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IRRADIATION CREEP BY STRESS-INDUCED PREFERENTIAL ATTRACTION DUE TO ANISOTROPIC DIFFUSION (SIPA–AD)

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An accepted mechanism for radiation creep is the dislocation climb enhancement via stress-induced preferential attraction (SIPA) of point defects. This attraction depends on the dislocation orientation with respect to the stress. It has been proposed as being induced by the second-order elastic interaction energy between the dislocation and the point defect, which is modelled as a polarizable inhomogeneity in a stress field (SIPA–I). An alternative mechanism is presented here: the stress-induced preferential attraction due to anisotropic diffusion (SIPA–AD). This is based on considering the point defect migration in an atomic lattice distorted by the dislocation and external stress fields; i.e. only the first-order size and shape interaction energy is considered but the discrete, anisotropic nature of the migration process is explicitly included. The dislocation sink strengths are calculated for different orientations and values of an external uniaxial stress and compared with the corresponding SIPA–I strengths for a characteristic fcc lattice. A simplified rate theory is used for modelling and comparing the irradiation creep predicted by SIPA–AD against the SIPA–I model. Larger creep rates and a different temperature dependence are found for SIPA–AD.

1. Introduction

There is a general understanding that the climb and possible glide of dislocations favourably oriented with respect to an external stress due to the stress-induced preferential attraction (SIPA) of point defects is the most feasible mechanism of radiation-induced creep under steady-state conditions. Heald and Speight [1] were the first to propose the SIPA as due to the stress-induced interaction energy between an inhomogeneity and a dislocation. Bullough and Willis [2] (BW) showed that for an elastic inhomogeneity this interaction depends on the dislocation orientation with respect to the external stress via the change of the crystal elastic constants induced by the defect; i.e. this stress-induced interaction energy is of second-order compared with the size one. Also the defect-induced change in elastic constants is generally an ill-defined quantity whose value and sign must be theoretically estimated [3] and it is very difficult to measure. On the other hand BW only evaluated an angularly averaged value of the stress-induced interaction energy between the dislocation and the point defect and they assumed the stress-induced change in the dislocation bias factor Z to be proportional to that energy. Wolfer and Ashkin [4] solved the steady-state diffusion equation by using a perturbative method and they obtained explicit solutions for the bias dependence of the trace and projected deviatory component of the stress. Recently Bullough et al. [5] also made an explicit numerical calculation of the bias. However, these two sets of calculations imposed different boundary conditions for the diffusion problem and they show systematic differences that we will discuss later. The stress-induced preferential attraction of an inhomogeneity by a dislocation due to its polarizability in a external stress field will be called in what follows SIPA–I. On the other hand Savino [6] has critically examined the diffusion equations on which the previously mentioned papers are based and he claims that terms which may be relevant to the bias are generally omitted in solving those equations. Lately Dederichs and Schroeder [7] (DS) rederived the equations for the diffusion of point defects in a stress field and they concluded that they reduce to the ones generally used [8] only for very simple or null stress fields or for isotropic distortion of the defect at equilibrium and at the saddle point configuration, (see section 2). Finally Tomé et al. [9] and Woo and Savino [10] used those equations to calculate the

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diffusion of intrinsic point defects towards a straight dislocation and dislocation loop in the presence of an external stress field.

Causey et al. [11] and Nichols [12] compared the creep values calculated through BW theory for the SIPA–I with experiments and, based on different arguments, they found those values are smaller than the measured ones. Also, according to the first authors, the wrong temperature dependence of those values is predicted. However Wolfer [13], based on his previous work [4], claims good agreement between SIPA–I theory and experiments. In this paper we will use the above mentioned calculations of Tomé et al. [9] to evaluate creep rates. Our purpose is to elucidate the relative importance of including the full equation of diffusion as deduced by DS in evaluating the dislocation sink strength for point defect, against the SIPA–I mechanism of BW. The first mechanism has been already proposed by Savino [6]; only the first-order size interaction energy is included in the model but the defect configurations at equilibrium and at the saddle point are explicitly considered. We shall call this mechanism SIPA–AD for "stress-induced preferential attraction due to anisotropic diffusion". The preference of the defect in a stress field to drift towards some dislocation orientations rather than others comes, in this mechanism, via the coupling of the dislocation drift with the effect of the external stress on determining preferential jumping directions for the defect.

The plan of the work is as follows: in section 2 the diffusion equations of different authors and the resulting dislocation strengths are compared and some new results concerning the calculations of Tomé et al. [9] presented. In section 3 a simplified model for the strain rate of an idealized crystal under irradiation and a uniaxial stress field is deduced. This strain rate is then evaluated by using the bias factors deduced within the different models and calculations and the results are critically compared.

2. Diffusion in dislocation and external strain fields

2.1. Diffusion equations

In order to calculate either the instantaneous or steady-state defect concentration for a medium evolving in time the single jump process at a site (either interstitial or lattice site) must be studied. If the defect walk takes place in a strained lattice, both the location within the strain field and the jumping direction are relevant. The interaction energy between a defect located at a site l and a strain field ϵ may be written in first order [6] as:

$$E_{\text{int}}^{\text{e,s}}(l, n) = P_n^{\text{e,s}} \cdot \epsilon(l) \qquad (1)$$

where $P_n^{\text{e,s}}$ is the dipole tensor for the defect either at the equilibrium (e) or at the saddle point configuration (s) with an orientation n among the possible n_0 orientations at the site. Only single thermally activated jumps are included by Savino [6] and DS. The defect concentration $c(\boldsymbol{r}, t)$ at a site $\boldsymbol{r}$ must satisfy for a time t the continuity equation

$$\frac{\partial c(\boldsymbol{r}, t)}{\partial t} = -\nabla \cdot \boldsymbol{J}(\boldsymbol{r}, t) \qquad (2)$$

with

$$\begin{aligned} \boldsymbol{J}(\boldsymbol{r}, t) = &-\sum_{j=1}^{N} \sum_{n=1}^{n_0} \sum_{m_{ij}=1}^{M_{ij}} \frac{\nu_0}{2n_0} \\ &\times \exp\left(-Q^{(n,m_{ij})}(\boldsymbol{r})/kT\right) \\ &\times \left[\exp\left(E^n(\boldsymbol{r}_i)/kT\right)c^n(\boldsymbol{r}_i, t)\right. \\ &\left.-\exp\left(E^n(\boldsymbol{r}_j)/kT\right)c^n(\boldsymbol{r}_j, t)\right]\boldsymbol{s}_{ij} \end{aligned}$$

