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Progress in modelling the microstructural evolution in metals under cascade damage conditions

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Abstract

In recent years, it has been shown that intra-cascade clustering of vacancies and self-interstitial atoms (SIAs), differences in the thermal stability and mobility of the resulting clusters and one-dimensional (1-D) diffusional glide of SIA clusters play a key role in damage accumulation in metals under cascade damage conditions. The model taking these aspects into account (production bias model, PBM) succeeded in rationalising striking features in the microstructural evolution in pure metals, where the conventional rate theory model failed: the high overall swelling even at low dislocation densities, the enhanced swelling near grain boundaries, the decoration of dislocations with SIA loops, saturation of void growth and void lattice formation. In the present paper, the main ideas and results of these considerations are reviewed. We discuss recent work on possible effects of deviations of SIA cluster diffusion from strictly 1-D by direction changes and/or self-climb and formulate a general reaction kinetics including 1-D and 3-D cluster diffusion. Such reaction kinetics may be considered to form the basis for a general description of cascade damage accumulation in metals and complex technical alloys.

1. Introduction

According to the picture suggested in the 1950s [1,2], a displacement cascade creates a vacancy rich core which may collapse to form a vacancy cluster, and self-interstitial atoms (SIAs) which were considered to leave the cascade region by replacement sequences or by thermally activated random migration. At the beginning of the 1970s, evaluations of diffuse X-ray scattering experiments on the basis of an advanced scattering theory [3] indicated that not only vacancies but also SIAs are able to cluster in the cascade region. Detailed results were, however, only published in the 1980s [4–6]. But it is now only 10 years ago that results of molecular dynamics (MD) simulations [7] presented in fall 1989 in Silkeborg during the workshop on 'radiation damage correlation for fusion conditions' initiated vigorous discussions on possible consequences of SIA clustering in cascades.

In the temperature range of void swelling, SIA clusters are stable while small vacancy clusters decay into single vacancies. Woo and Singh [8,9] introduced this asymmetry in the concurrent production of stable SIA clusters and unstable vacancy clusters in cascades as a 'production bias' representing a potential driving force for void swelling. It was soon recognised [10] that this driving force can only be maintained if a substantial fraction of SIA cluster is able to escape to sinks other than voids, and it was shown [11–13] that one-dimensional diffusional glide of planar SIA clusters in the form of small dislocation loops represents an efficient SIA removal mechanism. The 1-D motion of planar clusters had indeed been observed in MD simulations [14] which showed, in additions, that such clusters may change their diffusion direction (Burgers vector, BV).

Thus, a new type of defect reaction kinetics had to be considered where SIA clusters play an active role. This differs qualitatively from the conventional rate theory approach where both vacancies and SIAs are assumed to be produced as mono-defects, randomly in

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space and time, and clusters of both types of defects (except dis and tris) resulting from diffusional reactions of the (mobile) mono-defects are assumed to be immobile [15–18]. A special feature of the new kinetics is the (thermally activated) 1-D diffusion of SIA clusters by which the highly heterogeneous microstructural evolution in pure metals as well as the saturation of void swelling and void lattice formation becomes understandable [11].

In the last few years, the new approach, called production bias model (PBM), has been developed from qualitative and semi-quantitative considerations of defect accumulation [11–13] to quantitative treatments, particularly of the accumulation of vacancies in voids [19]. The decoration of dislocations with SIA loops [20,21] and its role in the deformation behaviour of metals [21,22] has been modelled. It has been shown recently that the effect of the recoil energy on the evolution of voids (in Cu) which has been clearly demonstrated experimentally only recently [23,24] can be quantitatively modelled in term of the PBM [25]. Both analytical and MC simulation studies have been started to clarify the role of direction (BV) changes and self-climb of SIA loops in their global reaction kinetics [26–30].

In the present paper, we review this development. We first, in Section 2, consider properties of cascade induced SIA clusters which play a key role in cascade damage accumulation. The main features of reaction kinetics, taking 1- to 3-D diffusion of SIA clusters into account, are described in Section 3. Applications of such reaction kinetics to the treatment of specific features in cascade damage accumulation are reviewed in Section 4. Finally, in Section 5, the present state of the art is summarised and a brief outline of problems to be treated in future is given.

2. Properties of cascade induced SIA clusters

In recent years, many MD simulations have been performed to study defect production in displacement cascades [7,31–34] as well as the properties of cascade induced defect clusters [31–39]. The main results of cascade simulations are:

1. Efficient intra-cascade recombination results in low damage efficiencies.
2. Substantial intra-cascade clustering of both vacancies and SIAs occurs directly in the cascade region.
3. The characteristics of defect production in cascades depends on crystal structure. Thus, in bcc, both intra-cascade recombination and clustering are not as efficient as in fcc [34,40].

The properties of clusters studied in the simulation [35–39] are:

1. the formation energies of their possible (meta-stable) configurations and their corresponding relative thermal stability,
2. the migration modes and energies of the mobile configurations.

