 order to model an infinite straight dislocation, periodic boundary conditions
 111 were applied in the direction of the Burgers vector and in the direction of
 112 the dislocation line, while a fixed boundary conditions were applied in the
 113 direction that is normal to the glide plane. A typical dislocation density in the
 114 simulation cell in this case is $1.5 \cdot 10^{15} \text{ m}^{-2}$. A combination of the conjugate
 115 gradient and quasi static relaxation with constant volume was applied to
 116 relax the crystal and obtain the equilibrium structure of the dislocation.

117 A vacancy is created by removing one atom from the lattice. An SIA is
 118 inserted as a dumbbell containing two atoms aligned along $\{100\}$ directions
 119 and placed at a distance of $0.2 a_0$ from each other, centred on a lattice site.
 120 Given the three different orientation of the dumbbells, we performed calcu-
 121 lations on each configuration, and used the average of these three obtained
 122 energies as input for the bias calculation. The interaction energy is defined
 123 as the difference between the formation energy of a PD with and without a
 124 dislocation. The interaction maps are calculated by positioning PDs on each
 125 lattice site.

126 Large scale molecular statics calculations were performed using the DYMOKA
 127 code [19]. Full interaction energy landscapes around the dislocation core for
 128 PDs were obtained using EAM potentials for Cu [20], Ni [21] and Al [22].
 129 The potentials reproduce the properties of defects in the bulk crystal in good
 130 agreement with reference data obtained from experiments and *ab initio* cal-

131 culations as shown in Tab.1.

132 Due to the splitting of the dislocation in an fcc lattice, the dislocation-PD
133 interaction range is relatively large, hence the fixed and periodic boundary
134 conditions should be carefully treated. The artificial contribution to the
135 interaction energy originated from the strain induced by the fixed boundary
136 conditions has been removed from the atomistic interaction energy maps as
137 described below.

138 Atoms located near the fixed atomic layers can not fully relax thus in-
139 troducing non-physical strain, which in turn affects the interaction energy.
140 Several positions were chosen along the direction normal to the dislocation
141 glide plane to compute the PD formation energy with the strained lattice
142 constants. Later, these data are used for the correction that removes the
143 impact of the fixed boundary conditions. To eliminate the contribution to
144 the interaction energy from the image dislocations, the isotropic elastic in-
145 teraction model is applied to create the two neighbouring image dislocations
146 whose contribution is correspondingly subtracted.

147 To obtain the bias numerically from FEM, it is unavoidable to deal with
148 the integration area which is denoted as the core region of the dislocation.
149 Inside the core boundary, the PDs are assumed to be absorbed and therefore
150 the PD concentrations are zero. A dislocation is usually seen as a cylinder for
151 simplification and the core radius is regarded as a variable in the previous
152 bias calculations [23]. We have studied the impacts of the choice of the
153 core geometry in a previous work [15]. In this work, considering that one

154 integration circle around both partial cores may not be representative for
 155 a large partial dislocation splitting such as in the austenitic alloy, we use
 156 two circles to represent the two partial dislocation core regions separately.
 157 To assign some physical meaning to the dislocation core radius we used an
 158 interaction energy gradient threshold [16]:

$$b\nabla|E| \geq k_{\text{B}}T \quad (1)$$

159 The radii determined by this criterion are different for different defect species
 160 and different interaction profiles. In our calculations for Cu, Ni and Al,
 161 the radii in atomistic interaction energies are 12 Å and 6 Å for SIAs and
 162 vacancies, respectively, while 8 Å and 4 Å are used in elastic interaction
 163 maps for SIAs and vacancies, respectively.

164 In order to study the influence of dislocation densities on the bias calcu-
 165 lation, different dislocation densities were generated by expanding the region
 166 described by the atomistic interaction and matching it to the anisotropic elas-
 167 tic solution in the outskirts. In this manner the near core region is described
 168 as accurately as possible while at the same time one can obtain dislocation
 169 densities on the same order of magnitude as in technological materials.

