A kinetic equation of reacting loops

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MANY electron transmission microscope studies have been made of the annealing behaviour of defect clusters in quenched or neutron-irradiated crystals. In order to calculate the time-dependent size spectra of loops, Zorski's statistical theory of dislocations [1] can be modified. A kinetic equation is derived for the distribution function representing the loop density per unit radius range.

Przeprowadzono wiele badań dotyczących zjawiska wyżarzania skupisk defektów w kryształach poddawanych obróbce cieplnej lub napromieniowaniu neutronami. Dla wyznaczenia zależnych od czasu widm rozmiarów pętli zmodyfikowano statystyczną teorię dyslokacji Zorskiego [1]. Wyprowadzono równanie kinetyki dla funkcji rozkładu, przedstawiającej gęstość pętli obliczaną dla obszaru o promieniu jednostkowym.

Проведено много исследований, касающихся явления отжига скоплений дефектов в кристаллах, подвергнутых термической обработке или облучению нейтронами. Для определения зависящих от времени спектров размеров петель модифицирована статистическая теория дислокаций Зорского [1]. Выведено уравнение кинетики для функции распределения, представляющей плотность петель, рассчитанную для области единичного радиуса.

1. Introduction

MANY electron transmission microscope studies have been made of the annealing behaviour of defect clusters in quenched or neutron-irradiated crystals. Aluminium [2] and molybdenum [3] are the crystals mainly observed. There has been found a decrease of the loop density and a corresponding growth of loops during a thermal annealing. Basically two mechanisms have been proposed for explaining the experimental results. The first one explains the loop growth or shrinkage by diffusion of point defects to and from the loop via the matrix [4]. For the second mechanism it is assumed that the motion of loops in the climb direction is caused by the diffusion of atoms along the dislocation lines of the loops (the so-called pipe diffusion [5]), which has a small activation energy. The driving force for the coalescence of loops is provided by the elastic interaction existing between loops.

The experiments by MAHER [3] indicate that the interstitial loop growth observed in molybdenum can only be interpreted in terms of the second mechanism.

All informations about the experiments are hidden in the time-dependent size spectra of loops. In order to calculate the size spectra it is necessary to develop a statistical theory of dislocation loops. ZORSKI [1] has proposed such a theory. Based on an equation of motion for loops interacting by a pure elastic force, ZORSKI obtained a coupled system of hydrodynamical equations for the determination of the averaged values of the loop density, loop velocity and the averaged displacement field.

This theory can be modified for an application to the experiments. Because of the relatively weak elastic forces between the loops, the loop motion in the crystal lattice can only be caused by a diffusion mechanism and inertial forces can be disregarded. Furthermore, loop reactions are to be taken into account.

Proceeding on this basis, a kinetic equation can be derived for the distribution function representing the loop density per unit radius range. The main assumption is that the density of the loops must be low enough to ensure that the mean path of the free diffusion is large compared to the effective range of the loop interaction defined below.

2. Loop motion in the crystal lattice

We consider a system of circular prismatic dislocation loops characterized by space vectors x, radii R and identical Burgers vectors b (Fig. 1).
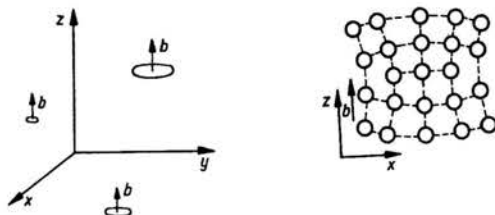

FIG. 1. Prismatic interstitial loops.

Loop motion in the crystal lattice can only be understood as a result of thermally activated processes. We have to distinguish between glide parallely to b due to nucleation of kink pairs and self-climb perpendicularly to b occuring by short circuit diffusion of atoms around the loop perimeter [5].