Small planar SIA clusters in the form of dislocation loops (coupled crowdions) have been found to be highly mobile [7,14,35–39] performing fast 1-D glide diffusion, occasionally interrupted by direction (BV) changes [14,37,38]. These findings are of special interest for the defect reaction kinetics forming the basis for modelling cascade damage accumulation.

It has been found that macroscopic continuum dislocation theory provides useful guidelines for estimating the formation and migration energies of SIA clusters in the form of dislocation loops [39]. In Fig. 1, the macroscopic pictures of the three main processes relevant for the cluster reaction kinetics are sketched. Fig. 1(a) indicates diffusional glide of a loop. Estimates of migration energies for this process on the basis of the Peierls energy per dislocation core atom yield values below kT_m for loops containing less than 100 SIAs even for bcc metals (T_m: melting temperature; $kT_m = 0.12$ and 0.17 eV for Cu and Fe, respectively). The atomistic details of loop glide may, however, be complicated [36,39]. The interaction of loops with other defects such as impurities will generally result in a decrease of the effective glide diffusivity.

Fig. 1(b) indicates random (conservative) self-climb by dislocation core diffusion [13]. Thus activation energies for this transversal diffusion mode may be considered to be comparable with those for self-diffusion along dislocations and grain boundaries which are in the range of 7–10 kT_m. The diffusion coefficients for a loop as a whole entity, D_{cl}, decreases with the number n of SIAs per loop as $D_{cl} \sim D_{cd}/n^{3/2}$, where D_{cd} is the dislocation core diffusion coefficient.

Fig. 1(c) illustrates a possible mechanism for a BV change of a loop from the point of view of dislocation theory. The change in BVs from $\boldsymbol{b}_1$ to $\boldsymbol{b}_2$ is considered to occur by the sweeping of a dislocation segment with the difference vector $\Delta\boldsymbol{b} = \boldsymbol{b}_2 - \boldsymbol{b}_1$ across the loop area. For fcc where $\boldsymbol{b} = \langle 1\,1\,0\rangle/2$, the activation energy $E_{\Delta b}$ for this transition is estimated to increase with n as $E_{\Delta b}/kT_m \sim 3\sqrt{n}$. Lower values are expected for a two-step process consisting of a transition from a first perfect to a faulted one and from there to another perfect configuration by the sweeping of partials across the loop area. This would hold in spite of the required stacking fault energy since this is restricted to rather small values for small loops even for high specific stacking fault energy. An analogous two-step process consisting of a transition from an immobile to a mobile and back to an (other) immobile configuration has been proposed for the piecewise 1-D diffusion interrupted by direction changes of single SIAs [36]

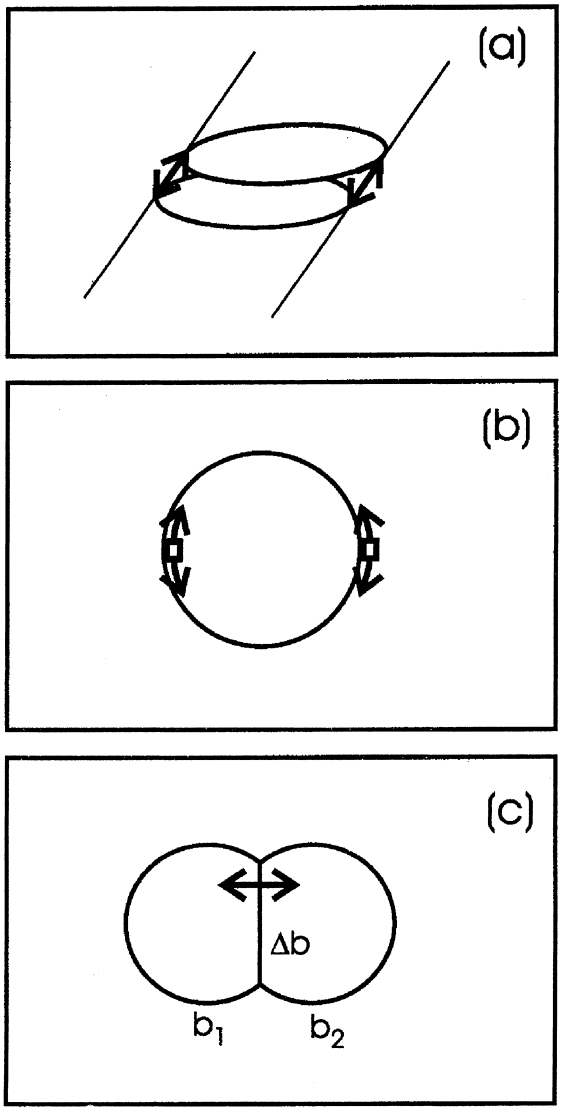

Fig. 1. Illustration of the main processes relevant for the reaction kinetics of SIA loops from the point of view of macroscopic dislocation theory: (a) diffusional glide as random jumps across the Peierls barrier, (b) random self-climb by diffusion of double jogs (core interstitials and vacancies), (c) Burgers vector change by the sweeping of a dislocation across the loop area.

and small loops [21]. The interaction of a loop with other defects may be expected to facilitate BV changes.