170 3. Results

171 3.1. Interaction energies

172 The interaction energies of PDs with an edge dislocation have been cal-
173 culated in Cu, Ni and Al. The comparison between anisotropic elastic and
174 atomistically obtained interaction energy map reveals that the elastic descrip-
175 tions of the atomistic features in the dislocation core region is insufficient, as
176 shown in Fig.1, Fig.2 and Fig.3 for Cu, Ni and Al, respectively. In these fig-
177 ures, sub-plots A and B are, respectively, atomistic- and elastic interaction of
178 dislocation and SIAs. C and D represent the vacancy-dislocation interaction
179 in the atomistic- and elastic models. The difference between A and B, and
180 between C and D are shown in E and F, respectively, in order to have a more
181 detailed view of where the divergence emerge. The difference attributed to
182 the insufficient description of the elastic core model.

183 In the atomistic calculations, the dislocation splits into two partials fol-
184 lowing the energy minimization in accordance with Frank’s rule. In copper
185 the stacking fault energy is $E_{\text{SF}}=44.4 \text{ mJ/m}^2$. The splitting distance result-
186 ing from the stacking fault is calculated to be $30 \text{ \AA}$ according to elasticity
187 theory [24] $d = \frac{Gb^2(2+\nu)}{8\pi(1-\nu)E_{\text{sf}}}$ where G is shear modulus, b is Burgers vector, ν
188 is the Poisson ratio and E_{sf} is the stacking fault energy. In our atomistic
189 calculations, the positions of the two partials are determined by identifying
190 atoms with maximal energies, which would occur in the dislocation core.
191 This gives a distance of $35 \text{ \AA}$ between the two partials. In the case of nickel,
192 the $E_{\text{SF}}=113 \text{ mJ/m}^2$ which corresponds to a splitting distance of $19 \text{ \AA}$ from

193 theoretical calculation while 22 Å is found from the atomistic calculations.
 194 For Al, the $E_{\text{SF}}=129.4$ mJ/m² which leads to a partial distance of 9 Å while
 195 the calculated distance is 14 Å. We consider these results to be in acceptable
 196 agreement and the regular underestimation of the stacking fault ribbon is
 197 due to the insufficiency of the isotropic elasticity theory.

198 3.2. B_d calculations and predictions

199 The bias factors computed using the atomistic interaction energies, ac-
 200 counting for the boundary conditions and image dislocations, are shown in
 201 Fig.4. The results corresponding to the dislocation density of 10^{14} m⁻² are
 202 obtained for the temperature range 603 – 1000 K. At the same temperature
 203 and dislocation density, $B_d^{\text{Al}} > B_d^{\text{Ni}} > B_d^{\text{Cu}}$ is observed. The dislocation bias,
 204 meanwhile, is proportional to the swelling rate of the material according to
 205 the SRT model. Under this presumption, these results suggest that copper
 206 should exhibit a lower swelling rate than nickel and aluminium under the
 207 same irradiation conditions. This is in agreement with neutron irradiation
 208 experiments described in [25] that shows that nickel is more prone to irradi-
 209 ation induced swelling as compared to copper. An analysis based on electron
 210 irradiation data [26] also indirectly suggests a larger bias for nickel than for
 211 copper. The B_d calculated using atomistic interactions are about 20% lower
 212 than these using the elastic interaction energies, which shows the inaccuracy
 213 of the elastic interactions used to obtain the dislocation bias. This shows,
 214 however, the opposite trend comparing to our previous work [15], where the

atomistic interaction energies result in higher dislocation bias compared to that using the elastic interaction energies. The reason stems from the choice of the dislocation core radius. In the previous work, the same dislocation radii are used for the integration while in the present work, the criterion of Eq.1 is used and the radii are thus different for atomistic- and elastic interaction energies. The criterion in the present work is better motivated comparing to the arbitrary choice in the previous work.