where ν_0 is the pre-exponential factor in the jump probability, $\boldsymbol{s}_{ij}$ is a vector that joins the i lattice site at $\boldsymbol{r}_i$ with the neighbour j site among N possible sites, n stands for the defect orientation at equilibrium and M_{ij} paths join site i with j; $Q^{(n,m_{ij})}$ is the saddle point energy for an $\boldsymbol{s}_{ij}$ jump via an m_{ij} path starting with the defect in an n orientation and $E^n(\boldsymbol{r}_i)$ is the defect formation energy with an orientation n at a site i. If the equilibrium defect orientation at a given site is attained within a few jumps

$$c^n(\boldsymbol{r}_i, t) = c(\boldsymbol{r}_i, t)\frac{\exp[-E^n(\boldsymbol{r}_i)/kT]}{\sum_m \exp[-E^m(\boldsymbol{r}_i)/kT]} \qquad (3)$$

where $c(\boldsymbol{r}_i, t)$ is the total defect concentration at site i.Eq. (2) may be reduced to:

$$\begin{aligned} \frac{\partial c(\boldsymbol{r}, t)}{\partial t} = \nabla_i\Bigg[&D_{ij}(\boldsymbol{r}) \\ &\times\left(\nabla_j c(\boldsymbol{r}, t) + \frac{c(\boldsymbol{r}, t)}{kT}\nabla_j \bar{E}(\boldsymbol{r})\right)\Bigg] \end{aligned} \qquad (4)$$

where

$$\begin{aligned} D_{km}(\boldsymbol{r}) = &\sum_{j=1}^{N} \sum_{n=1}^{n_0} \sum_{m_{ij}=1}^{M_{ij}} \frac{\nu_0}{2n_0} \\ &\times \exp\left\{-\left[Q_{(\boldsymbol{r})}^{(n,m_{ij})} - \bar{E}(\boldsymbol{r})\right]/kT\right\} s_{ij}^k s_{ij}^m \end{aligned} \qquad (5)$$

where s_{ij}^k is the k component of $\boldsymbol{s}_{ij}$. The average energy

$\bar{E}$ at the equilibrium site is defined as

$$\bar{E}(\boldsymbol{r}) = \frac{1}{n_0} \sum_{n=1}^{n_0} E^{(n)}(\boldsymbol{r}).$$

If the defect has a spherically symmetric configuration at the saddle point, which is not generally the case for vacancies and interstitials, and

$$\sum_{j=1}^{N} s_{ij}^{k} s_{ij}^{m} \propto \delta_{km},$$

eq. (4) reduces to the expression used by Wolfer and Ashkin [4] for calculating the dislocation drift at steady state:

$$\frac{\partial c(\boldsymbol{r}, t)}{\partial t} = \nabla^2[D(\boldsymbol{r})c(\boldsymbol{r}, t)] + \frac{1}{kT}\nabla[D(\boldsymbol{r})c(\boldsymbol{r}, t)] \cdot \nabla E^{s}(\boldsymbol{r}) + \frac{1}{kT}D(\boldsymbol{r})c(\boldsymbol{r}, t)\nabla^2 E^{s}(\boldsymbol{r}) \quad (6)$$

where they took $\partial c(\boldsymbol{r}, t)/\partial t = 0$, i.e. $c(\boldsymbol{r}, t) = c(\boldsymbol{r})$ and defined

$$D(\boldsymbol{r}) = D^0 \exp[-E^{m}(\boldsymbol{r})/kT] \quad (7)$$

being

$$E^{m}(\boldsymbol{r}) = E^{s}(\boldsymbol{r}) - \bar{E}(\boldsymbol{r}). \quad (8)$$

$E^{s}(\boldsymbol{r})$ is the energy of the defect at the saddle point and $\bar{E}(\boldsymbol{r})$ has been defined in eq. (5), both energies calculated in presence of a strain field. D^0 may be identified with the corresponding terms in (5). One must realize that, as also pointed by DS with respect to eq. (4), the solution of (6) depends on the interaction energy at the saddle point; the one at equilibrium enters only via the boundary condition on the variable:

$$\psi(\boldsymbol{r}, t) = D(\boldsymbol{r})c(\boldsymbol{r}, t).$$

Finally, Bullough et al. [5] solved the equation for $c(\boldsymbol{r})$ also under steady-state conditions and including a constant defect production term K

$$\nabla^2 c(\boldsymbol{r}) + \frac{1}{kT}\nabla c(\boldsymbol{r}) \cdot \nabla\phi + \frac{c(\boldsymbol{r})}{kT}\nabla^2\phi = -\frac{K}{D}. \quad (9)$$

In (9) the diffusivity D is taken as constant and ϕ is the interaction energy between the strain field and the point defect presumably at the equilibrium site as proposed in [8].

2.2. Dislocation sink strength

In a medium under irradiation there is a time and space dependent equiproduction, $K(\boldsymbol{r}, t)$, of interstitials and vacancies which either recombine among themselves or migrate towards existing or newly created sinks in the crystal (dislocation network, loops, grain boundaries, precipitates, etc.) with a flow vector $\boldsymbol{J}(\boldsymbol{r}, t)$. The interstitial $c_i(\boldsymbol{r}, t)$ and vacancy $c_v(\boldsymbol{r}, t)$ concentrations satisfy the coupled system of equations

$$\partial c_i(\boldsymbol{r}, t)/\partial t = -\nabla \boldsymbol{J}_i(\boldsymbol{r}, t) + K(\boldsymbol{r}, t) - \alpha c_i(\boldsymbol{r}, t)c_v(\boldsymbol{r}, t), \quad (10a)$$

$$\partial c_v(\boldsymbol{r}, t)/\partial t = -\nabla \boldsymbol{J}_v(\boldsymbol{r}, t) + K(\boldsymbol{r}, t) - \alpha c_i(\boldsymbol{r}, t)c_v(\boldsymbol{r}, t). \quad (10b)$$