A qualitatively new feature in the dynamics of nm-scale loops compared to the conventional macroscopic dislocation dynamics is that, at temperatures above $0.2T_m$, all the processes considered above for such small loops, i.e., diffusional glide, changes in BVs and self-climb may be assumed to occur by thermal activation.

3. Main features of SIA cluster diffusion reaction kinetics

In a realistic modelling of cascade damage accumulation as formulated in the PBM, intra-cascade clustering and the different thermal stabilities and mobilities of the resulting vacancy and SIA clusters must be taken into account. The thermally activated 1-D diffusion of SIA clusters represents a qualitatively new feature to be introduced into the defect reaction kinetics which deserves special attention.

3.1. Microstructural evidence for 1-D cluster diffusion

There is plenty of indirect evidence for 1-D SIA transport over large distances in pure metals under cascade damage conditions. For temperatures between 0.2 and $0.4T_m$, TEM studies have revealed a highly heterogeneous and segregated accumulation of vacancies and SIAs in regions separated by several μm. The most striking observations are:

1. Efficient void nucleation (without the assistance of helium) resulting in high swelling rates occurs already at very low doses (10^{-3}–10^{-2} dpa) even when the dislocation density is very low [41]. Under such conditions, a substantial fraction of the SIAs corresponding to the voids is missing in virtually dislocation-free regions.
2. SIA loops segregate to dislocations [41–44] which may initiate the formation of dislocation walls [43].
3. The accumulation of vacancies in voids is considerably enhanced in several μm wide regions adjacent to grain and sub-grain boundaries [44–47].

The common feature of these heterogeneous microstructures is their large spatial scale which is significantly (up to more than one order of magnitude) larger than what would be expected for a 3-D reaction kinetics as used in the conventional rate theory where the scale of spatial variations is of the order of the average distance between sinks (typically ~100 nm). The heterogeneous and segregated accumulation of vacancies and SIAs can only the understood in terms of a far ranging 1-D transport of SIA loops through the existing microstructure as will be explained in the following section.

3.2. 1-D vs. 3-D diffusion reaction kinetics

In order to illustrate the difference in the spatial scales of the microstructures resulting from the standard 3-D and the 1-D diffusion reaction kinetics, we consider the evolution of the concentration, c, of defects produced at a production rate P and performing 3-D or 1-D diffusion with diffusivity D, respectively, in a half-space containing a random distribution of sinks of strength k^2 and bounded by an ideal planar absorber, such as a grain boundary, at $x = 0$. The (strictly) 1-D diffusing defects are assumed to diffuse in x-direction. In the mean

field approximation, this problem is described by the diffusion reaction equation

$$\partial c/\partial t = P + D\partial^2 c/\partial x^2 - Dck^2, \quad (1)$$

subject to the initial and boundary conditions $c(x, t = 0) = c(0, t) = 0$. The simple steady-state solution of this problem is

$$c(x) = (P/Dk^2)[1 - \exp(-kx)]. \quad (2)$$

According to Eq. (2), the spatial scale of the concentration profile $c(x)$ is given by the mean diffusion range (mean free path)

$$\lambda \propto k^{-1}. \quad (3)$$

For 3-D diffusing defects, the sink strength $k_3^2 = \lambda_3^{-2}$ is proportional to the density of sinks. For a random distribution of spherical sinks such as voids of absorption radius r_{abs} (void radius) and number density, N, for instance, it is given by [15–17]

$$k_3^2 = \lambda_3^{-2} = 4\pi r_{\mathrm{abs}} N, \quad \text{i.e., } \lambda_3 \propto N^{-1/2}. \quad (4)$$

Differently from this, the mean diffusion range of 1-D diffusing defects is, similar as in collision theory, inversely proportional to the defect absorption cross-section, σ ($= \pi r_{\mathrm{abs}}^2$ for spherical sinks), and density, N,

$$k_1 \propto \lambda_1^{-1} = \sigma N, \quad \text{i.e., } \lambda_1 \propto N^{-1}. \quad (5)$$

The corresponding sink strength, k_1^2, is quadratic in the sink density establishing according to Eq. (1), together with the concentration of the mobile defects, reaction kinetics of third order [12,48].

Comparison of Eqs. (4) and (5) shows that

$$\lambda_1/\lambda_3 \propto (r_{\mathrm{abs}}^{1/2}/\sigma)N^{-1/2} \gg 1 \quad (6)$$

for low to medium sink densities. Accounting for the correct numerical factor of $\sqrt{2}$ in Eq. (5) [29] we find for voids inducing swelling S, $\lambda_1/\lambda_3 = \sqrt{(8/3S)} \approx 16$ for 1% swelling. A similar conclusion is obtained for a random distribution of dislocations where the absorption cross-section is to be substituted by an absorption diameter, d_{abs}, which needs to be determined experimentally or theoretically.

