Spin Effects in Plasticity

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The influence of a magnetic field on dislocation depinning from paramagnetic obstacles is studied. It is suggested that the depinning may take place due to the following mechanism. When a kink passes an obstacle the unsaturated electron bonds of the kink and the obstacle form a radical pair. Magnetic field-induced intercombination transitions from the binding to an antibinding state of the radical pair lead to an additional population of high spin antibinding states with lower binding energy. This results in a plasticity growth. A strong dependence of the amplitude-dependent internal friction of dislocations on the magnetic field is predicted. [S0031-9007(97)02777-4]

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A magnetic field influences the low temperature plasticity of metals due to two main factors. These are an increase of the electron component of the dislocation viscous drag (Kravchenko effect [1]) and enhancement of dislocation depinning from paramagnetic obstacles [2]. The role of the first mechanism is studied in much detail (see, e.g., reviews [3]). It contributes largely to the plasticity of pure metals at large pulse loads at which dislocations move with large velocities and their deceleration is due to viscous friction. The second, less studied, mechanism plays an important part under the conditions when the dislocations move slowly by means of thermally activated transitions over the local barriers under the action of a constant load. In this case their motion is hindered by point defects, called pinning obstacles, and the depinning processes become of crucial importance.

It is far from obvious that a magnetic field is capable of influencing the dislocation depinning. Most of the experiments have been carried out in fields not higher than 10 kOe (see, e.g., [4] and references therein). The Zeeman interaction is very small ($\mu_B H \leq 10^{-4}$ eV where μ_B is the Bohr magneton) compared to typical dislocation—pin binding energies, of the order of 0.1 eV or more. It is even 2 orders of magnitude smaller than the thermal energy kT at room temperature and can hardly influence the probability of the thermally activated transitions of dislocations over the local barriers. Nevertheless a strong influence of a magnetic field on the plasticity is observed.

A model [2] has been proposed which suggests that the magnetic field changes the spin multiplicity of the radical pairs formed by dangling bonds of dislocation cores and obstacles in such a way that depinning becomes more probable. Such ideas have been successfully applied to explain the influence of a magnetic field on radical chemical reactions [5].

Paramagnetic states in the dislocation cores of semiconductors are well known [6]. Arguments favoring the existence of paramagnetic states in dislocations in ionic crystals and metals have been presented in [7]. The role of paramagnetic obstacles can be played by various point defects with a nonzero magnetic moment. These may include transition metal impurities, vacancies and their complexes, dislocation intersections. A radical pair formed by dislocation core and obstacle dangling bonds may be either in a singlet (S) or in a triplet (T) electron spin state. At a large distance between the partners ($\geq 10^{-7}$ cm), S and T state energies practically coincide and the S-T transition is a resonance process (see, e.g., [5]). At a shorter distance the resonance is destroyed due to the exchange interaction. As a result the corresponding binding energies differ, the binding energy in the S state being usually appreciably higher [5,8].

A magnetic field influences the kinetics of the radical pair formation by lifting the ban on S-T intercombination transitions and results in an additional population of the T states. Since the latter are characterized by a much lower binding energy (if any) than the S state, the depinning of dislocations from the obstacles becomes more probable. This leads to an increase of the average dislocations free segment length and, hence, to an increase of the crystal plasticity. This mechanism has been used to explain the principal features of the magnetoplastic [2] and electroplastic [9] effects, the influence of a magnetic field on the amplitude-independent internal friction of dislocations [10], and the work hardening of metals [11].

In spite of a successful application of the model [2] for the explanation of various effects mentioned above, the model itself needs a sounder theoretical ground. Paper [2] proposes a simple formula for the depinning probability dependence on the magnetic field which contains only terms quadratic in the magnetic field. Application of this formula to fields that seem far beyond its region of validity leads to our surprise to a quite reasonable, quantitative interpretation of experimental data. Interpreting strong magnetic field experiments one has to assume that the average dislocation free segment length grows several times, sometimes even by an order of magnitude, which cannot be understood within the framework of the model [2].

