

Some implications of the second law of Newton on dislocation creep

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Abstract. We develop some elements of the statistical mechanics for mobile dislocations, which allow us to give a dynamical description of the center of mass of the mobile dislocation system with Newton's second law. The two fundamental equations of plastic deformation (*i.e.* the Orowan equation and the Fuchs and Ilshner equation) are given a new interpretation within the statistical mechanics framework. Also it is shown that the acceleration of mobile dislocations is responsible for the stability of the steady states under fluctuations.

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1. Introduction

Usually for steady state dislocation creep the acceleration of dislocations is neglected. However, for the transient stages of plastic deformation the situation is quite different. For these stages it is known that the accelerations of dislocations is important in cases where stress, σ , or the average internal stress, $\langle\sigma_i\rangle$, changes with time. During plastic deformation such changes in the stresses may occur in an abrupt way or in a more continuous way. For the first case we have situations such as a sudden change on the applied stress during a creep test [1], or an internal friction tests [2-4], and anomalies in the yield stress of superconductor materials near the transition temperature [5-8]. The second case usually presents the creep transient which arises during primary creep. The qualitative features of the deformation rate, $\langle\dot{\epsilon}\rangle$, have been explained considering the acceleration of dislocations for certain cases of creep transients [9-11]. Essentially Gasca-Neri, Ahlquist and Nix [10], and Mejía and Mendoza [11] follow the Fuchs and Ilshner approach [9], who performed a time derivation of the Orowan equation obtaining a mathematical expression for $d\langle\dot{\epsilon}\rangle/dt$, namely, starting from

$$\langle\dot{\epsilon}\rangle = \alpha b \rho_m \langle v \rangle. \quad (1)$$

The Fuchs and Ilshner equation reads

$$\frac{d\langle\dot{\epsilon}\rangle}{dt} = \alpha b \left(\langle v \rangle \frac{d\rho_m}{dt} + \rho_m \frac{d\langle v \rangle}{dt} \right), \quad (2)$$

where α is the average geometrical factor relating the tensile deformation to the shear deformation for polycrystalline samples, b is the magnitude of the Burgers' vector, ρ_m is the mobile dislocation density and, $\langle v \rangle$ is the average glide velocity of mobile dislocations.

Eqs. (1) and (2) are the fundamental equations on dislocation creep, and because of that it is interesting to make a brief mention about their original method of derivation and their meaning. The derivation of the Orowan equation, Eq. (1), is based on topological properties of the edge dislocations [12], and it yields the strain rate of the material under plastic deformation. On the other hand, the Fuchs and Ilshner equation, Eq. (2), is obtained from a mathematical manipulation of the Orowan equation (its time derivative), and it yields the rate of change of the strain rate.

From our point of view other interpretations for the fundamental equations on dislocation creep may be given, and we consider one that is based on a statistical approach for the description of the acceleration of mobile dislocations.

Our main purpose is to show that the Fuchs and Ilshner equation is the appropriate dynamical description for the motion of the center of mass of the mobile dislocation system through Newton's second law expressed in a volumetric way. Therefore, the Orowan equation may be interpreted in terms of the volumetric density of linear momentum of the mobile dislocations. Also we show that a theoretical explanation of the stability of the steady states is only possible if the acceleration of mobile dislocations is taken into account.

2. The second law of Newton and the equation of motion for the mobile dislocation system

We know that one-dimensional dislocations are solitons [13,14]. The first treatment in such a scheme was developed in 1939 by Frenkel and Kontorova [15]. The dynamical behavior of the mass center of a system of solitons is governed by Newton's second law [16]. Then the motion of a "gas" of one-dimensional dislocations can be described in terms of the dynamical properties of its center of mass. The previous ideas suggest that, in general, the mobile dislocation system from a real crystal under deformation obeys the second law of Newton too. In order to prove such a hypothesis our analysis starts from the equation of motion per unit length of an edge dislocation. Further, we develop some elements of the statistical mechanics of mobile dislocations.

In order to emphasize the physical ideas, let us consider the plastic deformation due to dislocations gliding in a material with only one active slip system.