Correspondingly, the motion of loops is determined by different diffusivities being

$$(2.1) \qquad D_g = a^2 \frac{L}{w} \nu_0 e^{-\frac{U}{KT}}$$

in glide direction [6] and

$$(2.2) \qquad D_c = \frac{a^5}{2R^3} \nu_0 e^{-\frac{Q}{KT}}$$

in climb direction [3], where

$\quad a \quad$ the lattice constant,
$L = 2\pi R \quad$ the length of the loop,
$\quad w \quad$ the critical length of a pair of kinks,
$\quad \nu_0 \quad$ the jump frequency,
$\quad U \quad$ the activation energy for a pair of kinks,
$\quad Q \quad$ the activation energy for circuit diffusion,
$\quad T \quad$ the annealing temperature.

Because of $U \approx Q$, loops are moving much faster in glide direction than in climb direction

$$(2.3) \qquad D_g \gg D_c.$$

The motion of interacting loops can be determined by the Einstein drift equation

$$(2.4) \qquad \frac{d}{dt}\mathbf{x}_\alpha = \frac{1}{KT}\left(D_g \sum_\alpha \sum_{(\beta)} \mathbf{F}_{g\,\alpha\beta} + D_c \sum_\alpha \sum_{(\beta)} \mathbf{F}_{c\,\alpha\beta}\right).$$

The forces $\mathbf{F}_g$ and $\mathbf{F}_c$ are parallel and perpendicular to $\mathbf{b}$, respectively. The sum is to be taken over all the loops. We do not take into account external forces.

Using the infinitesimal loop approximation for the elastic interaction energy, analytical expressions of the forces exerted by one loop having the position $\mathbf{x}$ and the radius R on the other loop having the position $\mathbf{x}'$ and the radius R' can be derived [7]

$$(2.5) \qquad \begin{aligned} F_g &= \frac{BR^2 R'^2}{|\mathbf{x}-\mathbf{x}'|^4}h(\theta), \\[2mm] F_c &= -\frac{BR^2 R'^2}{|\mathbf{x}-\mathbf{x}'|^4}g(\theta), \end{aligned}$$
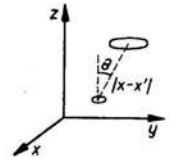
where

FIG. 2.

$$B = \frac{3\pi\mu b^2}{4(1-\nu)},$$

$$(2.6) \qquad h(\theta) = \cos\theta(3 - 30\cos^2\theta + 35\cos^4\theta),$$

$$g(\theta) = \sin\theta(1 + 10\cos^2\theta - 35\cos^4\theta).$$

The climb force $\mathbf{F}_c$ has the direction of the projection of $\mathbf{x}-\mathbf{x}'$ on the climb plane.

3. The kinetic equation

Let $\varrho(\mathbf{x}, R, t)$ denote the distribution function such that $\varrho(\mathbf{x}, R, t)d\tau dR$ is the number of loops having the positions $\mathbf{x}$ in the range $d\tau$ and radii between R and $R+dR$. Following Boltzmann's idea a kinetic equation can be derived

$$(3.1) \qquad \frac{\partial}{\partial t}\varrho(\mathbf{x}, R, t) + D_c(R)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varrho(\mathbf{x}, R, t) + D_g(R)\frac{\partial^2}{\partial z^2}\varrho(\mathbf{x}, R, t) = \left(\frac{\partial\varrho}{\partial t}\right)_{coll}.$$

The left-hand part describes the change of ϱ by diffusion without any interaction.

Now, an explicit expression must be developed for the right-hand term caused by the interaction of the loops. The calculation of $\left(\dfrac{\partial\varrho}{\partial t}\right)_{coll}$ is based on the assumption that only binary encounters need to be taken into consideration. Higher order encounters can be disregarded if the loop density is sufficiently low to ensure that the mean path of the free diffusion is large in comparison with the range of the interaction defined now.

3.1. The effective capture radius

In order to calculate binary encounters, it is necessary to study the coalescence of two loops moving by drift and diffusion. This problem cannot be solved analytically. But it is possible to disregard the diffusion of the loops for small distances and the only motion is a drift along the lines of force (drift approximation [8]). Correspondingly, the random diffusion is the essential part for large distances.