The aim of this communication is to provide a more solid basis for our understanding of the microscopic physics underlying various plasticity related processes by formulating a model generalizing the model [2]. The multiplicity of the T states is introduced explicitly and the nonstationary character of the states is taken into account.

At low temperatures and stresses a dislocation gets free from an obstacle when a kink passes the obstacle [12]. Stresses drive the kinks along the dislocation lines until they collide with obstacles. We assume that unsaturated electronic bonds of the colliding kink and obstacle form a radical pair which, at equilibrium distance in the pair, is binding only in the singlet spin configuration. If the radical pair is formed in a triplet configuration the kink passes the obstacle nearly freely and the dislocation depins. When the kink passes the region where a resonance between the S and T states takes place an external magnetic field may induce S-T transitions of the radical pairs. This process increases the proportion of the radical pairs formed in the T states which causes depinning of the dislocations and, hence, the average dislocation free segment length grows.

Excluding very weak magnetic fields (hundreds Oe) the intercombination transitions are caused mainly by the difference of the Zeeman frequencies of the electronic states forming the radical pair (Δg mechanism [5]). This mechanism results in transitions between the S state and the triplet state T_0 with the zero projection of the total spin on the direction of the magnetic field. Transitions to the $T_\pm$ states with unit spin projections are in this case forbidden. The lifetime of the S state, $T_1(S)$, is controlled mainly by the Δg mechanism, whereas additional mechanisms make the lifetime of the T_0 state, $T_1(T_0)$, much shorter. As shown in [13] lattice vibrations cause a modulation of the exchange interaction in the radical pair that results in the most efficient spin-lattice relaxation. The corresponding relaxation transitions are allowed only between states with the same parity, i.e., between the T_0 and $T_\pm$ states, whereas S-T transitions are forbidden. Therefore a transition from the S to T_0 state caused by the Δg mechanism is followed by a spin-lattice relaxation to a $T_\pm$ state in which a kink passes the obstacle.

The population dynamics of the radical pair spin states in a magnetic field are controlled by the following equation for the density matrix

$$i\,\frac{\partial \rho_{\mu\nu}}{\partial t} = \frac{1}{\hbar}\,[\hat{\mathcal{H}}, \hat{\rho}]_{\mu\nu} - i\,\frac{\rho_{\mu\nu}}{T_{\mu\nu}}\,, \tag{1}$$

where

$$T_{\mu\nu} = T_1(\mu)\delta_{\mu\nu} + T_2(1 - \delta_{\mu\nu}).$$

Here $\hat{\mathcal{H}}$ is the spin Hamiltonian of a radical pair, and $T_1(\mu)$ and T_2 are the times of the longitudinal and transverse spin relaxations. The Greek indices take values of S, T_0. It is mentioned above that $T_1(S) \gg T_1(T_0)$ which allows one to neglect the longitudinal relaxation of the S state and use the notation $T_1 = T_1(T_0)$ in what follows.

The magnetic field H causes S-T_0 transitions in the course of the radical pair formation when the resonance between these two states has not been destroyed by the exchange interaction. The corresponding matrix element is [5]

$$\langle S|\hat{\mathcal{H}}|T_0\rangle = \tfrac{1}{2}\,\Delta g\,\mu_B H\,,$$

where Δg is the difference of the g factors of the radical pair states.

Colliding kinks and obstacles form uncorrelated radical pairs which populate equally each of the four states, $(S,\ T_{0\pm})$, therefore the initial conditions for the density matrix are

$$\rho_{SS}(0) = \rho_{T_0T_0}(0) = \tfrac{1}{4}\,, \tag{2}$$

the off-diagonal elements being assumed to be zero.