The large spatial scale in 1-D diffusion reaction kinetics at low to moderate sink densities is the reason for the heterogeneous and segregated defect accumulation under cascade damage conditions. It should, however, be emphasised that the local details of some features of the microstructure such as the decoration of dislocations with SIA loops and the enhanced swelling near grain boundaries cannot be adequately described within the framework of a mean field approximation as formulated in Eq. (1) but require special treatments taking the specific local conditions into account [12,20,21].

3.3. Reactions of SIA clusters with dislocations

According to the preceding discussion, important parameters in the 1-D diffusion reaction kinetics of SIA clusters are the cross-sections and diameters for the reaction of the clusters with their reaction partners. For the reaction of SIA clusters with voids, the geometrical cross-section represents a reasonable approximation to the absorption cross-section. The reactions of 1-D diffusing SIA clusters with dislocations, on the other hand, are controlled by the long range elastic interaction between these defects and are therefore much more complicated.

Several characteristic regions where the reactions of mobile SIA clusters with dislocations differ distinctly may be identified as illustrated in Fig. 2. In the region far away from the dislocation where the mutual elastic interaction energy is small compared with the thermal energy, $|E_{\mathrm{el}}(r)| \ll kT$, a cluster in the form of a glissile loop may be expected to perform a thermally activated random glide motion. A loop may be considered to be (temporarily) trapped by a dislocation when the attractive interaction energy is large compared with the thermal energy, $-E_{\mathrm{el}}(r) \gg kT$. The size of the thus defined 'trapping region' characterised by a 'trapping diameter' d_{tr}, has been estimated on the basis of several approximate assumptions including elastic isotropy, straightness of dislocations and the 'infinitesimal loop' (elastic

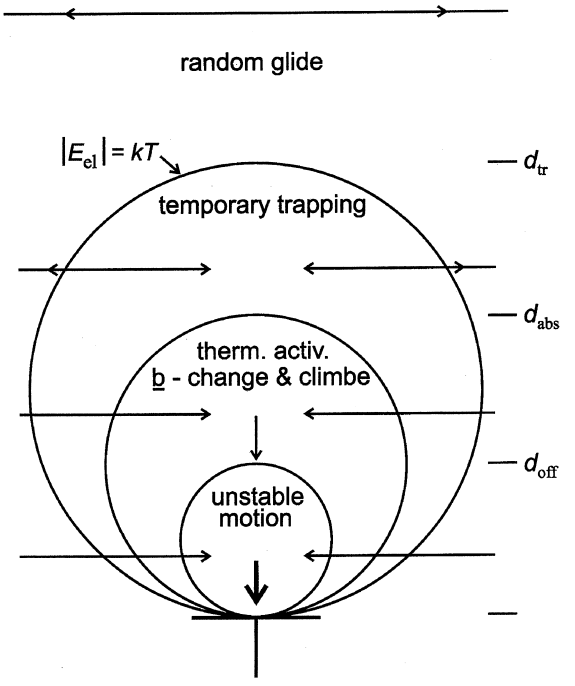

Fig. 2. Sketch of characteristic regions in the interaction of a glissile loop with a dislocation.

dipole) approximation [11–13] (which may be dropped in numerical calculations [49]). Within these approximations, d_{tr} varies with the number n of SIAs in the cluster and temperature as $d_{tr} \propto n/T$ and can reach values of several 10s of nm in the relevant ranges of cluster size and temperature.

A loop trapped in the strain field of a dislocation can, however, only reach the dislocation by changing its direction and/or by climbing substantially before it would have a chance to get detrapped by thermal activation. Only in the region where the rate of direction changes or substantial self-climb is higher than the rate of detrapping, the loop is likely to get incorporated into the dislocation [20,21]. The thus defined 'absorption diameter', d_{abs}, is expected to increase with increasing frequency of BV changes and increasing climb rate and may even reach the trapping diameter, $d_{abs} \to d_{tr}$. In the outer part of the 'absorption region', direction changes will still need thermal activation while the loop motion is expected to become unstable below a critical 'stand-off distance', d_{off} [20–22,49].

According to this picture, the following hierarchy of spatial scales has to considered in the treatment of the local reaction kinetics of SIA loops with dislocations:

$$0 < d_{off} < d_{abs} < d_{tr}. \tag{7}$$

In the region $d_{off} < d < d_{tr}$, accumulation of SIA loops may occur under appropriate conditions [20,21] (Section 4.1). The most important parameter for global reaction kinetics, particularly for void growth and swelling, is the absorption diameter d_{abs} which is expected to depend, via the frequency of BV changes and the rate of self-climb, on loop size and temperature. Information on this parameter can be obtained by evaluating swelling saturation (Section 4.4).

3.4. General reaction kinetics accounting for deviations of cluster diffusion from 1-D

In Section 3.2, the two extremes of pure 1-D and 3-D reaction kinetics of clusters with random distributions of sinks have been compared. BV changes and self-climb disturb the global 1-D reaction kinetics, and increasing rates of these processes induce a continuous transition from 1-D to 3-D reaction kinetics. For 1-D diffusion of loops interrupted by BV changes, the character of the reaction kinetics depends on the relationship between the following three main types of length scales involved:

1. the mean 1-D diffusion lenth, l, covered during the time between two BV changes, τ_{ch}, in a sink-free virtual crystal, $l = 2D_1\tau_{ch}$;
2. the mean 1-D diffusion range (mean free path) in a given microstructure $\lambda_1 = (\sigma N)^{-1}$;
3. the effective linear dimension of the sinks considered, the absorption radius r_{abs} (or diameter d_{abs}).