Determining the capture radius or the range of interaction of the coalescence process for two loops, we consider at first loops in the same climb plane, specially a pinned loop R at the origin, and the other loop R' at the distance r. The force F_c is reduced to ($\theta = \pi/2$)

$$(3.2) \qquad F_c = -\frac{BR'^2 R^2}{r^4}$$

and is attractive only.

The range of interaction can be characterized by the path r_0, defined by the requirement, that the loop be moving by drift in the same time as due to diffusion only. That means, the radius r_0 is determined by

$$(3.3) \qquad t_{\text{drift}}(r_0) = t_{\text{diff}}(r_0),$$

where t_{diff} is the time in which a diffusing loop situated at $x = 0$, at $t = 0$ will be found in the root-mean-square distance r_0, given by

$$r_0^2 = 4D_c t_{\text{diff}}.$$

The time $t_{\text{drift}}(r_0)$ is the solution of the drift equation

$$(3.4) \qquad \frac{dr}{dt} = -\frac{D_c}{KT}\frac{BR^2 R'^2}{r^4}, \qquad \begin{array}{l} r(0) = r_0, \\ r(t)_{\text{(drift)}} \approx 0. \end{array}$$

The result is, according to (3.3),

$$(3.5) \qquad r_0^3 = \frac{R^2 R'^2}{l_0}, \qquad l_0^{-1} = \frac{5B}{4KT}.$$

The definition of r_0 (3.5) is equivalent to a condition for the elastic interaction energy $V(r)$ caused by F_c

$$(3.6) \qquad -V(r_0) = \frac{4}{15}KT < KT$$

and means that, if r fulfills the condition (3.6), the potential energy will be less than the thermal energy of the loop in the lattice, and the effect of the potential will be relatively unimportant. A more exact definition of the capture radius could be obtained on the basis of the idea of Ham [9].

In the case that both loops, having the different diffusion constants $D_c = D_c(R)$ and $D_c' = D_c(R')$, are moving, the radius r_0 and the drift time t_{drift} satisfy the condition

$$(3.7) \qquad r_0^5 = \frac{(D_c + D_c')R^2 R'^2}{l_0} t_{\text{drift}}$$

following from the solution of the modified Eq. (3.4). Now, t_{diff} is the time in which both independently diffusing loops found at $x = 0$ at $t = 0$ will appear in the root-mean-square distance r_0. Thus

$$(3.8) \qquad r_0^2 = (D_c + D_c')t_{\text{diff}}$$

and the capture radius (3.5) is not changed when both loops are moving.

3.2. The effective capture volume

In general, we have to consider loops in different climb planes. Figure 3 shows the direction of the forces as a function of θ[Eq. (2,5)].

$$F_c(\pi - \theta) = F_c(\theta), \qquad F_g(\pi - \theta) = -F_g(\theta),$$
$$\theta_g^{(1)} \approx 30°, \qquad \theta_c \approx 53°,$$
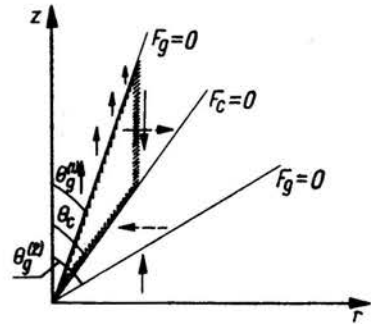$$\theta_g^{(2)} \approx 70°.$$

FIG. 3.

A coalescence of two loops is possible due to a combination of glide and climb in the angle range

$$(3.9) \qquad \theta_c < \theta < \pi - \theta_c.$$

Because of $D_g \gg D_c$ (2.3), the loops move fast in the glide direction in comparison with the motion in the climb direction. Therefore a loop moves near $\theta_g^{(2)}$ resp. $\pi - \theta_g^{(2)}$ before the coalescence. Thus the time in which a loop arrives at the origin, is approximately given by the time of motion along the line $\theta = \theta_g^{(2)}$ resp. $\theta = \pi - \theta_g^{(2)}$.