The kinks move in the random field of internal stresses and, hence, times of their passage through the resonance region are randomly distributed. The radical pair leave the resonance region in a monomolecular way, so that the Poisson time distribution should be used, and the average S state population in a magnetic field becomes

$$\rho_{SS}(H) = \frac{1}{\tau_0}\int_0^\infty \rho_{SS}(\tau)\exp\left(-\frac{\tau}{\tau_0}\right)d\tau\,, \tag{3}$$

where τ_0 is the average time for the radical pairs to pass the resonance region. The population $\rho_{SS}(t)$ of the S state at a time t is obtained from Eq. (1). The quantity $\rho_{SS}(H)$ plays an important role in what follows, since it characterizes the proportion of the strong bonds between the obstacles and dislocations formed in the S configurations which cannot be broken at low temperatures and stresses.

One can readily see that the function $\rho_{SS}(H)$ is actually (to within the factor $1/\tau_0$) the Laplace transform of $\rho_{SS}(t)$. This opens a simple way to calculate this function directly. Carrying out the Laplace transformation of Eq. (1) for the density matrix with the initial condition (2), one obtains a set of linear equations for which the solution is

$$\rho_{SS}(H) = \frac{1}{4}\,\frac{(1 + \frac{T_1}{\tau_0})(1 + \frac{T_2}{\tau_0}) + \frac{H^2}{H_m^2}}{(1 + \frac{T_1}{\tau_0})(1 + \frac{T_2}{\tau_0}) + (1 + \frac{\tau_0}{2T_1})\frac{H^2}{H_m^2}}\,, \tag{4}$$

where

$$H_m = \frac{\hbar}{\Delta g\,\mu_B\sqrt{T_1T_2}} \tag{5}$$

is a characteristic magnetic field making the intercombination processes efficient.

At low stresses and temperatures, dislocations are depinned from the obstacles only in a T state of the radical pair. The total probability that the dislocation remains pinned is

$$W(H) = (1 - p) + p\rho_{SS}(H), \tag{6}$$

where p is the probability that there is a kink in the vicinity of the obstacle. The dislocation remains pinned to an obstacle if either no kink passes the obstacle [the first term in (6)] or a kink is near an obstacle but the radical pair is formed in the S state [the second term in (6)].

Now the relative change of the average dislocation free segment length in a magnetic field is estimated as

$$L_c(H) = L_c(0)\,\frac{W(0)}{W(H)} = L_c(0)\,\frac{(1 - p) + p\rho_{SS}(0)}{(1 - p) + p\rho_{SS}(H)}, \tag{7}$$

since it is inversely proportional to the pinning probability (6).

In a strong magnetic field ($H \gg H_m$) Eq. (7) yields a saturated value of the average free segment length,

$$L_c(\infty) = L_c(0)\,\frac{(1 - p) + p\rho_{SS}(0)}{(1 - p) + p\frac{\rho_{SS}(0)}{1+\tau_0/2T_1}}. \tag{8}$$

In a weak magnetic field ($H \ll H_m$) one arrives at the equation

$$L_c(H) = L_c(0)\left(1 + \frac{H^2}{H_0^2}\right), \tag{9}$$

in which

$$H_0 = H_m \times \sqrt{\frac{(1 - p) + p\rho_{SS}(0)}{p\rho_{SS}(0)}\left(\frac{2T_1}{\tau_0}\right)\left(1 + \frac{T_1}{\tau_0}\right)\left(1 + \frac{T_2}{\tau_0}\right)}. \tag{10}$$

For the typical values $\Delta g \sim 10^{-3}$ [5] of the g factor difference and $T_1 \approx T_2 \approx 3 \times 10^{-9}$ s [14] for the spin-lattice relaxation times in metals, Eq. (5) yields $H_m \sim$ 30 kOe. Comparing the approximate formula (9) with the exact Eq. (7) one sees that for fields $H \leq 0.3H_m \sim$ 10 kOe they differ not more than by 10% (see Fig. 1). The approximate Eq. (9) agrees very well with the available experimental data till rather high magnetic fields $H \leq 10$ kOe , which is much larger than H_0.