The three physically meaningful relationships between these length scales enable us to distinguish the following three characteristic cases in the reaction kinetics as illustrated in Fig. 3:

1. The pure (correlated) 1-D case defined by $l \gg \lambda_1$ (Fig. 3(a)). In this case, a given straight 1-D diffusion line is terminated by two unambiguously defined

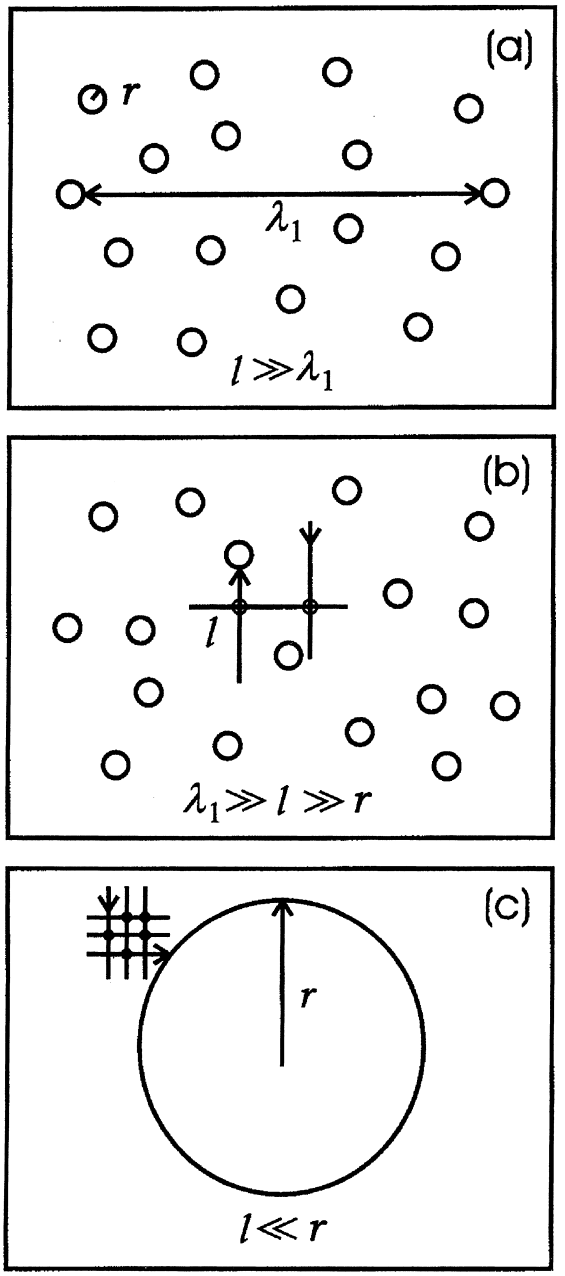

Fig. 3. Illustration of the three characteristic cases in the reaction kinetics of a piecewise 1-D diffusing defect with an immobile sink: (a) correlated 1-D, (b) uncorrelated 1-D, (c) 3-D.

individual sinks. Due to the two sink correlation associated with this, 1-D reaction kinetics are of third order [12,48]. Including the correct numerical factors of 2, the partial sink strength of a sink of configuration i may be written as [29]

$$k_{1i}^2 = 2/\lambda_1\lambda_{1i}. \tag{8}$$

2. The 'uncorrelated 1-D' case defined by $\lambda_1 \gg l \gg r_{\rm abs}$ (Fig. 3(b)). The correlation between sinks characteristic for pure 1-D reaction kinetics is broken by direction changes, but an important feature of 1-D, the dependence of sink strengths and reaction rates on absorption cross-sections and diameters is maintained. In this case, adequately called 'uncorrelated 1-D reaction kinetics', the total line length covered by a cluster during its life time, λ_1, consists, on the average, of $n \sim \lambda_1/l$ straight portions of mean length l. Accordingly, the cluster life time may be expressed as $\tau_{\rm life} \sim n\tau_{\rm ch} \sim (\lambda_1/l)\tau_{\rm ch} \sim l\lambda_1/D_1$, resulting with $k^2 \sim 1/D_1\tau_{\rm life}$ in $k_i^2 \sim 1/l\lambda_{1i}$ or more precisely in [29]

$$k_i^2 = 2\sqrt{2}/l\lambda_{1i}. \tag{9}$$

Comparison with Eq. (8) shows that the sink strength in this intermediate case is increased by a factor of $\sqrt{2}\lambda_1/l$ relative to the correlated (pure) 1-D case. This behaviour has been confirmed by recent MC simulations [27,28].

3. The 3-D case defined by $r_{\rm abs} \gg l$ (Fig. 3(c)) where the sink strength has the well-known behaviour as, for instance, given by Eq. (4).