The equation of motion per unit length of an edge dislocation [17,18] is

$$m \frac{dv}{dt} = (\tau - \tau_{il})b - F_d, \quad (3)$$

where m is the mass per unit length of dislocation (assumed to be constant), v is the glide velocity, τ is the applied shear stress on the glide plane, and τ_{il} is the local internal shear stress which opposes to τ . F_d is a dissipative force due to glide, which is called the drag force per unit length [1]. For our purpose it is enough to know that in general F_d has a zero value only when a dislocation has no gliding or vibrational movement (an exception is treated by Flytzanis *et al.* [19] for the soliton-like motion of a dislocation in a lattice at 0 Kelvin degrees).

In a solid undergoing deformation, there exists a local inhomogenous density of mobile dislocations gliding at different velocities depending on the local configuration of dislocations they face. Taking this information in consideration *Li* [21], describes certain features of plastic deformation by using a distribution function of the radii of curvature. We generalize such scheme by defining a distribution function $N(\mathbf{r}, v)$ for the number of unit lengths of mobile dislocations having a position between \mathbf{r} and $\mathbf{r} + d\mathbf{r}$ and velocities between v and $v + dv$. Then the mobile dislocation density, ρ_m , and the average of any function of the system are defined respectively by

$$\rho_m = \int \int N(\mathbf{r}, v) d^3\mathbf{r} dv, \quad (4)$$

$$\langle \phi \rangle = \frac{\int \int N(\mathbf{r}, v) \phi d^3\mathbf{r} dv}{\int \int N(\mathbf{r}, v) d^3\mathbf{r} dv}. \quad (5)$$

Now, with the theoretical elements previously described, we proceed to analyze the dynamical behavior of the mobile dislocation system. This can be obtained by making a summation of the volumetric force acting on mobile dislocations when its density is constant and the volumetric force necessary to incorporate or desincorporate dislocations to the gliding process. During a creep test in general ρ_m is not a constant. but we may choose an interval of time $\delta t'$ small enough so that creation or annihilation events are negligible and ρ_m remains constant. If for this $\delta t'$ it is supposed that all mobile dislocations glide with an average velocity, $\langle v \rangle$, then the volumetric force acting on ρ_m is given by ρ_m times the average of Eq. (3), and using Eq. (5), one gets

$$m\rho_m \frac{d\langle v \rangle}{dt} = \rho_m [(\tau - \langle \tau_{il} \rangle)b - \langle F_d \rangle], \quad (6)$$

where the principle of superposition of forces [22], was used; this principle is valid in the linear theory of elasticity [23].

If we consider an interval of time dt bigger than $\delta t'$ then the value of ρ_m is not a constant. During this interval of time ρ_m can change due to an increment or a

decrement in the quantity of mobile dislocations. The increment of ρ_m is denoted by $d\rho_m^+$ and is due to generation of new dislocations and liberation of dislocations previously immobilized. The decrement on ρ_m is denoted by $d\rho_m^-$ and is due to immobilization of previously mobile dislocations.

The force per unit length required to accelerate a newly generated dislocation (or liberated one) is mdv/dt as given by Eq. (3). Supposing that all these dislocations start from rest and reach the average glide velocity, $\langle v \rangle$, in a infinitesimal fraction of dt , and using the principle of superposition of forces, the volumetric density of force acting on $d\rho_m^+$ is $m\langle v \rangle \frac{d\rho_m^+}{dt}$. A similar analysis can be done for $d\rho_m^-$. This analysis gives us the volumetric density of force acting on a fraction of mobile dislocations in order to immobilize them. This volumetric force is equal to $-m\langle v \rangle \frac{d\rho_m^-}{dt}$. Then the total volumetric force on the mobile dislocation system because of the total change in its density is

$$m\langle v \rangle \left(\frac{d\rho_m^+}{dt} - \frac{d\rho_m^-}{dt} \right) \equiv m\langle v \rangle \frac{d\rho_m}{dt}. \quad (7)$$