To assess the impacts of elastic constants and the partial splitting distances on the bias calculations, the elastic constants of Cu, Ni and Al, as well as variable partial core distances are used in the elastic model to simulate materials with different SFEs, considering that the SFE is the major component in determining the partial splitting distance. As shown in the inset figures in Fig.5, the elastic constants of Cu are used to generate the elastic interaction model with partial distances of 14 Å, 22 Å and 35 Å, respectively. The bias factors are calculated correspondingly at the temperature of 815 K and 1000 K with the dislocation density of 10^{14} m^{-2} . At both temperatures, the bias decreases as the partial distances increase. The same trend is observed when the elastic constants of Ni and Al are used. Comparing the B_d calculated with interactions that are generated using Cu, Ni and Al elastic constants at the same partial distance, it is seen that $B_d^{\text{Cu}} > B_d^{\text{Ni}} > B_d^{\text{Al}}$ in the defined temperature range. At $d = 35 \text{ Å}$, the B_d calculated using elastic constants of Cu is about 7% larger than that using elastic constants of Ni while the B_d calculated using elastic constants of Ni is about 6% larger than that of Al. In

238 these constructed interaction models, all calculation parameters are the same
 239 except the elastic constants used to describe the interaction. Therefore, in
 240 this case, the difference in B_d originates only from the variation of the elastic
 241 constants. To identify the most important elastic properties in determining
 242 the B_d , an empirical parameter $[B/G]$ is selected in order to obtain an ap-
 243 proximately linear relation related to the dislocation bias factors, where B
 244 is the bulk modulus and G is the shear modulus. Given that the interaction
 245 energy of a dislocation and a SIA is determinant in the bias calculation, the
 246 capture efficiency Z_{SIA} is further studied as a function of the unitless param-
 247 eter $[B/G]$. This parameter takes into account that the interaction energy is
 248 decided by the relaxation volume in the isotropic elastic interaction model,
 249 and the relaxation volume can be seen as a balance between compressing
 250 the two central atoms and their neighbours, and shearing of the surrounding
 251 crystal. As shown in Fig.6, by constructing elastic interactions with 14, 22
 252 and 35 Å partial distances, and using the elastic constants from Ni, Al and
 253 Cu, the Z_{SIAs} are proportional to the empirical parameter $[B/G]$. The values
 254 of this parameter for Ni, Al and Cu are marked on the x-axis. For typical
 255 austenitic alloys, the $[B/G]$ value is in the range of 2 and 2.3 as shown in
 256 the Tab.2. Therefore the capture efficiency Z_{SIA} for the alloy is supposed
 257 to located about 1% below Ni in Fig.6. The typical range is marked on the
 258 x-axis in the figure.

259 As it is seen from Fig.5, the difference in B_d induced by employing dif-
 260 ferent elastic constants are much less pronounced compared to that induced

261 by the variance of the partial distance. Further studies are made by extend-
 262 ing the partial distances and calculating the corresponding B_d with elastic
 263 interactions constructed using the elastic constants from Ni since Ni locates
 264 closest to the austenitic alloy in Fig.6 and it is the austenitizer in austenitic
 265 alloys. When the partial distance is small enough, the two partials collapse
 266 back to a single core dislocation. The single core dislocation bias is relatively
 267 large: around 35% as shown in Fig.7. As the partial distance increases,
 268 the calculated B_d decreases and converges to a certain level. The reason is
 269 probably that as the partial distance increases, the overlap effect on lattice
 270 sites decreases, therefore the interaction energies around the partial cores
 271 decrease. Since the diffusion potential is an exponential function of the in-
 272 teraction energy, it gets weaker as a consequence of the partial separation.
 273 When the two partial cores are far enough from each other, they are seen
 274 as twice the dislocation densities with half the Burgers vector on each par-
 275 tial dislocation, comparing to the case when partial distance is zero with
 276 one strong dislocation core. At a large partial distance, the decrease of B_d
 277 due to SFE decrease is eliminated by the increase of B_d due to the disloca-
 278 tion density increase. From Fig.7 the B_d converges to about 0.1 after the
 279 partial distance reaches 100 Å. The converged value 0.1, compared to the
 280 non-splitting full core value 0.35, has been lowered with a factor of about 3.
 281 This implies that the stacking fault distances plays a more significant role
 282 than the elastic properties when assessing dislocation bias factors.