Rate theory of a "lossy" medium seems to be the appropriate theoretical approach to eqs. (10) for obtaining an approximate quantitative solution which reveals the relative importance of different sinks. Wiedersich [14] was the first to apply that theory for solving radiation damage problems. Lately, especially after the work of Brailsford and Bullough [15], its use has been widely adopted. Within the rate theory approach the complex set of eqs. (10) is replaced by two equations for the concentration of defects in a medium with a local homogeneous distribution of sinks, which have an effective capture probability of the point defects k_j^2. Then, instead of (10) the equations

$$\frac{\partial\langle c_i\rangle}{\partial t} = -\sum_j k_{ij}^2 D_i\langle c_i\rangle - \alpha\langle c_i\rangle\langle c_v\rangle + K, \quad (11a)$$

$$\frac{\partial\langle c_v\rangle}{\partial t} = -\sum_j k_{vj}^2 D_v\langle c_v\rangle - \alpha\langle c_i\rangle\langle c_v\rangle + K + \sum_j K_j^e \quad (11b)$$

for the average vacancy, $\langle c_v\rangle$, and interstitial, $\langle c_i\rangle$, concentration are solved; where k_{ij}^2, k_{vj}^2 are the j sink strengths or capture probabilities for interstitials and vacancies respectively, D_i and D_v the interstitial and vacancy diffusivities which are assumed as temperature but not space dependent, α the recombination factor, K the average defect production rate and K_j^e the vacancy thermal emission from the j sink. Then the whole complexity of eqs. (10) is translated into obtaining realistic values for the different sink strenghts which obviously are not independent. Brailsford [16] and Brailsford and Bullough [17] extensively discuss the assumptions involved in calculating those strengths and their interrelations. The simplest approach is neglecting recombination and assuming a single sink type uniformly distributed in the medium. In addition, under uniform and constant irradiation dose K at reactor temperature, steady-state conditions are reached almost immediately after switching on the irradiation – see however Rauch and Simon [18]. Under those assumptions (11) reduces to:

$$K = k^2 D\langle c\rangle. \quad (12)$$

Table 1
Parameters of the calculation in section 3
(a) Definition of symbols

Symbol	Definition	Units
$\langle c_i \rangle$, $\langle c_v \rangle$	Interstitial and vacancy averaged concentration	1/atom
k_i^2, k_v^2	Interstitial and vacancy total sink strength	$1/m^2$
k_{iD}^2, k_{vD}^2	Interstitial and vacancy network dislocation strength	$1/m^2$
k_{iG}^2, k_{vG}^2	Interstitial and vacancy grain boundary strength	$1/m^2$
D_i, D_v	Interstitial and vacancy diffusivities	$m^2\ s^{-1}$
α	Recombination coefficient	atom s^{-1}
K	Defect production rate	$atom^{-1}\ s^{-1}$
K_v^e	Vacancy emission	$atom^{-1}\ s^{-1}$
ρ_D	Total dislocation density	m^{-2}
Z_i, Z_v	Interstitial and vacancy dislocation bias factor	–
Z_i^0, Z_v^0	Interstitial and vacancy dislocation bias factor for zero external stress	–
Z_{iI}, Z_{iII}, Z_{iIII} Z_{vI}, Z_{vII}, Z_{vIII}	Interstitial and vacancy bias factor for different dislocation orientations	–
Z_1^e, Z_2^e, Z_3^e	Vacancy emission factor for different dislocation orientations	–
d_G	Average grain diameter	m
d_1, d_2, d_3	Grain dimension in different directions	m
σ_0	External uniaxial stress	Pa
σ	External hydrostatic component of the stress	Pa
σ'	External deviatoric stress tensor	Pa

(b) Constants for the dislocation bias
(b1) SIPA-AD model
Dipole tensors [3]

Defect	P_1 (eV)	P_2 (eV)	P_3 (eV)	e_1	e_2	e_3	n	s
Vacancy (equilibrium)	−0.15	−0.15	−0.15	(100)	(010)	(001)	1	–
Vacancy (saddle point)	0.00	−1.28	4.68	$(1\bar{1}0)$	(110)	(001)	–	e_2
Dumb-bell interstitial (equilibrium)	14.4	14.4	14.4	(100)	(010)	(001)	3	–
Dumb-bell interstitial (saddle point)	12.6	17.3	15.7	$(1\bar{1}0)$	(110)	(001)	–	e_2

P_i: eigenvalue; e_i: eigenvector in cartesian lattice axes; n: number of defect orientations at a given site; s: jump direction.

(b2) SIPA based models

(b2.1) Savino–Laciana [19] based on BW model
Relaxation volume:
Interstitial: $e_i^0 = v_i/\Omega = 0.8$
v_i: interstitial relaxation volume
Vacancy: $e_v^0 = v_v/\Omega = 0.$
v_v: vacancy relaxation volume
Bias factor: $Z_i^0 = 1.2$, $Z_v^0 = 1$
Elastic constants of the defect (K^*, μ^*):
Rigidity: $K^* = K + \Delta K$
Interstitial: $\Delta K_i = 0$
Vacancy: $\Delta K_v = 0$
Shear modulus: $\mu^* = \mu + \Delta\mu$
Interstitial: $\Delta\mu_i = -\mu$
Vacancy: $\Delta\mu_v = 0$
K, μ: elastic constants of perfect crystal

(b2.2) Bullough et al. [23]
Same parameters as (b2.1)

(b2.3) Wolfer and Ashkin [4]
Bias factors, defect relaxation volumes: same as (b2.1)
Dislocation core radius
$a = 10b$
Polarizabilities
$\alpha_v^K = -150$ eV, $\alpha_v^\mu = -15$ eV
$\alpha_i^K = 100$ eV, $\alpha_i^\mu = -150$ eV

Table 1 (continued)

(c) Material constants for the calculations

Diffusivities:	Grain size:
$D_v = \nu_0 a_0^2 \exp-(E_m/kT)$	$d_G = 5\times10^{-6}$ m
$D_i = \frac{2}{3}\nu_0 a_0^2 \exp-(E_m^i/kT)$	Dislocation Burgers vector:
ν_0: 5×10^{12} s^{-1}	$b = a_0/2$
a_0: 3.6×10^{-10} m	Shear modulus
E_m: 1.3 eV	$\mu = 56$ GPa
E_m^i: 0.25 eV	Poisson's ratio:
Recombination factor:	$\nu = 0.364$
$\alpha = 30\nu_0[\exp-(E_m^i/kT)+\exp-(E_m^v/kT)]$	Young's modulus:
Formation energy for vacancies:	$E = 2\mu(1+\nu)$
$E_f^v = 1.4$ eV	Atomic volume:
Defect production rate	$\Omega = (a_0/2)^3$
$K = 10^{-7}$ dpa s^{-1}	

The condition of uniform sink distribution implies that a region round the sink core may be defined in which all the defects produced are absorbed by that sink. Then $\langle c \rangle$ may be calculated by solving in that region eq. (2) at steady-state either in its full expression or with the approximations (4), (6) or (9), with appropriate boundary conditions and defect production rate, i.e.