The increasing reaction rate in the transition from pure 1-D to 3-D reaction kinetics is due to the increasing search-and-find efficiency of the migrating defects with increasing frequency of their direction changes. For reactions with dislocations, the transition from 1-D to 3-D is accentuated by the fact that, in this case, in addition to the decrease of l, $d_{\rm abs}$ increases with increasing frequency of direction changes, $d_{\rm abs} \to d_{\rm tr}$.

It is emphasised here that the difference between the correlated and uncorrelated 1-D cases does not affect the partitioning of mobile defect over different types of immobile sinks since in the corresponding sink fractions common factors such as the global mean free path λ_1 and the mean diffusion length l cancel. This was tacitly assumed in our previous work [11–13,19]. The difference will, however, play a role in reactions between mobile clusters. Thus, the reduction of the mobile cluster density in the uncorrelated 1-D kinetics, due to an increase of the sink strength of immobile sinks, will suppress the agglomeration of such clusters.

A recent theoretical analysis of the dependence of the sink strength on the frequency of direction changes [30] suggests that the transition from 1-D to 3-D may be described by the following general interpolation formula

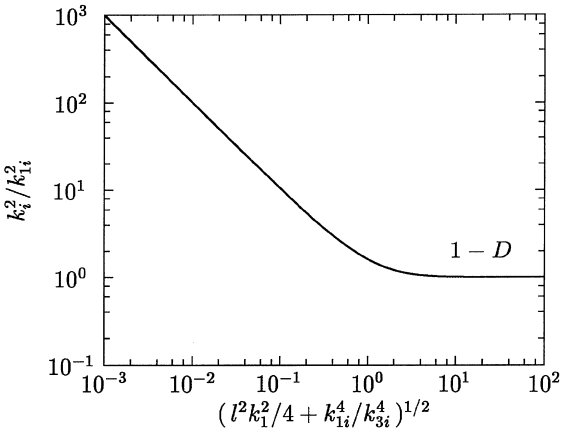

Fig. 4. Master curve interpolating between 1-D and 3-D reaction kinetics.

$$y = 0.5\left\{1 + \sqrt{(1 + 4/x^2)}\right\}, \tag{10a}$$

with

$$y = k_i^2/k_{1i}^2, \quad x^2 = (l^2k_1^2/4 + k_{1i}^4/k_{3i}^4). \tag{10b}$$

This function is plotted in Fig. 4. It represents a master curve for the dependence of the sink strength on the three main spatial scales l, λ_1 and $r_{\rm abs}$ involved. This is presently being tested by MC simulations. Diffusion of SIA loops by random self-climb may be included [30]. Such a function will form the basis for generalising the PBM. We emphasise here that the reaction kinetics in a void lattice require a special treatment [26,29].

3.5. Parameters controlling the character of cluster reaction kinetics

The main parameters controlling the character of the SIA cluster reaction kinetics, via the length scales, l, λ_1 and $r_{\rm abs}$ (or $d_{\rm abs}$) are crystal structure, microchemistry (impurities), microstructure, and temperature. The mean 1-D diffusion length between BV chages, $l = 2D_1\tau_{\rm ch}$, depends via D_1 and $\tau_{\rm ch}$ on temperature. Since the activation energy for BV changes is higher than that for diffusional glide, l is expected to decrease with increasing temperature, thus changing the kinetics towards that for 3-D diffusion. This trend is strengthened by the increase of the microstructural length scales λ_1 and $r_{\rm abs}$ with increasing temperature under otherwise constant conditions.

The effect of crystal structure (for instance bcc vs. fcc) on the mean 1-D diffusion length is not yet clear even though there is some indication from void growth saturation data (Section 4.4) that the ability of SIA loops for changing their BV is higher in fcc than in bcc [26]. On the other hand, there is clear evidence from MD

simulations that intra-cascade recombination and clustering are more efficient in fcc than in bcc [34] which is most likely the reason for some characteristic differences in the microstructural evolution of both crystal structures [40].

The interaction of SIA loops with impurities and precipitates is expected to reduce l efficiently by a reduction of both the effective loop diffusivity D_1 (by temporary binding) and the time between BV changes τ_{ch}, changing the diffusion reaction kinetics of SIA loops from 1-D towards 3-D. In parallel with this transition, the character of the microstructural evolution changes from a highly heterogeneous for pure metals to a more homogeneous one for alloys.

4. Review of modelling cascade damage accumulation

In the preceding section, we have described the main features of general reaction kinetics accounting for 1-D diffusion, BV changes and self-climb of SIA clusters produced in cascades. Detailed quantitative modelling of cascade damage accumulation as formulated in the PBM requires the specification of parameters characterising defect production in cascades, the stability and mobility of point defects and their clusters produced in cascades and the interaction of all defect species relevant for the microstructural evolution (production and sink terms in diffusion reaction equations of the form of Eq. (1)). For studying specific features of the microstructure and trends in their evolution, the generally complicated systems of equations can be substantially simplifed. In the following, we summarise the treatment of some typical examples.