Using Eqs. (6) and (7), the total force per unit volume acting on the mobile dislocation system, $\langle f \rangle$ is

$$\langle f \rangle = m\rho_m \frac{d\langle v \rangle}{dt} + m\langle v \rangle \frac{d\rho_m}{dt} = \frac{d}{dt}(m\rho_m\langle v \rangle) = \frac{d}{dt}\langle p \rangle. \quad (8)$$

In other words, using the Orowan equation

$$\langle f \rangle = \frac{m}{\alpha b} \frac{d}{dt}\langle \dot{\epsilon} \rangle. \quad (8.a)$$

In this frame, the Orowan and Fuchs and Ilshner equations appear with an additional interpretation to the one described in section 1. The physical meaning of the Fuchs and Ilshner equation is as follow. Since $\frac{d\langle \dot{\epsilon} \rangle}{dt} \sim \langle f \rangle$, this equation is related to the volumetric net force which describes the dynamical behavior of the center of mass of the mobile dislocation system. And, the key element for this interpretation is that the volumetric linear momentum which appears in the second law of Newton is related to the strain rate as given by the Orowan equation.

In the next section, it will be shown that one condition for the stability of steady states under fluctuations is given by the Fuchs and Ilshner equation. This result will be obtained by using a creep model independent from our model. Also it is shown that the acceleration of mobile dislocations plays a fundamental role in a plastic deformation during steady state, contrary to previous theoretical considerations.

3. Fluctuations, acceleration of dislocations and stability of steady states

Usually, the creep tests are carried on annealed samples by applying constant stress, σ , and temperature, T , at temperature above 0.5 the melting temperature in Kelvin degrees. During a creep test the values of σ and T fluctuate around the chosen values, because of intrinsic characteristics of any experimental system. These changes in σ and T occur also during steady states and induce microstructural changes in the sample under plastic deformation, in such a way that the stability of steady states under fluctuations is an experimental fact commonly observed. A theoretical demonstration of this fact was achieved only in recent times [24].

This demonstration due to Montemayor-Aldrete *et al* [24] was obtained by analyzing the implications of the condition of compatibility of two complementary creep schemes. The first one with a microscopical emphasis on the microscopical defects of the crystals under deformation [1]. The second with macroscopical emphasis in the description of the curves of deformation versus time, during transient and steady stages of deformation [25]. Montemayor-Aldrete *et al.* have shown that for steady state creep, the microstructural-defect-vector \mathbf{S} is a constant vector, where \mathbf{S} is given by $\mathbf{S} = (S_1, S_2, \dots, S_n)$ with $S_1 = \rho_m$, $S_2 = \rho_T$ (ρ_T the total dislocation density), $S_3 = R$ (R the cell size of dislocations), etc. Hence, all the elements of a defect configuration which might be considered relevant for the description of plastic deformation are specified. Also for steady state this model has shown that every function ϕ with \mathbf{S} dependence is also a constant. There ϕ can be $\langle \dot{\epsilon} \rangle$, or the creation rate of entropy of the system, the volumetric density of kinetical energy of mobile dislocations, etc.

In this section we apply an approximation of the model described above, in order to show that the stability of steady states under fluctuations involves acceleration of dislocations and needs to be explained by using the Fuchs and Ilschner equation.

For Steady State the model gives a continuity equation for each component S_i of \mathbf{S}

$$\frac{\partial S_i}{\partial t} + \sum_{j \neq i}^n \frac{\partial S_i}{\partial S_j} \frac{dS_j}{dt} = 0, \quad (9)$$

where $j \neq i$; also, every function ϕ with \mathbf{S} dependence obeys the following equation

$$\frac{d\phi}{dt} = \sum_j^n \frac{\partial \phi}{\partial S_j} \frac{dS_j}{dt} = 0. \quad (10)$$

In order to obtain practical conclusions from Eqs. (9) and (10), the vector \mathbf{S} will be approximated by its two first components, then $\mathbf{S} = (\rho_m, \rho_T)$. Following the Bird, Mukherjee and Dorn approach [26], the average value of the internal shear stress, $\langle \tau_i \rangle$ is proportional to $(\rho_T)^{1/2}$. From the analysis of Ahlquist, Gasca-Neri and Nix [27], the average velocity of mobile dislocations is proportional to $(\alpha\sigma - \langle \tau_i \rangle)^n$. Therefore, (ρ_m, ρ_T) can be transformed into another space given by $\mathbf{S} = (\rho_m, \langle v \rangle)$.