$$\partial c(r, t)/\partial t = -\nabla \cdot J(r) + K = 0 \qquad (13)$$

$$J(r)|_{r=a} = 0 \qquad (14)$$

for a at the boundary between zones belonging to different sinks. A second boundary condition is needed at the sink core where the defect would be unstable. The approach sketched above, with

$$c(r_0) = c_0 \qquad (15)$$

constant concentration, generally null, at the dislocation core radius (r_0) was adopted by Tomé et al. [9] and Bullough et al. [5] for calculating the sink strength. They solve (13) for a lattice with a homogeneous dislocation density, and under a uniaxial external stress, with boundary conditions (14) and (15), and obtain the sink strength from (12). The dislocation lines can be taken as parallel, centred at a cylinder of radius

$$a = (\pi\rho_D)^{-1/2} \qquad (16)$$

and with the same Burgers vectors. Under those conditions Tomé et al. [9] replace the $J(r)$ of eq. (2) in (13) and calculate c_i, c_v and finally k_{iD}^2, k_{vD}^2 by using (12). Bullough et al. [5] solve (9) by taking the boundary condition (14) over an infinite parallelepiped of side $2a$. The full defect anisotropy and the different defect orientations at equilibrium and saddle point are included by Tomé et al. [9] in the diffusion calculation but only first-order and shape effects in the interaction energy between the defect and the dislocation; Bullough et al. [5] included the defect polarizability by the stress in the calculation of the interaction energy but they modelled the defect as an isotropic inhomogeneity and did not include the interaction energy at the saddle point configuration in their diffusion equations. Both calculations model the dislocation by its distortion in an elastic, isotropic medium.

For the calculation of k_D^2, Wolfer and Ashkin [4] adopt an approach different from that sketched in eqs. (12)–(14). They consider a dislocation located in a region where defects are neither produced nor absorbed except at the dislocation core. This region of size a, eq. (16), is itself imbedded in the effective medium defined by eq. (12) and the boundary condition at a

$$c(a) = \langle c \rangle \qquad (17)$$

is imposed. The sink strength is obtained by:

$$k_D^2 = J/D\langle c \rangle \qquad (18)$$

where J is the defect flux for any closed surface round the dislocation core in the region defined above. Wolfer and Ashkin claim that this model is more realistic than the periodic boundary one previously sketched because of the random distribution of dislocations in the medium. However in the recent review of Brailsford and Bullough [17] this approach for the sink strength calculation is severely criticized as not self-consistent.

2.3. Calculations

We shall adopt the Tomé et al. [9] calculations of the straight edge dislocation sink strength for vacancies and interstitials. The split dumb-bell interstitial and vacancy dipole tensors at the equilibrium and at the saddle point configurations reported by Schober [3] are used. Among the set of Schober's values we choose for this work those based on a modified Morse potential for a Cu lattice, table 1. The dislocation has a ⟨110⟩ Burgers vector, lies on a {111} plane and the isotropic elastic model is assumed for its strain field. The dislocation point defect interaction energy is calculated by using (1).

An external uniaxial stress

$$\sigma_{ij} = \sigma_0 \delta_{ik} \delta_{jk} \tag{19}$$

is assumed to be applied in a k direction, which induces a homogeneous strain field in an isotropic continuum

$$\epsilon_{kk} = \epsilon_0 = \sigma_0/E, \quad \epsilon_{mm} = -\nu\epsilon_0, \quad \epsilon_{km} = 0 \quad \text{if } k \neq m \tag{20}$$

where E is the Young's modulus and ν is the Poisson's ratio. Averaged elastic constants for Cu are used and the strain (20) is added to the dislocation field when the energies (1) are calculated. Dislocation concentrations ranging from 2.5 to 36×10^{14} m^{-2} (i.e. regions with $a \simeq 3.55 \times 10^{-8}$ m to $a \simeq 9.43 \times 10^{-9}$ m) are adopted for the calculation. Three orientations are taken for the stress: (I) parallel to the Burgers vector, (II) perpendicular to the Burgers vector and the dislocation line and (III) perpendicular to the Burgers vector and parallel to the dislocation line. The sink strengths obtained by the

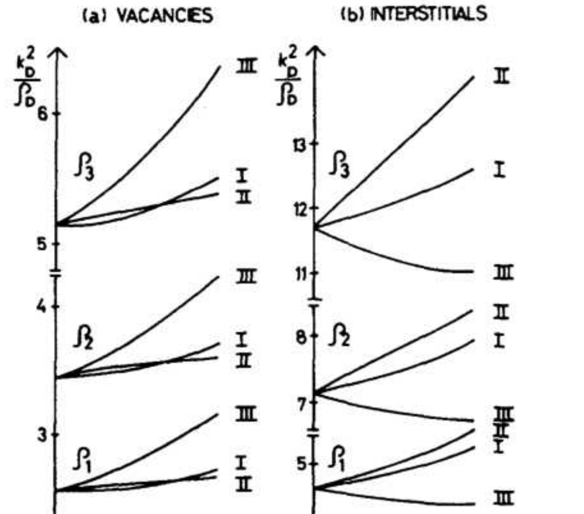

Fig. 1. Dislocation sink strength $k_D^2/\rho = Z_D$ as a function of the external strain field. (a) Vacancies, (b) Interstitials, $T = 300$ K, $\rho_1 = 2.5 \times 10^{14}$ m^{-2}, $\rho_2 = 9.5 \times 10^{14}$ m^{-2}, $\rho_3 = 36 \times 10^{14}$ m^{-2}. Orientations I, II and III as described in the text.

numerical calculations are plotted in fig. 1 as a function of the crystal uniaxial strain ϵ_0. This plot has been shown already in [9] but it is repeated here for the sake of completeness. It can be seen that the strengths not only show a dependence on the external stress but they appear to be somewhat larger than the values generally fitted to experiments in the literature [20].

The SIPA-I model as discussed by BW provides expressions for the dislocation sink strengths in the presence of an external stress. These have been calculated by Bullough and Hayns [23] assuming, as BW did, that the defect can be modelled by an isotropic distortion centre. This centre is taken for the vacancy case to have a negligible interaction with the dislocation while it is strong for the interstitial, which is taken to be soft in shear. The limiting case is considered of assuming the interstitial shear modulus as null. If the sink strength is written as

$$k_D^2 = Z\rho_D \tag{21}$$

the bias factors for the vacancy remain constant while those for the interstitial deduced on the basis of the BW model under different orientations (I, II and III above) of the external uniaxial stress are [19]:

$$Z_{iI} = Z_i^0 \left(1 + \frac{5\sigma_0(2-\nu)}{2\mu e^0(7-5\nu)} \right) \tag{22a}$$

$$Z_{iII} = Z_i^0 \left(1 - \frac{5\sigma_0(1+\nu)}{2\mu e^0(7-5\nu)} \right) \tag{22b}$$

$$Z_{iIII} = Z_i^0 \left(1 - \frac{5\sigma_0(1-2\nu)}{2\mu e^0(7-5\nu)} \right) \tag{22c}$$

where μ is the crystal shear modulus, ν the Poisson modulus, Z_i^0 the interstitial bias for the dislocation in a stress-free lattice and e^0 the relative volume expansion (v/Ω) induced by the defect. These expressions for Z_i are independent of temperature and dislocation density while Z_i depends linearly on the external stress and is inversely proportional to e^0. The basis on which the expressions (22) are deduced have been criticized by Nichols [12].