283 With the above analysis, it is possible to predict the dislocation bias on

284 the austenitic alloys. Using equation $d = \frac{Gb^2}{4\pi E_{sf}}$ [24], an approximate value for
 285 equilibrium separation is calculated to be 127 Å by inserting $G=77.5$ GPa,
 286 $b=2.5$ Å and $E_{sf}= 30$ mJ/m². The parameters are shown in Tab.2. As seen
 287 in Fig.7, an equilibrium distance of 127 Å corresponds to a bias factor about
 288 0.1 when using the elastic interaction model with the elastic constants of Ni.
 289 When we substitute the elastic constants of Ni with that of an austenitic
 290 alloy, as discussed already, the B_d might be about 1% lower than it is using
 291 Ni elastic constants, which is negligible. Therefore, the bias factor calculated
 292 using the elastic interactions for austenitic alloy is estimated to be 0.1. The
 293 tolerance of this prediction is relatively high since the separation distances of
 294 austenitic alloys lie on the plateau region in Fig.7. To benchmark the predic-
 295 tion, a FeNiCr alloy EAM potential [21] is used to construct a Fe-10Ni-15Cr
 296 alloy. The elastic constants calculated from the EAM potential are used in
 297 the elastic interaction model to obtain the interaction energies of this alloy.
 298 This is used to estimate the bias factor and we obtain a value of 0.093 with an
 299 equilibrium partial distance of 104 Å, which is in agreement with the above
 300 prediction value of 0.1. This implies that even without a proper EAM poten-
 301 tial, by applying the elastic constants and SFE obtained from experiments,
 302 it is possible to predict the dislocation bias for a fcc alloy. However, the
 303 predicted values are obtained by using only the elastic interaction energies.
 304 From the comparison of B_d values using atomistic- and elastic interaction
 305 models in Cu, Ni and Al, the dislocation bias are about 20 % higher using
 306 the elastic interaction energies than using the atomistic ones. Therefore, the

307 more realistic dislocation bias in the alloy should be about 20 % lower than
 308 what we predicted using the elastic interaction energies. This results in an
 309 estimation of $B_d \approx 0.08$ in the actual austenitic alloy at the temperature of
 310 815 K and a dislocation density of 10^{14} m^{-2} .

311 4. Conclusions

312 In this work, an efficient and easily reproducible approach is proposed
 313 to perform a systematic study of the dislocation bias factors in fcc Cu, Ni
 314 and Al model lattices. The atomistic interaction energies between an edge
 315 dislocation and point defects are calculated and applied to obtain the dis-
 316 location bias factor for the three model lattices. The results are compared
 317 with the bias calculated using anisotropic interaction models. It is found
 318 that $B_d^{\text{Al}} > B_d^{\text{Ni}} > B_d^{\text{Cu}}$ at the same temperature and dislocation density, which
 319 is in agreement with experiments.

320 The elastic models are applied to study the fundamental parameters that
 321 influence the B_d values by changing the elastic constants and the partial dis-
 322 location distances in the anisotropic model. The results show that the B_d
 323 is more sensitive to the change of equilibrium partial dislocation separation
 324 distances than to the change of elastic constants, regardless of temperatures.
 325 As the separation distance gets larger, the bias tends to converge. When the
 326 two partial cores are far enough from each other, they will act as indepen-
 327 dent dislocations with half the Burgers vector, but in a system with twice
 328 the dislocation density, compared to the case when partial distance is zero.

Therefore the bias factor tends to increase. However, the trend is balanced by the tendency of decrease induced by larger separation distance.

By estimating the partial dislocation separation of the austenitic alloy, a prototype of 316 stainless steel, we predict the dislocation bias to be about 0.1 at temperature close to the swelling peak (815 K) and typical dislocation density of 10^{14} m^{-2} . This value is in agreement with the dislocation bias calculated from numerical FEM using the elastic interaction model. By taking into account the overestimation of the bias induced by using elastic interaction energies, a more realistic bias value of 0.08 is predicted under the same conditions.

