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KINETIC STRESS TENSOR IN STATISTICAL THEORY OF SCREW PARALLEL DISLOCATIONS

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1. Introduction

This paper is continuation of and supplement to [1]. In [1] a statistical analysis of parallel straight screw dislocations in an infinite linear solid body $\mathscr{B}$ was perfomed following essentially the ideas explored in [2] and [3]. As a consequence, the field equations governing the mean (continuum average) behaviour were derived. However, a set of field equations derived by means of statistical methods cannot be a full set and we had to specify some constitutive relation for kinetic stress tensor

$$\overset{K}{\sigma}_{ij}(x_m, t) \overset{\text{def}}{=} -m_{ip} \sum_{\Gamma} \langle (\dot{\underset{\Gamma}{\zeta}}_j - V_j)(\dot{\underset{\Gamma}{\zeta}}_p - V_p) \underset{\Gamma}{\delta} \rangle . \tag{1.1}$$

In the above expression m_{ip} is mass of dislocation line per unit length, $\dot{\underset{\Gamma}{\zeta}}(j=1, 2)$ is the velocity of dislocation line Γ, $\underset{\Gamma}{\delta}$ — Dirac delta function and V_j the average dislocation velocity in x_m at instant t. In the above mentioned paper we assumed the constitutive relation for $\overset{K}{\sigma}_{ij}$ in the form

$$\overset{K}{\sigma}_{ij} = -m_{ij}\, p(\alpha), \quad p(\alpha) = p_0 (\alpha/\alpha_0)^{\gamma} \equiv B \alpha^{\gamma}, \tag{1.2}$$

where α is the average dislocation density while p_0, α_0 and γ are some constants.

We are going to reexamine this assumption in the following text.

2. Statistical equilibrium

Let V be the volume of the considered solid body $\mathscr{B}$. The body contains N parallel screw dislocations and no external forces or other influences are acting on $\mathscr{B}$. The total energy of all the dislocations per unit length amounts to [4]:

$$H_0 = K + U, \tag{2.1}$$

where

(2.2) $$K=\frac{1}{2}\sum_{\Gamma=1}^{N} m_{ip}\,\dot{\underset{\Gamma}{\zeta_i}}\,\dot{\underset{\Gamma}{\zeta_p}}$$

is total kinetic energy of all the dislocations and

(2.3) $$U=U(\underset{\sim}{\zeta}_1-\underset{\sim}{\zeta}_2,\underset{\sim}{\zeta}_1-\underset{\sim}{\zeta}_3,\ldots,\underset{\sim}{\zeta}_{N-1}-\underset{\sim}{\zeta}_N)\equiv$$

$$\equiv U(\zeta_{12},\zeta_{13},\ldots,\zeta_{N-1,N})=\sum_{\substack{\Gamma,\Delta=1\\ \Gamma<\Delta}}^{N} U(\zeta_{\Gamma\Delta})\equiv$$

$$\equiv\sum_{\substack{\Gamma,\Delta=1\\ \Gamma<\Delta}}^{N} U_{\Gamma\Delta}=\frac{1}{2}\sum_{\substack{\Gamma,\Delta=1\\ \Gamma\neq\Delta}}^{N} U_{\Gamma\Delta}$$

is total potential energy of the dislocation distribution. In (2.2)

(2.4) $$m_{ip}=\delta_{ip}m^*=\delta_{ip}(\rho_0 b^2/4\pi)\ln(r/b),$$

where b is Burgers vector, ρ_0 — density of matter and r — some characteristic length. On the other hand, potential energy for two parallel screw dislocations with the same Burgers vectors equals:

(2.5) $$U_{\Gamma\Delta}=\frac{\mu b^2}{4\pi}\left\{2\left(r_{\Gamma\Delta}-\sqrt{1+r_{\Gamma\Delta}^2}\right)+\ln\frac{1+\sqrt{1+r_{\Gamma\Delta}^2}}{\sqrt{1+r_{\Gamma\Delta}^2}-1}\right\},\quad r_{\Gamma\Delta}\equiv\frac{\zeta_{\Gamma\Delta}}{L},$$

where $\zeta_{\Gamma\Delta}$ is the shortest distance between Γ and Δ dislocations and L — the dislocation length.