The result is

$$(3.10) \qquad r_0(\theta) \approx r_0(\theta_g^{(2)}).$$

The calculation of $r_0(\theta_g^{(2)})$ is quite similar to that of $r_0(\pi/2)$, but Eq. (3.4) is to be modified by

$$(3.11) \qquad r^4 \rightarrow (r^2 + z^2)^2 = \frac{r^4}{\sin^4 \theta_g^{(2)}} .$$

Thus [instead of (3.5)], we obtain the radius r_c for the three-dimensional capture

$$(3.12) \qquad r_c^3 = \frac{R^2 R'^2}{l}, \qquad l^{-1} = \frac{5 B \sin^4 \theta_{gi}^{(2)} g(\theta_{gk}^{(2)})}{4KT} .$$

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Defining the boundary of the so-called effective capture volume in the z-direction in such a manner as r_0 in the climb direction, we find

$$(3.13) \qquad z_g \approx r_c \tan\theta_g^{(1)}.$$

Now, a circular cylinder having the radius r_c and the height $2z_g$ can be associated with the loops R and R'. Because of the repulsive forces (Fig. 3), the bases of the cylinder act on the random diffusing loops like reflecting walls. Fig. 3 shows that only the loops R' passing the lateral area of the cylinder in the range $\theta_c < \theta < \pi-\theta_c$ coalesce with the loop R.

Let us note that this approximation of the effective capture volume is rough in the surroundings of the points $(r_0, \theta_g^{(1)})$ because the repulsive force vanishes for $\theta = \theta_g^{(1)}$.

3.3. The collision parts

It is convenient to introduce

$$(3.14) \qquad \left(\frac{\partial\varrho}{\partial t}\right)_{\text{coll}} = \left(\frac{\partial\varrho}{\partial t}\right)_{\text{coll}}^{+} - \left(\frac{\partial\varrho}{\partial t}\right)_{\text{coll}}^{-},$$

where $(\partial\varrho/\partial t)_{\text{coll}}^{-} dR$ is the number of loops deflected out of, and $(\partial\varrho/\partial t)_{\text{coll}}^{+} dR$ the number deflected into, the radius range R to $R+dR$ per unit volume per unit time.

The evaluation of the collision parts requires the knowledge of the loop current density on the lateral area $(\theta_c < \theta < \pi-\theta_c)$ of the effective reaction volume. We have to take into account that, contrary to the usual Boltzmann's equation due to the capture, the number of loops near the surface of the reaction volume could decrease in a small range in such a manner that it cannot be described by the mean density $\varrho(\mathbf{x}, R, t)$. But this diluting effect is compensated by the fast diffusion in the glide direction $(D_g \gg D_c)$. Thus the current density on the surface of the effective reaction volume is determined by the mean density of the loops multiplied by their velocity in the climb direction given by Eq. (2.4) specified for two loops

$$(3.15) \qquad v = \frac{D_c}{KT} F_c.$$

In order to evaluate $(\partial\varrho/\partial t)_{\text{coll}}^{-}$, we consider the encounters taking place in the volume element $d\tau$ between the loops in the radius range R to $R+dR$ and loops of all radii; in general, each of such encounters leads to the loss of one loop from the specified radius range.