4.1. Decoration of dislocations with SIA loops

Decoration of dislocations with SIA loops is perhaps the most striking feature providing evidence for 1-D diffusion of SIA clusters. It has been shown that this effect cannot be rationalised in terms of single SIA production, diffusion and clustering, but may be attributed to the trapping and agglomeration of glissile, cascade-induced SIA loops in the strain field of dislocations [20,21]. The trapping and the subsequent detrapping or absorption of an individual cascade induced loop has been described in Section 3.3. In the region $d_{off} < d < d_{tr}$ (Fig. 2), agglomeration and growth of loops occur when the probability for the arrival of a second loop in the interaction range of a first trapped loop is larger than the probability for detrapping and absorption of the latter. This occurs at high loop arrival rates realised at high loop production rate and/or sink density. The reduction of the probability for detrapping and absorption with increasing loop size and density results in the stabilisation of the evolving dislocation decoration. Loop accumulation cannot occur in the region of unstable loop motion, $d < d_{off}$, where the motion of the loops is unstable and fast and their density correspondingly low.

The incorporation of further loops into the region of loop accumulation ceases when the attractive stress field of the leading dislocation is compensated by the loops decorating it. Subsequently, loop trapping can only occur ahead of the existing structure which thus grows away from the leading dislocation eventually forming a dislocation wall. A quantitative treatment of the problem is complicated since loop diffusion and agglomeration has to be considered to occur in the inhomogeneous stress field of the dislocation and the evolving loop structure.

4.2. Effects of grain boundaries on void swelling

Grain boundary (GB) effects on swelling such as the enhanced swelling near GBs and the increase of swelling with decreasing grain size occurring under cascade damage conditions are also striking examples for effects which cannot be modelled in terms of the conventional rate theory approach where intra-cascade clustering and 1-D diffusion of SIA clusters are ignored. Quite the contrary, within the conventional approach a reduction of swelling is expected when approaching a GB [50] or decreasing the grain size [51].

On the other hand, these phenomena can be easily rationalised in terms of the 1-D diffusional glide of cascade induced SIA clusters and their escape and annihilation at GBs [12,52]. According to Section 3.2, the width of the zone of enhanced swelling adjacent to GBs, w, is expected to be given by the mean 1-D diffusion range of the clusters, λ_1, and to decrease with dose when the microstructure develops. This, together with the assumption that the voids evolving in the zone of enhanced swelling form the dominant sinks for clusters there, is confirmed by the close correlation between w and λ_1 deduced from the observed void structure. Deviations at low doses where λ_1 is large have been attributed to sinks other than voids, such as sessile SIA loops [12]. However, also BV changes of the clusters which would reduce the spatial scale of the structure according to Eq. (11) together with Eq. (5), may play a role in these deviations. For Al and Cu, these deviations give a lower bound estimate for the mean 1-D diffusion length l of the order of several μm. For small grains where the zone width would be of the order of the grain size, the GB effect reduces to a grain size effect on swelling [45,51].

4.3. Bulk swelling in pure metals

Within the conventional rate theory approach, the driving force for (bulk) swelling is attributed to the single defect dislocation bias. This is, however, only

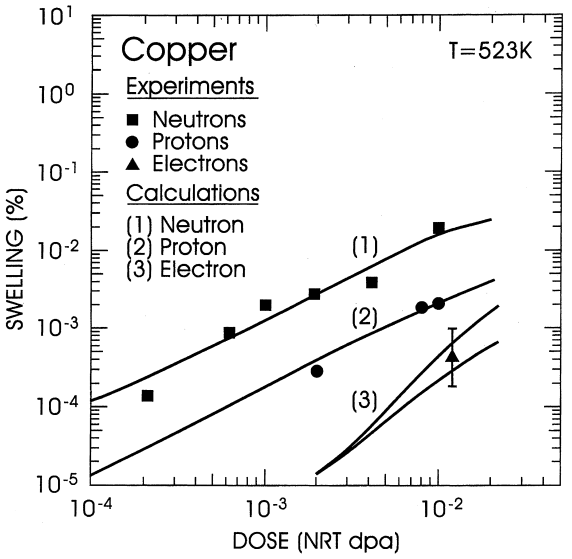

Fig. 5. Experimental and theoretical results demonstrating the effect of recoil energy on void swelling in pure Cu irradiated at 523 K with 2.5 MeV electrons, 3 MeV protons and fission neutrons [23–25]. Swelling for electron irradiation is calculated in terms of the conventional single defect dislocation bias. For proton and neutron irradiations, 1-D diffusing cascade induced SIA clusters are taken into account.

valid for the case of single Frenkel pair production as occurring under electron irradiation. Under cascade damage conditions, the main contribution to the driving force for swelling is due to differences in the thermal stability and mobility of cascade induced vacancy and SIA clusters and the capture of 1-D diffusing SIA clusters by other clusters or dislocations. In the PBM, these features are explicitly taken into account.