Bullough et al. [5] numerical calculations of the dislocation sink strength are performed as a function of the dislocation concentration and of a parameter

$$p = \mu\Omega e^0/kT \tag{23}$$

which is related to the temperature T and the lattice expansion induced by the defect $(v = \Omega e^0)$. The same assumptions about the defect polarizabilities as those previously outlined are adopted by those authors.

Finally, the expression of Wolfer and Ashkin [4] for the bias is

$$Z = Z^0 + \delta Z(\sigma_H) + \delta Z(\sigma') \tag{24}$$

where the hydrostatic component of the stress, $\sigma_H = \frac{1}{3} T_r(\sigma)$, contributes to the bias as

$$\delta Z(\sigma_H) = -\frac{(b/4r_0)^2}{\ln(a/r_0)} \left(\frac{1-2\nu}{2\pi(1-\nu)kT} \right)^2 \alpha^K v \sigma_H \tag{25}$$

and the deviatory tensor σ' as

$$\delta Z(\sigma') = -\frac{1}{3} \frac{(b/4r_0)^2}{\ln(a/r_0)} \frac{(1+\nu)\alpha^\mu v \sigma'_{ij}}{[2\pi(1-\nu)kT]^2} \times \left[2\hat{b}_i \hat{b}_j - (1-4\nu)\hat{l}_i \hat{l}_j \right] \tag{26}$$

where r_0 is the dislocation core radius, $2a$ is the average distance between dislocation lines, v is the defect relaxation volume, α^K and α^μ are the defect bulk and shear polarizabilities and the vectors $\hat{l}$ and $\hat{b}$ have unit modulus and they are parallel to the dislocation line and Burgers vector respectively.

3. Specimen deformation

3.1. Rate theory

A simplified model is adopted for the crystal. Straight edge dislocations uniformly distributed in space and grain boundaries are taken as interstitial and vacancy sinks. At steady-state and assuming a spatially homogeneous defect production rate, eqs. (11) reduce to

$$K - k_i^2 D_i \langle c_i \rangle - \alpha \langle c_i \rangle \langle c_v \rangle = 0 \tag{27a}$$

$$K + K_v^e - k_v^2 D_v \langle c_v \rangle - \alpha \langle c_i \rangle \langle c_v \rangle = 0 \tag{27b}$$

with

$$k_{i,v}^2 = k_{i,vD}^2 + k_{i,vG}^2$$

where subscript D stands for dislocation and G for grain boundaries (for the meaning of different symbols see table 1). The dislocation distribution is taken as composed of six different orientations, made by three Burgers vectors in the cartesian axes and two possible dislocation lines orthogonal to each vector. A uniaxial stress σ_0, eq. (20), is assumed to be applied parallel to one of those axes, say axis 1.

Then:

$$k_{i,vD}^2 = Z_{i,v}\rho_D = \frac{1}{3}\rho_D (Z_{i,vI} + Z_{i,vII} + Z_{i,vIII}) \tag{28}$$

where I, II and III stand for the dislocation orientations with respect to the stress axis as discussed in section 2.3. ρ_D is the total dislocation density. The grain boundary sink strength is taken as

$$k_G^2 = 6 k_D / d_G \tag{29}$$

the grains are taken as parallelepipeds with their main axes 1, 2, 3 parallel to the specimen axes and the previously mentioned cartesian axes [24]

$$d_G^{-1} = \left(d_1^{-1} + d_2^{-1} + d_3^{-1} \right)/3. \tag{30}$$

If we allow for vacancy emission from dislocations and grain boundaries

$$K_v^e = D_v (\rho_D/3) c_v^e (Z_1^e + Z_2^e + Z_3^e) + 2 D_v k_D \times (Z_1^e/d_1 + Z_2^e/d_2 + Z_3^e/d_3) \tag{31}$$

where

$$c_v^e = \exp(-E_f^v/kT) \tag{32}$$

E_f^v is the vacancy formation energy and

$$Z_1^e \simeq \exp b^3 \sigma_0 / kT$$
$$Z_2^e \simeq Z_3^e \simeq 1. \tag{33}$$

If the specimen deformation is due to dislocation climb and defects absorption at grain boundaries the strain rate can be easily deduced:

$$\dot{\epsilon}_1 = \dot{\epsilon}_{cD} + \dot{\epsilon}_{cG1} + \dot{\epsilon}_{TD} + \dot{\epsilon}_{TG1} \tag{34a}$$

$$\dot{\epsilon}_2 = \dot{\epsilon}_3 = -\tfrac{1}{2}\dot{\epsilon}_{cD} + \dot{\epsilon}_{cG2,3} - \tfrac{1}{2}\dot{\epsilon}_{TD} + \dot{\epsilon}_{TG2,3}. \tag{34b}$$

The first and second terms in (34) are due to irradiation creep by dislocation climb

$$\dot{\epsilon}_{cD} = \tfrac{1}{3}\rho_D \{ D_i \langle c_i \rangle [\tfrac{2}{3} Z_{iI} - \tfrac{1}{3}(Z_{iII} + Z_{iIII})] - D_v \langle c_v \rangle [\tfrac{2}{3} Z_{vI} - \tfrac{1}{3}(Z_{vI} + Z_{vIII})] \} \tag{35}$$

and grain boundary defect absorption

$$\dot{\epsilon}_{cG1} = \tfrac{2}{3} \left\{ k_{iD} D_i \langle c_i \rangle \left[\frac{2}{d_1} - \left(\frac{1}{d_2} + \frac{1}{d_3} \right) \right] - k_{vD} D_v \langle c_v \rangle \left[\frac{2}{d_1} - \left(\frac{1}{d_2} + \frac{1}{d_3} \right) \right] \right\}. \tag{36}$$