The number of the loops reacting with a considered loop having a radius R in the given interval in time dt is determined by the number of loops of all radii R' passing the lateral area of the cylinder associated to the loop R and by a corresponding term caused by the motion of the loop R itself into the reaction volume of any other loop. Thus

$$(3.16) \qquad \left(\frac{\partial\varrho}{\partial t}\right)_{\text{coll}}^{-} = \left(\frac{\partial\varrho}{\partial t}\right)_{\substack{\text{coll} \\ \to R}}^{-} + \left(\frac{\partial\varrho}{\partial t}\right)_{\substack{\text{coll} \\ R\to}}^{-}$$

$$= \varrho(\mathbf{x}, R, t) \int dR' \varrho(\mathbf{x}, R', t) \int\int dF'\big(v(\mathbf{x}', R') + v(\mathbf{x}', R)\big).$$

The first surface integral taken over the lateral area of the cylinder of the radius r_c and the height $2z_c$

(3.17)
$$z_c = r_c \tan \theta_c$$

yields with (15), (3.1) and (3.12)

(3.18)
$$\iint dF' v(z', R') = 2\pi r_c 2 \int_0^{z_c} dz' \frac{D'_c}{KT} F_c(z', r_c)$$

$$\approx 2\pi r_c \cdot 2z_c \frac{D'_c}{KT} F_c(0, r_c) = 4\pi r_c \tan\theta_c r_c \frac{D'_c}{KT} \frac{BR^2 R'^2}{r_c^4}$$

$$= 4\pi r_c D'_c \tan\theta_c \frac{4}{5\sin^4\theta_g^{(2)} g(\theta_g^{(2)})}.$$

Thus we obtain from (3.16)

(3.19)
$$\left(\frac{\partial \varrho}{\partial t}\right)^-_{\text{coll}} = \alpha \varrho(\mathbf{x}, R, t) \int dR' \varrho(\mathbf{x}, R', t) r_c(R, R')(D'_c + D_c),$$

$$\alpha = \frac{16}{5} \pi \frac{\tan\theta_c}{\sin^4\theta_g^{(2)} g(\theta_{g1}^{(2)})}.$$

The evaluation of the collision part $(\partial \varrho/\partial t)^+_{\text{coll}}$ describing the creation of loops R due to coalescence of loops R' and R'' can be performed in the same way, if the condition of the conservation of the number of atoms forming the loops is fulfilled; that means

(3.20)
$$R^2 = R'^2 + R''^2.$$

It is found to be (appendix)

(3.21)
$$\left(\frac{\partial \varrho}{\partial t}\right)^+_{\text{coll}} = \frac{1}{2} \alpha \int_0^R dR' \frac{R}{\sqrt{R^2 - R'^2}} r_c(\sqrt{R^2 - R'^2}, R') \times$$

$$\times [D_c(R') + D_c(\sqrt{R^2 - R'^2})] \varrho(\mathbf{x}, \sqrt{R^2 - R'^2}, t) \varrho(\mathbf{x}, R', t).$$

Comparing with (3.19), it can be seen that the arguments are changed only because of the reaction condition (3.20) except the factor $R/\sqrt{R^2 - R'^2}$.

Finally, inserting (3.14) with (3.19) and (3.21) into (3.1), we find

(3.22)
$$\left[\frac{\partial}{\partial t} + D_c(R)\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + D_g(R)\frac{\partial^2}{\partial z^2}\right]\varrho(\mathbf{x}, R, t)$$

$$= \frac{1}{2}\alpha \int_0^R dR' \frac{R}{\sqrt{R^2 - R'^2}} r_c(\sqrt{R^2 - R'^2}, R')(D_c(R') + D_c(\sqrt{R^2 - R'^2})) \times$$

$$\times \varrho(\mathbf{x}, \sqrt{R^2 - R'^2}, t)\varrho(\mathbf{x}, R', t)$$

$$- \alpha \int_0^\infty dR' r_c(R, R')(D_c(R) + D_c(R'))\varrho(\mathbf{x}, R, t)\varrho(\mathbf{x}, R', t),$$

where

$$(3.23) \quad r_c^3 = \frac{R^2 R'^2}{l}, \quad l^{-1} = \frac{15\pi}{16} \frac{\sin^4\theta_g^{(2)} g(\theta_g^{(2)})}{1-\nu} \frac{\mu b^2}{KT} \approx \frac{4}{1-\nu} \frac{\mu b^2}{KT},$$

$$\alpha \approx \frac{16}{5}\pi \frac{\tan\theta_c}{\sin^4\theta_g^{(2)} g(\theta_g^{(2)})} \approx 10.$$

4. Discussion

The conditions for the validity of the kinetic Eq. (3.22) are the same as for Boltzmann's equation. The mean path of the free diffusion must be large compared to the effective range of the loop interaction r_c; therefore we have to assume

$$(4.1) \qquad nr_c^3 \ll 1,$$

where n denotes the mean loop density.