Let us now imagine that body $\mathcal{B}$ is divided into two parts D and D', the part D being of volume ΔV that is much smaller that V and containing n dislocations ($n\ll N$). Their total energies per unit length are

(2.6) $$H\equiv H_D=\frac{1}{2}\sum_{\Gamma=1}^{n} m_{ip}\,\dot{\underset{\Gamma}{\zeta_i}}\,\dot{\underset{\Gamma}{\zeta_p}}+\frac{1}{2}\sum_{\substack{\Gamma,\Delta=1\\ \Gamma\neq\Delta}}^{n} U_{\Gamma\Delta},$$

(2.7) $$H_{D'}=\frac{1}{2}\sum_{\Gamma=n+1}^{N} m_{ip}\,\dot{\underset{\Gamma}{\zeta_i}}\,\dot{\underset{\Gamma}{\zeta_p}}+\frac{1}{2}\sum_{\substack{\Gamma,\Delta=n+1\\ \Gamma\neq\Delta}}^{N} U_{\Gamma\Delta}\equiv H',$$

(2.8) $$H_{DD'}=\frac{1}{2}\left(\sum_{\substack{\Gamma,\Delta=1\\ \Gamma\neq\Delta}}^{N}-\sum_{\substack{\Gamma,\Delta=1\\ \Gamma\neq\Delta}}^{n}-\sum_{\substack{\Gamma,\Delta=n+1\\ \Gamma\neq\Delta}}^{N}\right)U_{\Gamma\Delta},$$

so that

(2.9) $$H_0=H+H'+H_{DD'},$$

where $H_{DD'}$ is the interaction energy between D and D'. Assuming that interaction between D and D' is weak and that there are no external influences on $\mathcal{B}$ we have

(2.10) $$H_0 = \text{const} \simeq H + H',$$

and dislocations may be regarded so as to be in a statistically defined equilibrium· On the other hand

(2.11) $$n + n' = N,$$

where $n \in \Delta V$, $n' = N - n \in (V - \Delta V)$ and n can change with time. Consequently, there exists a strong analogy with an insulated thermodynamic system of particles $D + D'$ consisting of a small system D, heat reservoir D' and a perforated partition between them allowing particles to come from D to D' and vice versa.

Let $\Omega'(N-n, H_0 - H)$ denote the numb:r of states accessible to reservoir D' if the system D contains n dislocations and has some specified energy H.*

The corresponding probability for system D to have energy H and number of dislocations n is

(2.12) $$P_D(n, H) = C'\,\Omega'(N-n, H_0 - H) \equiv C'\,\Omega'(n', H').$$

Now, since $n \ll N$ and $H \ll H_0$ the expression on the right side of (2.12) may be replaced by its first order approximation

(2.13) $$\ln \Omega'(N-n, H_0 - H) = \ln \Omega'(N, H_0) - H\{\partial \ln \Omega'/\partial H'\}_0 - \\ - n\{\partial \ln \Omega'/\partial n'\}_0.$$

Denoting the above constants by

(2.14) $$\beta \equiv \{\partial \ln \Omega'/\partial H'\}_{H=0,\, n=0}, \quad \gamma \equiv \{\partial \ln \Omega'/\partial n'\}_{H=0,\, n=0},$$

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*) If kinetic energy of dislocations is disregarded, then for a crystal with n parallel screw dislocations and $\mathcal{N}^2$ atoms in cross section the number of accessible states amounts to

(a) $$\Omega = (\mathcal{N}^2)!/(\mathcal{N}^2 - n)!\, n!$$

The corresponding so called "configuration" entropy [5] equals

(b) $$S = k \ln \Omega,$$

where k is Boltzmann's constant. By means of Stirling's epproximation we finally have