The last two terms in (34) model the thermal creep due to vacancy emission at dislocations and grain boundaries

$$\dot{\epsilon}_{TD} + \dot{\epsilon}_{TG1} = \tfrac{2}{9}\rho_D D_v c_v^e (Z_v^e - 1) + k_{vD} D_v \langle c_v \rangle \left[\frac{2 Z_1^e}{d_1} - \left(\frac{1}{d_2} + \frac{1}{d_3} \right) \right]. \tag{37}$$

For illustration it is interesting to solve the case of equiaxed grains. If, in this case, the solutions for c_i and c_v in (27) are inserted in (35), the irradiation creep strain rate can be written as:

$$\dot{\epsilon}_{cD} = \rho_D \left[A k_i^2 k_v^2 (Z_i'/k_i^2 - Z_v'/k_v^2) - A_e k_i^2 k_v^2 (Z_i'/k_i^2 + Z_v'/k_v^2) \right] \tag{38}$$

where:

$$Z'_{i,v} = \tfrac{2}{3} Z_{i,vI} - \tfrac{1}{3}[Z_{i,vII} + Z_{i,vIII}] \tag{39}$$

$$A = \tfrac{1}{3}\frac{D_v D_i}{2\alpha}\left\{\left[(1+\xi)^2 + \eta\right]^{1/2} - 1\right\}$$

$$A_e = \tfrac{1}{3}\frac{D_v D_i}{2\alpha}\xi$$

$$\eta = \frac{4\alpha K}{D_i D_v k_i^2 k_v^2}$$

$$\xi = \frac{\alpha K_v^e}{D_i D_v k_i^2 k_v^2}.$$

We see that eq. (38) is composed of two terms respectively proportional to the parameters A and A_e. This parameter A_e depends on ξ, which gives the ratio between the vacancy–interstitial recombination rate multiplied by the thermal emission ($\alpha c_i c_v K^e$) and the product of vacancy and interstitial fluxes to sinks ($D_v k_v^2 c_v D_i k_i^2 c_i$). On the other hand A depends on ξ and η; the last, η, gives a ratio similar to ξ but between the recombination multiplied by the vacancy production rate ($\alpha c_i c_v K$) and the defect fluxes to sinks ($D_v k_v^2 c_v D_i k_i^2 c_i$). For normal reactor core conditions the ratio K_v^e/K is very small. Then only in the very high temperature limit the term with the emission parameter A_e may dominate over the one with A. However in this *very high temperature* limit the creep will be mainly given by the thermal contributions and, for the dislocation climb, the emission of vacancies by dislocations favourably oriented with respect to the stress (eq. (37), Nabarro creep) is expected to dominate.

At not very high temperatures the term in eq. (38) which contains the parameter A is larger than the one proportional to A_e. We see that the irradiation creep requires the *deviatory bias*, Z'_i, eq. (39) for interstitials to be larger than Z'_v for vacancies, which may be negative. These deviatory bias parameters compare the defect drifts towards the orientation I of the dislocation with the average ones towards II and III.

The not very high temperature range may be divided into an *intermediate–high temperature region* and a *low temperature region* with the limit among them depending on sink concentration. The *intermediate–high temperature region* corresponds to small interstitial–vacancy recombination against sink absorption, $\eta \ll 1$. If the only sinks are dislocations, eq. (38) reduces in this limit to

$$\dot{\epsilon}_{cD} \simeq \frac{K}{3}\left(\frac{Z'_i}{Z_i} - \frac{Z'_v}{Z_v}\right) \tag{40}$$

where

$$Z_{i,v} = (Z_{i,vI} + Z_{i,vII} + Z_{i,vIII})/3.$$

The *low temperature region* is determined by $\eta \gg 1$. In this limit eq. (38) becomes

$$\dot{\epsilon}_{cD} \simeq \frac{\rho_D}{3}\left(\frac{D_v D_i K}{\alpha}\right)^{1/2} k_i k_v \left(\frac{Z'_i}{k_i^2} - \frac{Z'_v}{k_v^2}\right) \tag{41}$$

and the recombination factor, table 1, may be expressed as [24]:

$$\alpha = (N/a_0^2) D_i \tag{42}$$

where N is a number between 30 and 100 and it depends on the recombination volume. If the only defect sinks are the network dislocations, inserting (42) in (41) we obtain:

$$\dot{\epsilon}_{cD} \simeq \left[D_v K Z_i Z_v N^{-1}\right]^{1/2} \frac{a_0}{3}\left(\frac{Z'_i}{Z_i} - \frac{Z'_v}{Z_v}\right). \tag{43}$$

By comparing (40) with (43) we conclude that for both expressions the creep is proportional to the difference $[(Z'_i/Z_i) - (Z'_v/Z_v)]$ but while at high temperatures it is linear with K, at low temperatures it goes like $K^{1/2}$ and it must show a strong temperature dependence via the $D_v^{1/2}$ term [11]. The limit T_c between high and low temperature ($\eta \doteq 1$) also depends on the energy E_m. Using eq. (42) and because of the temperature dependence of $k_i^2 k_v^2$, T_c can be obtained from the implicit equation

$$\nu_0 a_0^2 \exp\left(-\frac{E_m}{kT_c}\right) = \frac{4NK}{a_0^2 k_i^2 k_v^2}. \tag{44}$$

3.2. Strain rate calculation

In order to illustrate the relative importance of the different straining mechanisms and to compare the predictions of the different dislocation bias models previously sketched, we perform in this section some calculations of the strain rates previously deduced. Parameters characteristic of a standard cubic metal are chosen and summarized in table 1.

In fig. 2 eq. (40) is plotted as a function of the dislocation density. One must bear in mind that the creep rate at the plotting temperature will be proportional to (40) but its value may still have a stronger temperature dependence, eq. (43). However eq. (40) allows for a clear comparison of the bias influence on the creep. The creep predicted by the SIPA–I models developed by Wolfer and Ashkin [4], Bullough et al. [5] and Savino et al. [19] (based on BW's theory) are compared with the SIPA–AD one. In the SIPA–I based calculation the Z'_v term is null when the parameters of table 1 are chosen for the material. For comparison with