The structure of the collision parts in the kinetic equation leads to the time

$$(4.2) \qquad \tau^{-1} = \alpha nr_c D_c$$

characterizing the time of the change of the loop density. The time of a collision of two loops is given by $t_{\mathrm{drift}}(r_c) = t_{\mathrm{diff}}(r_c) \approx r_c^2/D_c$. This yields with (4.1)

$$(4.3) \qquad \tau = \frac{t_{\mathrm{drift}}}{\alpha nr_c^3} \gg t_{\mathrm{drift}}.$$

Thus the condition for binary encounters is fulfilled because the characteristic time is much greater than the collision time.

Finally, the time-dependence of the properties of the loop distribution may be discussed. The balance equation for a loop property $Q(R)$ can be found directly from the kinetic Eq. (3.22) by multiplying both sides of the equation by $Q(R)$ and integrating over R. Thus

$$(4.4) \quad \frac{\partial}{\partial t}\int_0^\infty dR Q(R)\varrho(\mathbf{x}, R, t) + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\int_0^\infty dR Q(R) D_c(R)\varrho(\mathbf{x}, R, t)$$

$$+ \frac{\partial^2}{\partial z^2}\int_0^\infty dR Q(R) D_g(R)\varrho(\mathbf{x}, R, t)$$

$$= \frac{1}{2}\alpha\int_0^\infty dR \int_0^R dR' Q(R) \frac{R}{\sqrt{R^2-R'^2}} r_c(\sqrt{R^2-R'^2}, R')(D_c(R') + D_c(\sqrt{R^2-R'^2})) \times$$

$$\times \varrho(\mathbf{x}, \sqrt{R^2-R'^2}, t)\varrho(\mathbf{x}, R', t)$$

$$-\alpha\int_0^\infty dR \int_0^\infty dR' Q(R) r_c(R, R')(D_c(R) + D_c(R'))\varrho(\mathbf{x}, R, t)\varrho(\mathbf{x}', R', t).$$

Substituting $R'' = \sqrt{R^2 - R'^2}$ in the integral before the last one and using the symmetry of the integrand, the equation becomes

$$(4.5) \quad \frac{\partial}{\partial t} \int_0^\infty dR Q(R) \varrho(\mathbf{x}, R, t) + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \int_0^\infty dR Q(R) D_c(R) \varrho(\mathbf{x}, R, t)$$

$$+ \frac{\partial^2}{\partial z^2} \int_0^\infty dR Q(R) D_s(R) \varrho(\mathbf{x}, R, t)$$

$$= \alpha \int_0^\infty dR'' \int_0^\infty dR' [Q(\sqrt{R''^2 + R'^2}) - Q(R') - Q(R'')] r_c(R'', R') \times$$

$$\times D_c(R') \varrho(\mathbf{x}, R'', t) \varrho(\mathbf{x}, R', t).$$

The number of loops is given by

$$(4.6) \qquad\qquad N(t) = \int d\tau \int_0^\infty dR \varrho(\mathbf{x}, R, t).$$

Thus Eq. (4.4) yields by integration over $\mathbf{x}$ with $Q = 1$

$$(4.7) \qquad \frac{\partial N}{\partial t} = -\alpha \int d\tau \int_0^\infty dR'' \int_0^\infty dR' r_c(R'', R') D_c(R') \varrho(\mathbf{x}, R'', t) \varrho(\mathbf{x}, R', t).$$

The right-hand side is less than zero, such that

$$(4.8) \qquad\qquad\qquad \frac{\partial N}{\partial t} < 0.$$

The number of loops decreases with the time due to the coalescence.