(c) $$S \simeq k\,\mathcal{N}^2 \ln (\mathcal{N}^2/(\mathcal{N}^2 - n)) + k n \ln ((\mathcal{N}^2 - n)/n) = \\ = -k\,\mathcal{N}^2 \{\alpha \ln \alpha + (1-\alpha) \ln (1-\alpha)\}$$

where $\alpha = n/\mathcal{N}^2$ is the dislocation density.

we obtain

$$\Omega'(N-n, H_0-H)=\Omega'(N, H_0)\exp(-\beta H-\gamma n) \tag{2.15}$$

and

$$P_D(n, H)=C\exp(-\beta H-\gamma n). \tag{2.16}$$

Therefore, as should be expected, we obtained "grand canonical" distribution for dislocation lines. The constants β and γ define statistical equilibrium between the systems D and D' and in the case of molecules of a gas they are given the names: temperature parameter $\beta=1/kT$ and chemical potential parameter — γ/β of the systems considered. The first defines the equality of temperatures in equilibrium and the second one is connected with diffusion (chemical concentration).

The mean energy $\overline{H}$ and the mean number of dislocations $\overline{n}$ in ΔV are

$$\overline{H}=\frac{\Sigma H\exp(-\beta H-\gamma n)}{\Sigma\exp(-\beta H-\gamma n)}=-\frac{\partial}{\partial\beta}\ln\Sigma\exp(-\beta H-\gamma n), \tag{2.17}$$

$$\overline{n}=\frac{\Sigma n\exp(-\beta H-\gamma n)}{\Sigma\exp(-\beta H-\gamma n)}=-\frac{\partial}{\partial\gamma}\ln\Sigma\exp(-\beta H-\gamma n). \tag{2.18}$$

As usually, the expression

$$Z\equiv\Sigma\exp(-\beta H-\gamma n) \tag{2.19}$$

is called partition function of the system. The summation should be taken over all possible states of the system D. For fixed n we have for the partition function

$$Z=\frac{1}{n!}\int\cdots\int\exp(-\beta H)\exp(-\gamma n)\frac{1}{h^{2n}}d^2\underset{\sim}{\zeta}_1\ldots d^2\underset{\sim}{\zeta}_n d^2\underset{\sim}{p}_1\ldots d^2\underset{\sim}{p}_n= \tag{2.20}$$
$$=\frac{\exp(-\gamma n)}{n!\,h^{2n}}\int\cdots\int\exp(-\beta H)\,d^2\underset{\sim}{\zeta}_1\ldots d^2\underset{\sim}{p}_n,$$

where h^2 is the area of a cell into which ΔA (cross section of ΔV) is subdivided and $n!$ appears because of indistinguishability of dislocation lines in ΔV. Further, (2.20) may be splitt into

$$Z=\frac{\exp(-\gamma n)}{n!\,h^{2n}}\left\{\int\cdots\int\exp\left(-\frac{1}{2}\beta m^*\sum_{\Gamma=1}^{n}\dot{\zeta}_{i\,\Gamma}\dot{\zeta}_{i\,\Gamma}\right)d^2\underset{\sim}{p}_1\ldots d^2\underset{\sim}{p}_n\right\}Z_U= \tag{2.21}$$
$$=\frac{\exp(-\gamma n)}{n!}\left(\frac{2\pi m^*}{\beta h^2}\right)^n Z_U,$$

where

$$Z_U\equiv\int\cdots\int\exp\left[-\frac{\beta}{2}\sum_{\substack{\Gamma,\Delta=1\\ \Gamma\neq\Delta}}^{n}U(\zeta_{\Gamma\Delta})\right]d^2\underset{\sim}{\zeta}_1\ldots d^2\underset{\sim}{\zeta}_n. \tag{2.22}$$