Since the efficiency of intra-cascade clustering of SIAs and vacancies depends on the recoil energy, defect accumulation, and particularly vacancy accumulation in voids, should depend on the type of irradiation (mass, charge and energy of particles) and the PBM should be able to reproduce such differences. This has been tested recently by studying swelling in pure Cu irradiated at 523 K with 2.5 MeV electrons, 3 MeV protons and fission neutrons at comparable damage rates to a dose level of ~0.01 NRT dpa [23,24]. For these conditions, Fig. 5 demonstrates the sensitivity of the experimentally observed swelling to recoil energy [23,24] and the capability of PBM to reproduce these observations [25].

4.4. Saturation of void growth and void lattice formation in pure metals

A special feature resulting from the combination of 3-D vacancy with (correlated and uncorrelated) 1-D SIA cluster reaction kinetics is the saturation of void growth and swelling observed in some pure metals under cascade damage condition [53]. This effect is due to the increasing efficiency of voids for capturing 1-D diffusing SIAclusters relative to their capturing of 3-D migrating vacancies. Void growth ceases when the partitioning of SIAs and vacancies over randomly distributed voids and dislocations becomes equal. This condition results in a simple relation between the maximum void radius, r_v^{max}, and the absorption diameter of dislocations, d_{abs}, independent of void and dislocation densities [11,26]:

$$r_v^{max} \approx \pi d_{abs}. \tag{11}$$

This relation may be used to estimate d_{abs} from observed maximum void sizes. For Ni and Mo, for instance, observed maximum void radii of 13 and 4 nm [53] result in d_{abs} values of 4 and 1.3 nm, respectively. Unfortunately, the available data do not allow conclusions on the dependence of d_{abs} on relevant parameters as discussed in Section 3.5.

Also void lattice formation [54] may be considered to be induced by the 1-D diffusion of SIA clusters in the form of loops [26,29]. The equality of structure and orientation (isomorphy) of a void lattice with the underlying crystal lattice in bcc, fcc and hcp may be explained by the 'alignment' of voids in the directions of motion of loops which are the close packed directions. Upon ordering, the character of the cluster reaction kinetics changes qualitatively which therefore needs a special treatment. Saturation of void growth and swelling in void lattices require BV changes and/or self-climb of SIA loops [26,29].

4.5. Swelling of alloys

As discussed in Section 3.5, the interaction of SIA clusters with impurities and precipitates in complex metallic alloys would tend to change the cluster diffusion reaction kinetics from 1-D towards 3-D. Such a transition would have important consequences for the swelling behaviour of alloys. Swelling would no longer saturate as for 1-D SIA cluster diffusion and the preferential absorption of SIA clusters by dislocations would become qualitatively analogous to that of 3-D diffusing single SIAs [26]. The corresponding cluster dislocation bias is, however, substantially larger than the single defect dislocation bias because of the stronger elastic interaction of clusters with dislocations. With the expected large values of the cluster dislocation bias (which may be deduced from estimated values of the trapping diameter, $d_{abs} \rightarrow d_{tr}$) the low cascade damage efficiency no longer represents a problem in explaining high swelling rates of about 1%/dpa in various types of steels [55]. Detailed modelling of swelling of alloys under cascade damage conditions on the basis of the general reaction kinetics described in Section 3.4 is in progress.

5. Summary and perspectives

Since the importance of intra-cascade SIA clustering was recognised 10 years ago, considerable progress has been achieved in modelling cascade damage accumulation in metals. This is true for both the short term/small scale simulation of the cascade defect dynamics and for modelling the long term/large scale microstructural evolution.

Numerous MD simulations have clearly demonstrated the intra-cascade clustering of SIAs, their 1-D diffusion, the occurence of direction changes and the role of other defects in these processes. The so-called PBM taking 1-D diffusion of cascade induced SIA clusters into account succeeded to rationalise some striking features in the microstructural evolution in pure metals such as enhanced swelling near grain boundaries, decoration of dislocations with SIA loops, saturation of void growth and void lattice formation which cannot be understood in terms of the conventional rate theory, and has been shown to allow a quantitative treatment of void swelling in dependence upon temperature, grain size, recoil energy and dose.

In recent work, the impact of deviations of SIA cluster diffusion from strictly 1-D by direction changes and/or self-climb has been studied by both MC simulations and analytical treatments. A general 1-D to 3-D diffusion reaction kinetics has been formulated which is now available to model cascade damage accumulation even in complex technical alloys.

Detailed and comprehensive modelling of the microstructural evolution in alloys at swelling temperatures, including void nucleation and the evolution of the overall dislocation structure will be one important task of future work. More attention than hitherto has to be devoted to cascade damage accumulation at lower temperature ($T \leqslant 0.2T_m$) which has been mainly neglected so far. For a deeper understanding of the deformation characteristics of metals under cascade damage, the interactions and reactions of dislocations with defect clusters have to be modelled in greater detail. Another direction of future work will be the investigation of the role of 1-D diffusion and direction changes of SIA clusters in partial and complete ordering of vacancy loops and voids and the generalisation of the cluster diffusion reaction kinetics for modelling such phenomena.

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