The area of a loop is πR^2. Hence

$$(4.9) \qquad\qquad s(\mathbf{x}, t) = \int_0^\infty dR \pi R^2 \varrho(\mathbf{x}, R, t)$$

gives the sum over the areas of the loops at the position $\mathbf{x}$ per unit volume.

Choosing $Q = \pi R^2$, the collision parts in (4.5) vanish and it follows

$$(4.10) \quad \frac{\partial}{\partial t} s + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \int_0^\infty dR \pi R^2 D_c(R) \varrho(\mathbf{x}, R, t) + \frac{\partial^2}{\partial z^2} \int_0^\infty dR \pi R^2 D_s(R) \varrho(\mathbf{x}, R, t) = 0.$$

This result is in accordance with the fact that loop reactions do not change the area of loops. The loop area in any volume can only be changed by diffusion of the loops through the surface of this volume.

The mean value of R^2 is defined by

$$(4.11) \qquad\qquad \overline{R^2}(t) = \frac{1}{N(t)} \int d\tau \int_0^\infty dR R^2 \varrho(\mathbf{x}, R, t).$$

Then

$$(4.12) \qquad\qquad N \frac{\partial \overline{R^2}}{\partial t} = \frac{\partial}{\partial t} \int d\tau \int_0^\infty dR R^2 \varrho(\mathbf{x}, R, t) - \overline{R^2} \frac{\partial N}{\partial t}.$$

Taking into account Eqs. (4.8) and (4.10), there follows

(4.13)
$$N\frac{\overline{\partial R^2}}{\partial t} = -\overline{R}^2\frac{\partial N}{\partial t} > 0.$$

The area per loop increases with time.

Acknowledgements

Appendix

The number z of loops produced per unit volume per unit time with the radii $R' \leqslant R$ and $(\partial\varrho/\partial t)^+_{\text{coll}}$ are connected by

$$z(R) = \int\limits_0^R dR'\left(\frac{\partial\varrho}{\partial t}\right)^+_{\text{coll}}$$

or

$$\frac{dz(R)}{dR} = \left(\frac{\partial\varrho}{\partial t}\right)^+_{\text{coll}}.$$

Comparing with the evaluation of $(\partial\varrho/\partial t)^-_{\text{coll}}$, the number $z(R)$ of loops becomes

$$z(R) = \frac{1}{2}\alpha\int\limits_0^\infty dR'\int\limits_0^\infty dR''r_c(R', R'')(D_c(R')+D_c(R''))\times$$
$$\times\theta(R-\sqrt{R'^2+R''^2})\,\varrho(\mathbf{x}, R', t)\varrho(\mathbf{x}, R'', t),$$

where

$$\theta(R) = \begin{cases} 0 & R < 0, \\ 1 & R > 0, \end{cases}$$

and

$$\frac{d\theta(R)}{dR} = \delta(R).$$

The additional factor $1/2$ results from the fact that the motion of the loop R' to R'' as well as the motion of the loop R'' to R' are counted twice in the double integral.

Thus it follows that

$$\left(\frac{\partial \varrho}{\partial t}\right)^{+}_{\text{coll}} = \frac{1}{2}\alpha \int\limits_{0}^{\infty} dR' \int\limits_{0}^{\infty} dR'' \, Z_c(R', R'') r_c(R', R'') (D_c(R')+D_c(R'')) \times$$

$$\times \delta(R-\sqrt{R'^2+R''^2}) \varrho(\mathbf{x}, R', t) \varrho(\mathbf{x}, R'', t).$$

Using the formula

$$\delta(w(y)) = \sum_{i} \frac{\delta(y-y_i)}{\left|\dfrac{\partial w(y)}{\partial y}\right|_{y=y_i}},$$

where y_i are the zeros of the function $w(y)$, we find the result (3.21).

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