In this study, we have shown that the SFE has an important effect on dislocation bias because it is related to the equilibrium splitting of partials. However, we have not considered the effect of the SF interface itself on defect capture. There is a possibility that the SF surface either facilitates or hinders defect diffusion to the partial cores, and it may also serve as a recombination area for PDs, thereby influencing the resulting bias of the dislocation. These aspects are left to future studies.

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Figure 1: Edge dislocation – point defect interaction energies for the different approaches in Cu model lattice, A) Atomistic SIA; B) Elastic SIA; C) Atomistic vacancy; D) Elastic vacancy; E) Difference between A and B; F) Difference between C and D.

Figure 2: Edge dislocation – point defect interaction energy maps for the different approaches in Ni model lattice, A) Atomistic SIA; B) Elastic SIA; C) Atomistic vacancy; D) Elastic vacancy; E) Difference between A and B; F) Difference between C and D.

Figure 3: Edge dislocation – point defect interaction energy maps for the different approaches in Al model lattice, A) Atomistic SIA; B) Elastic SIA; C) Atomistic vacancy; D) Elastic vacancy; E) Difference between A and B; F) Difference between C and D.

Figure 4: Temperature dependence of B_d for the atomistic and elastic cases at the dislocation density of 10^{14} m^{-2} .

Figure 5: B_d varies with partial dislocation separation distances. The B_d are calculated from anisotropic elastic interaction models using elastic constants from Cu, Ni and Al. The insets depict the interactions calculated using elastic constants from Cu with a separation of 14 Å, 22 Å and 35 Å respectively.

Figure 6: Z_{SIA} as an approximate linear function of an empirical parameter B/G at different partial separation distances. Typical B/G values for austenitic alloy is marked on the x-axis.

Figure 7: B_d calculated from constructed elastic model as a function of partial distances at 815 K and 1000 K and the dislocation density of 10^{14} m^{-2} .

Table 1: Fundamental parameters of Cu, Ni, Al from EAM potentials.

	Cu		Ni		Al	
	EAM	Ref	EAM	Ref	EAM	Ref
a_0 (Å)	3.615	3.615 ^{c}	3.519	3.519 ^{a}	4.032	4.032 ^{c}
$E_{\text{vac}}^{\text{for}}$ (eV)	1.27	1.27 ^{f}	1.48	1.79 ^{a}	0.68	0.66 ^{m}
$E_{<100>\text{SIA}}^{\text{for}}$ (eV)	3.063	2.8-4.2 ^{g}	4.08	4.08 ^{k}	2.68	2.59 ^{l}
E_{coh} (eV/at.)	3.54	3.54 ^{d}	4.45	4.45 ^{a}	3.36	3.36 ^{j}
E_{SF} (mJm ⁻²)	44.4	45 ^{e}	113	128 ^{b}	129.4	144 ^{i}

Notes: The Ref values are from experimental measurements (marked as bold) and other calculations. *a* is from [27]; *b* is from [28]; *c* is from [29]; *d* is from [30]; *e* is from [31]; *f* is from [32]; *g* is from [33]; *h* is from [34]; *i* is from [35]; *j* is from [36]; *k* is from [37]; *l* is from [38].

Table 2: Fundamental parameters of Cu, Ni, Al and typical austenitic alloy.

	Cu	Ni	Al	Austenitic alloy
$\Delta V_{\text{vac}}^{\text{Relax}}$ (atomic volume)	-0.3	-0.07	-0.4	-0.2 ^a
$\Delta V_{\text{SIA}}^{\text{Relax}}$ (atomic volume)	1.8	1.2	2.1	1.4 ^a 1.5 ^e
$G^{\text{effective}}$ (GPa)	41	75	29	70 ^a 75 ^b 77 ^c
B (GPa)	138	180	79	160 ^a 157 ^b 159 ^c
$T_m/2$ (K)	815	1000	603	973
E_{sf} (mJ/m ²)	44	113	129	18 ^a 30 ^d

Notes: 316 type alloy is used as a representative for the austenitic alloy here. *a* is from the EAM potential; *b* is from [39], *c* is from [40], *d* is from [41]. *e* is from [42]. Note that the compositions are slightly different in the different references.