Now the value of the resonance passage time τ_0 is estimated. The kink density in crystals with low Peierls barriers is rather high [12] and the probability that there is a kink near an obstacle is close to unity, $p \approx 1$. The experimental value of H_0 is about several kOe [2,9,10], whereas the characteristic field H_m is several tens of kOe. Then Eq. (10) results in $\tau_0 \approx 10^{-7}$ s since it must be 2 orders of magnitude larger than $T_1 \approx 10^{-9}$ s. The model discussed here is valid if the average resonance passage time τ_0 for a radical pair is smaller than its lifetime

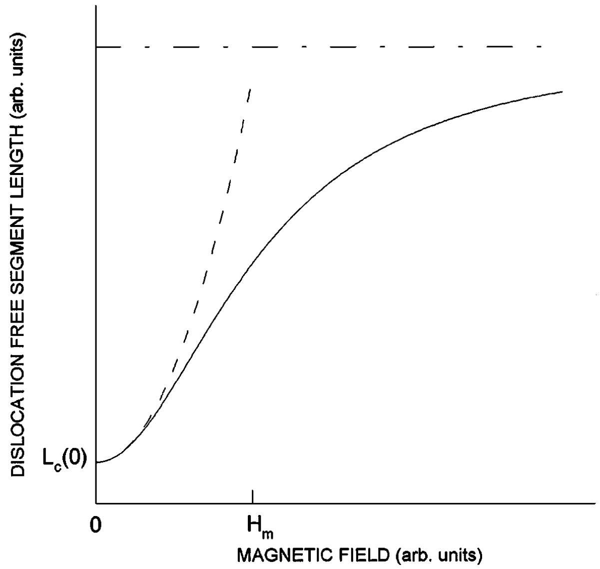

FIG. 1. Schematic representation of the dependence of the average dislocation free segment length on the magnetic field. The solid curve represents the dependence (7), whereas the dashed curve represents the quadratic dependence (9). Two curves deviate considerably only at rather large magnetic fields. The horizontal dash-dotted line shows the limiting value $L_c(\infty)$ for the dependence (7).

in a $T_\pm$ state. Such times, or even much larger ones, for the spin-lattice relaxation are well known for the forbidden transitions [15]. If the magnetic-field-induced S-T resonance transitions occur over the length which is on the order of the lattice spacing ($\sim 10^{-8}$ cm) then the time $\tau_0 \approx 10^{-7}$ s corresponds to a kink velocity about 0.1 cm/s. These are velocities which are readily achievable under realistic conditions [12].

The interpretation of various experiments on the influence of a magnetic field on the plasticity requires an assumption that the average dislocation free segment length $L_c(H)$ increases by an order of magnitude. The model described in this paper allows one to explain such an increase because, with $\tau_0/T_1 \sim 100$, Eqs. (7) and (4) at the high value $H = H_m$ yield the free segment length $L_c(H_m) \approx L_c(0)\tau_0/4T_1$ which is much larger than $L_c(0)$.

An experimental test of the model can be carried out by measuring the magnetic field dependence of the average dislocation free segment length, for which the amplitude-dependent internal friction is most appropriate. According to the Granato-Lücke theory [16], its decrement is

$$\Delta_H = \frac{A}{L_c}\left(\frac{\Gamma}{\sigma_0}\right)\exp\left(-\frac{\Gamma}{\sigma_0}\right), \tag{11}$$

where Γ characterizes the breakaway stress regime, A is a constant of the specimen, and σ_0 is the stress amplitude of the ultrasound. Γ is inversely proportional to the free segment length and, hence, it should be a function of the magnetic field,

$$\Gamma(H) = \Gamma(0)\,\frac{L_c(0)}{L_c(H)}. \tag{12}$$

Therefore, the decrement (11) depends exponentially on the free segment length $L_c(H)$, (12). This can make measurement of the amplitude-dependent internal friction a very sensitive technique for studying the average dislocation free segment length dependence in a broad range of magnetic fields.

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