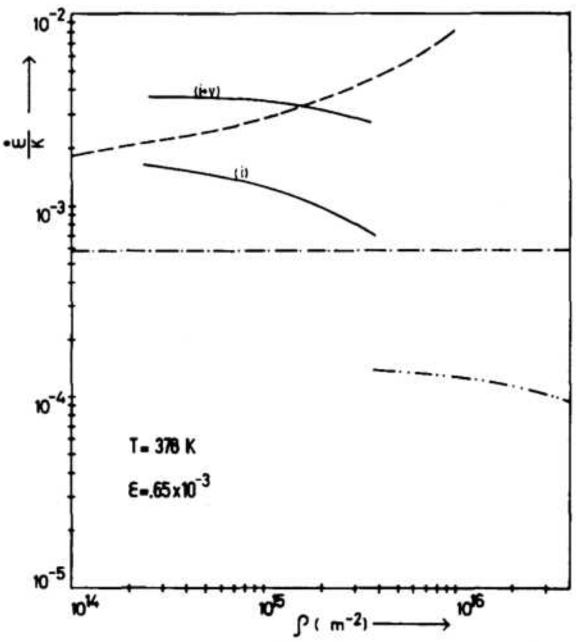

Fig. 2. Creep rate due to dislocations, eq. (40) in units of damage rate, against dislocation density. Temperature $T=$ 378 K, external induced strain: $\epsilon_0=0.65\times10^{-3}$. –·–·– Bullough et al. [5] calculations for SIPA; –·–·– Savino and Laciana [19] model based on Bullough et al. [23] and BW SIPA-I model; — — — Wolfer et al. [4] model based also on SIPA but with different boundary conditions for the calculation of the dislocation absoreption than Bullough et al. [5]; ——— our model, (i+v): including the full equation (40), (i): including only the Z_i'/Z_i term. This last approach consistent with the previously mentioned models that take $v_v=0$ (see table 1).

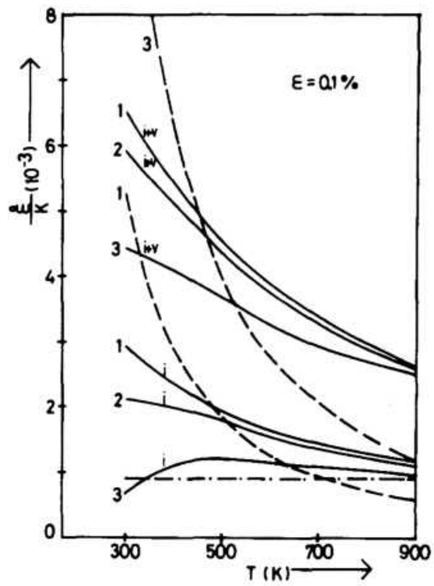

Fig. 3. Creep rate due to dislocations, eq. (40), against temperature; external strain, $\epsilon_0=0.1\%$. Symbols are the same as used in fig. 2. 1, 2, 3, stand for $\rho_D=\rho_1$, ρ_2, ρ_3 of fig. 1.

the SIPA–AD model we plot, the full equation (40) – (i + v) in fig. 2 – and a reduced one neglecting the vacancy contribution, $Z_v'=0$ and labelled as (i) in fig. 2. It can be seen that the SIPA–I bias as deduced by Savino et al. [19] provides a Z_i'/Z_i factor independent of the dislocation density; on the other hand the model of Bullough et al. [5] and the calculations by Tomé et al. [9] of the SIPA–AD predict an inverse dependence of the creep rate (40) on dislocation density, while the SIPA–I model of Wolfer and Ashkin [4] predicts the opposite behaviour. Our fig. 2 can also be compared with fig. 2 of Nichols [12]; the results labelled as Bullough–Hayns by Nichols are of $\dot{\epsilon}/K\simeq5.5\times10^{-4}$, i.e. very similar to those predicted by Savino et al. [19], while Nichols's values for the SIPA–I creep are approximately 5 to 10 times smaller and they increase with dislocation density. Finally it can be seen that although Bullough et al. [5] use the same boundary conditions as Tomé et al. [9] their predicted strain rates are about an order of magnitude smaller. This result seems to show that including the full lattice symmetry in the diffusion equations is numerically more important than allowing for second-order effects in the interaction energy.

In fig. 3 eq. (40) is now plotted against temperature. Different dislocation densities are included ($\rho_1=2.5\times10^{14}$ m^{-2}, $\rho_2=9.5\times10^{14}$ m^{-2}, $\rho_3=35.8\times10^{14}$ m^{-2}) for the same models of fig. 2, except for Bullough et al. [5] calculations where the temperature dependence was not reported. The general trend is either an inverse temperature dependence of Z' with T (Wolfer et al. [4], Tomé et al. [9]) or a constant value for the simplified model of Savino et al. [19]. In our model by comparing the (i + v) curves against the (i) ones it becomes apparent that the contribution of the vacancies to the dislocation climb (creep rate) is comparable to that of the interstitials.

In fig. 4 we plot once more eq. (40) against the value of the externally induced elastic strain of the specimen for the external strain, eq. (20), $\epsilon_0\leq0.4\%$. It can be seen it increases linearly with ϵ_0 at high temperature ($T=$ 900 K) while it has a parabolic dependence for low temperature ($T=300$ K).

Finally, in fig. 5 we plot separately eq. (37) for $\dot{\epsilon}_{TD}$, and (38) for $\dot{\epsilon}_{cD}$. The irradiation-produced vacancies and interstitials are assumed either to recombine among themselves or to be absorbed by network dislocations

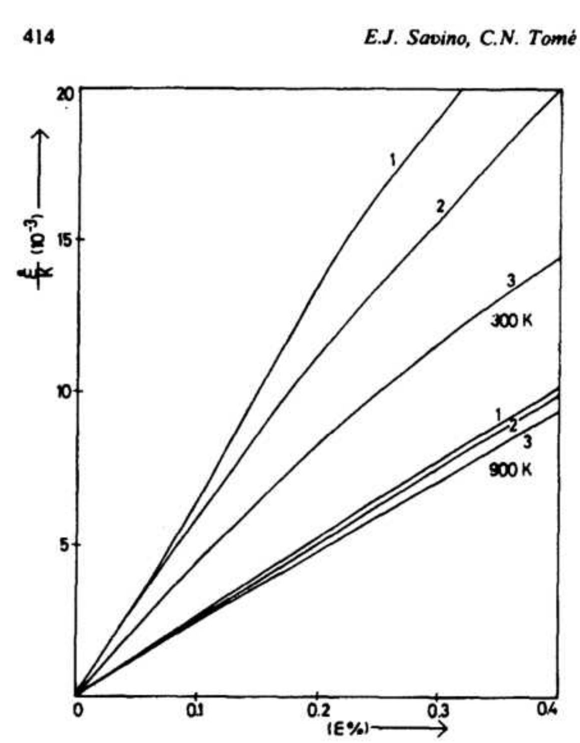

Fig. 4. Creep rate due to dislocations, eq. (40) against external strain at two temperatures (300 and 900 K) and three different dislocations densities; 1: ρ_1, 2: ρ_2, 3: ρ_3 of fig. 1.