Suppose that some external parameter of system D, say x, is changed by infinitesimal amount δx. The corresponding macroscopic work δW done by the system D as a result of this change amounts to

$$\delta W = \frac{\Sigma \exp(-\beta H - \gamma n)\,(-\partial H/\partial x)\,\delta x}{\Sigma \exp(-\beta H - \gamma n)} = \tag{2.23}$$

$$= \frac{\delta x}{\beta}\,\frac{\Sigma \exp(-\gamma n)\,\partial\{\exp(-\beta H)\}/\partial x}{\Sigma \exp(-\beta H - \gamma n)}$$

and if $\partial n/\partial x = 0$, then

$$\delta W = \frac{1}{\beta}\,\frac{\partial}{\partial x}\{\ln \Sigma \exp(-\beta H - \gamma n)\}\,\delta x = \frac{1}{\beta}\left(\frac{\partial}{\partial x}\ln Z\right)\delta x = Q_x\,\delta x, \tag{2.24}$$

where Q_x is the mean generalized force.

Let us now return to (1.1). Taking into account (2.4) and the equal probability of all the directions for velocities of dislocation lines it is reasonable to assume that kinetic stress tensor has the following form

$$\overset{K}{\sigma}_{ij}(x_m, t) = -m^* \sum_{\Gamma} \langle (\dot{\zeta}_i - V_i)_{\Gamma}\, (\dot{\zeta}_j - V_j)_{\Gamma}\, \delta_{\Gamma} \rangle = \delta_{ij}\,\overset{K}{\sigma}. \tag{2.25}$$

Now, if $x = \Delta A$ then $Q_x = \overset{K}{\sigma}$ and by means of (2.21) and (2.24) we have

$$\overset{K}{\sigma} = \frac{1}{\beta}\,\frac{\partial}{\partial(\Delta A)}\ln Z = \frac{1}{\beta}\,\frac{\partial}{\partial(\Delta A)}\ln Z_U. \tag{2.26}$$

From (2.5) and (2.22) it is seen that

$$\ln Z_U = f_1(\beta, \Delta A), \tag{2.27}$$

or, with $\alpha = n/\Delta A$,

$$\ln Z_U = f(\alpha, \beta), \tag{2.28}$$

so that

$$\overset{K}{\sigma} = \frac{1}{\beta}\,\frac{\partial}{\partial \alpha} f(\alpha, \beta) = kT\,\frac{\partial}{\partial \alpha} f(\alpha, kT). \tag{2.29}$$

Finally, if dislocation "gas" is sufficiently dilute a rather good approximation to it would be a van der Waals gas and by means of "virial expansion" [7], [8] we obtain

$$\overset{K}{\sigma} = \frac{1}{\beta}\left\{\frac{n}{\Delta A} - \frac{1}{2}\,\frac{n^2}{(\Delta A)^2}\,I(\beta)\right\} = \tag{2.30}$$

$$= \frac{1}{\beta}\left\{\alpha - \frac{1}{2}\,\alpha^2 I(\beta)\right\} \equiv kT\left\{\alpha - \frac{1}{2}\,\alpha^2 I(kT)\right\}.$$

We may conclude this paper by the following statement. Even in the very simplified case when no obstacles to dislocation motion are taken into account, temperature and thermal activation appear as mostly significant. The above expressions (2.29) and (2.30) might be improved by applying the same method to more realistic dislocation and other defects arrangements.

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LE TENSEUR CINETIQUE DU TENSION DANS LA THEORIE STATISTIQUE DES DISLOCATIONS SPIRALES PARALLELS

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Résumé

La fonction constitutive pour le tenseur cinétique du tension de la disposition de dislocation est dérivée au moyen de la fonction d'après l'équilibre défini par la statistique.

On a montré que cette fonction dépend de la densité des dislocations ainsi que de la température.

КИНЕТИЧКИ ТЕНЗОР НАПОНА У СТАТИСТИЧКОЈ ТЕОРИЈИ ЗАВОЈНИХ ПАРАЛЕЛНИХ ДИСЛОКАЦИЈА

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Резиме

Конститутивна функција за кинетички тензор напона дислокационог распореда је изведена помоћу функције раздељивања на основу статистички дефинисане равнотеже. Показано је да ова функција зависи од густине дислокација и температуре.

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