And using Eqs. (9), the following set of conditions for the stability under fluctuations for components of the defect vector \mathbf{S} in steady state is obtained:

$$\begin{aligned} \frac{d\rho_m}{dt} &= \frac{\partial\rho_m}{\partial t} + \frac{\partial\rho_m}{\partial\langle v \rangle} \frac{d\langle v \rangle}{dt} = 0; \\ \frac{d\langle v \rangle}{dt} &= \frac{\partial\langle v \rangle}{\partial t} + \frac{\partial\langle v \rangle}{\partial\rho_m} \frac{d\rho_m}{dt} = 0. \end{aligned} \tag{11}$$

Now taking ϕ as $\phi = \langle \dot{\epsilon} \rangle = \alpha b \rho_m \langle v \rangle$ and using Eq. (10), the condition for stability of $\langle \dot{\epsilon} \rangle$ is obtained, namely

$$\begin{aligned} \frac{d\langle \dot{\epsilon} \rangle}{dt} &= \frac{\partial\langle \dot{\epsilon} \rangle}{\partial\rho_m} \frac{d\rho_m}{dt} + \frac{\partial\langle \dot{\epsilon} \rangle}{\partial\langle v \rangle} \frac{d\langle v \rangle}{dt} \\ &= \alpha b \left(\langle v \rangle \frac{d\rho_m}{dt} + \rho_m \frac{d\langle v \rangle}{dt} \right) = 0, \end{aligned} \tag{12}$$

which is the Fucks and Ilschner equation.

The set of Eqs. (11) and (12) assure that every steady state in dislocation creep is stable under fluctuations. The equations of the components of \mathbf{S} , Eqs. (11) can be interpreted as follows: when in a given place of the sample the steady state value of ρ_m changes, it induces a flux on the other component of \mathbf{S} (that is in $\langle v \rangle$) which will tend to nullify the initial variation in ρ_m from its steady state value. Thus we conclude that the steady state for every S_i is the result of a dynamic equilibrium between a tendency to build up a defect structure and a tendency to destroy it, just as would be expected from irreversible thermodynamics [28].

4. Conclusions

The analysis of the previous sections gives us the following conclusions:

i) The dynamic description of the center of mass of the mobile dislocation system, can be obtained by using Newton's second law. This analysis, and a statistical mechanical approach, provides a more intuitive insight to the physical content of the Orowan and the Fuchs and Ilschner equations.

ii) The acceleration of mobile dislocations is responsible for the stability of steady states under fluctuations.

The above conclusions encourage further investigation for the approach taken in this paper. Here we developed a steady state application, but it is clear that the same approach can be used for the analysis of transient stages like:

1) The study of the dynamical behavior of mobile dislocations at the inflection point in Sigmoidal Creep Curves for viscous glide and for Power Law-Creep.

2) Further theoretical developments of our scheme in order to be able to describe the time evolution of the mobile dislocation density during a total unloading test.

Work along these lines is already in progress. In the first case, an analysis for viscous glide in Germanium, and Power-Law creep in Cu-16at%Al; and in the second case an analysis of experimental data for Al-11%wtZn.

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Resumen. Desarrollamos algunos elementos de la mecánica estadística de dislocaciones móviles. Ello nos permite dar una descripción de la dinámica del centro de masa del sistema de dislocaciones utilizando la segunda ley de Newton. Dentro del marco teórico de la mecánica estadística, damos una nueva interpretación de las dos ecuaciones fundamentales de la deformación plástica (*i.e.* la ecuación de Orowan y la ecuación de Fuchs e Ilshner). También se muestra que la aceleración de las dislocaciones móviles es la responsable de la estabilidad de los estados estacionarios ante fluctuaciones.