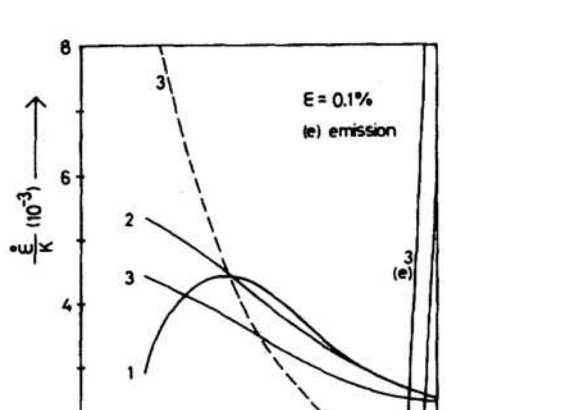

Fig. 5. Strain rates against temperature. Eq. (38) for $\dot{\epsilon}_{cD}$ and eq. (37) for $\dot{\epsilon}_{TD}$ (e) are plotted. — — —: Wolfer et al. [4] model, ———: SIPA-AD model for dislocation bias. 1, 2, 3 stand for the dislocation densities as in fig. 1.

and grain boundaries. If the creep rates predicted by the different SIPA models are compared among themselves it is found, that, except for the results of Wolfer et al. [4] at low temperature and large dislocation density the SIPA-AD mechanism provides a larger contribution to the irradiation creep by dislocation climb than the SIPA-I. At sufficiently large temperature the thermal creep ($\dot{\epsilon}_{TD}$) due to dislocation climb by thermal vacancy emission (Nabarro creep) becomes larger than the climb induced by irradiation [12]. This determines that for our model and that of Wolfer et al. [4] the creep rate may have a relative minimum at intermediate temperatures, while the simple calculation of Savino and Laciana [19], based on the BW model, predicts a steady increase of the creep rate with temperature.

4. Summary and conclusions

In this paper and a previous one [9] we have been able to calculate the interstitial and vacancy sink strengths of three different edge dislocation with (110) Burgers vector oriented parallel or perpendicular to an external uniaxial stess. The calculations summarized in section 2 are based on a model for point defect diffusion in a strained crystal which includes the discrete character of the defect jump. The preferential migration of point defects towards some dislocation orientations in a stress field is called by us "stress-induced preferential attraction due to anisotropic diffusion" (SIPA-AD). For modelling the strain rate under irradiation due to dislocation climb, the straight edge dislocations chosen for the calculation are assumed to have their Burgers vectors and dislocation lines oriented in three perpendicular directions in space with respect to the stress axis, one of those parallel to that axis. Within that approach and using the dislocation sink strengths previously deduced, the strain rate of a crystal containing a cubic homogeneous network of edge dislocations with Burgers vector oriented in the three perpendicular cubic directions is deduced via a rate theory approach and calculated in section 3. As shown by Wolfer [21] and Woo [22] modelling a real crystal by this simplified dislocation network is somewhat unrealistic and better approaches can be obtained when expressions for the dislocation sink strengths at any orientation with respect to the stress are available. However, as we rely on a numerical calculation for every dislocation orientation, we consider this model as a useful approach for revealing the relevance of different mechanisms of strain rate enhancement by dislocation climb under irradiation, which is the purpose of this paper. In this sense the most relevant comparison is between the creep rates resulting from our model for the dislocation sink strength based on the SIPA–AD mechanism against the strength deduced by Bullough et al. [5] based on the SIPA–I due to the defect polarizability by the strain field. Both sets of calculations adopt similar boundary conditions for deducing the steady-state defect concentration under irradiation in the neighbourhood of a dislocation. From the results shown in the previous section we must conclude that the SIPA–AD provides larger contribution to the climbing than the SIPA–I.

Although for our calculations we have used some point defect parameters characteristic of Cu we can compare the calculated creep rate values with the available experimental results in steel. We follow previous theoretical papers of Bullough and Hayns [23], Nichols [12] and Wolfer [13]; these authors compare their models of the SIPA–I with experiments by Mosedale et al. [26], Stralsund [27] and Gilbert et al. [28]. This comparison serves to test whether a mechanism predicts the right order of magnitude for the irradiation creep. While Bullough and Hayns [23], based on BW model of the SIPA–I, claim that it provides a good fit to the experimental results, Nichols [12] asserts that it is highly unlikely to be the main contribution to the observed creep rates and Causey et al. [11] conclude that it predicts not only too low values in some temperature ranges but also the wrong temperature dependence. On the contrary we found that the SIPA–AD predicts a reduction of the strain rate $\dot{\epsilon}_{cD}$ with temperature consistent with the results for the creep rate refered by Causey et al. [11]. From fig. 5 it can be seen that at 700 K and under an external stress of approximately 150 MPa, allowing for dislocation climb, defect recombination and grain boundary absorption, the SIPA–AD predicts creep rates $\dot{\epsilon}/K$ between 1 and 3×10^{-3}. If we take the measurements of Gilbert et al. [28] referred to by Nichols [12], of $\dot{\epsilon}_{radiation} \simeq 7 \times 10^{-11}\ s^{-1}$ near 700 K and at 100 MPa and we assume a production of freely migrating defects characteristic of fast reactors: $K \simeq 1 \times 10^{-7}$ dpa s^{-1}, we obtain $\dot{\epsilon}/K \simeq 7 \times 10^{-4}$ as a characteristic experimental value. Also the values of Mosedale et al. [26], used by Bullough and Hayns [23] and Nichols [12], vary between $\dot{\epsilon}/K \simeq 7 \times 10^{-5}$ and $\dot{\epsilon}/K \simeq 8 \times 10^{-4}$. Those of Stralsund [27], used by Wolfer for comparing with his SIPA–I model, are larger, $\dot{\epsilon}/K \simeq 2 \times 10^{-3}$. We see that the creep rate values predicted by our simple calculation based on the SIPA–AD model are comparable with or larger than the experimental ones. Also the calculations of Wolfer et al. [4], based on the SIPA–I model but on different boundary conditions than those of Bullough and Hayns [23] or Bullough et al. [5] for calculating the defect diffusion towards the dislocation and deducing the sink strengths, predict strength values and creep rate dependence on temperature similar to ours. However, as discussed by Brailsford and Bullough [17], the boundary conditions used by those authors imply a point defect source at infinity which is far from the actual irradiation conditions.

Acknowledgements

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Discussion

W. Mansel: How are your calculations influenced by assuming that the dislocations are of vacancy type or interstitial type?

E. Savino: Only straight dislocations were included in the calculations.