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STORED ENERGY AND RECRYSTALLIZATION

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ABSTRACT

Simple statistical considerations show that the recrystallized grain size of a deformed single crystal of a metal can be expressed as a function of the potential energy stored within the metal as a result of the deformation. A parabolic relation between the stored energy and the magnitude of the deformation is suggested and a formula relating recrystallized grain size with deformation is derived which agrees with the empirical rule formulated by Walker.

1. INTRODUCTION

In a recent publication Leighly, Walker, and Marx[1] have attempted to derive an explanation for the observed relation between the recrystallized grain size of a metal and the amount of deformation which the metal had been subjected to before the recrystallizing anneal. The postulation by these authors on the mechanism for nucleation is that the total energy stored in a unit volume of metal, by cold working, is distributed statistically over the whole volume of the specimen and that a fraction of the higher energy points functions as nuclei for recrystallization.

In the present paper we have attempted to solve the problem on similar lines but with a more detailed consideration of the basic ideas involved. It is known

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that the evaluation of the partition function for energy distribution in a crystal lattice deformed in any manner is extremely complicated because of the alteration of the vibrational frequencies of the atomic oscillators from their normal values due to the deformation process. The best that can be done is to consider a deformed static lattice and to superpose the normal thermal vibrations of the oscillators upon it. The partition function can then be approximately evaluated.[2] To this approximation the energy in any state of the crystal can always be expressed as the sum of a static potential energy (energy when the atoms are at rest at their lattice positions) and the total vibrational energy of the various oscillators. The static potential energy then includes the internal energy produced by external forces acting on the crystal and is thus essentially independent of temperature.

On this basis we can then regard the total energy W (per unit volume) of a deformed metal crystal to be made up of two parts: (1) the thermal energy W_T, which depends only on temperature and thus on the frequency of the atomic oscillations; and (2) a temperature-independent stored energy W_S, which is a function of the total plastic deformation in the metal.† If we divide a unit volume of the solid into N submicroscopic cells of equal size and assign to all these cells the same *a priori* probability of reaching an energy level ϵ_N, then the distribution of energy corresponding to a state of maximum thermodynamic probability at a given temperature T may be expressed by the standard equation of statistical mechanics:

$$\frac{\Delta N}{N} = \frac{1}{f} \cdot e^{-\epsilon_N/kT} \tag{1}$$

where $\Delta N/N$ is the fraction of cells with an energy ϵ_N and f is the partition function of the distribution given by the general equation

$$\bar{\epsilon} = W/N = kT^2 \frac{\partial}{\partial T} (ln\, f) \tag{2}$$

k is Boltzmann's constant, and T the absolute temperature.

Then,

$$ln\, f = \int \frac{W}{NkT^2} \cdot dT \tag{3}$$

Substituting $W = W_T + W_S$, and integrating with respect to T we get

$$ln\, f = \phi(W_T) - \frac{W_S}{NkT} + ln\, C \tag{4}$$

where $ln\, C$ is an integration constant and $\phi(W_T) = \int \frac{W_T}{NkT^2} dT$ is related to the partition function $f(T)$ of a continuous solid at a temperature T as obtained from Debye's theory. Substituting for f in equation (1) we get

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† The static energy is considered to be the zero of our energy scale.

$$\frac{\Delta N}{N} = \frac{1}{C \exp\{\phi(W_T)\}} \cdot \exp\{-(\epsilon_N - W_s/N)/kT\} \tag{5}$$

We now make the assumption that the nuclei for new strain-free grains are formed in those cells where the energy ϵ_N reaches a value q. We may divide q into temperature-dependent and temperature-independent parts: $q = q_T + q_s$, where q_T is the vibrational internal energy of the Nth cell and q_s is the maximum mechanical energy that can be stored within the cell. Then,

$$\frac{\Delta N}{N} = C' \exp\{-[q_T/kT + \phi(W_T)]\} \exp\{-(q_s - W_s/N)/kT\} \tag{6}$$

Since q_T will always be close to the average internal energy per cell of the whole volume at a constant temperature T, we can treat the temperature-dependent part of equation (6) as a virtual constant for our purpose. Then,

$$\Delta N = NK \exp\{-(q_s - W_s/N)/kT\} \tag{7}$$

where,

$$K = C' \exp\{-[q_T/kT + \phi(W_T)]\} \tag{8}$$

Equation (7) is the fundamental equation for any process of nucleation in which the stored energy of deformation is the driving agency in forming unstrained nuclei. The condition for the same *a priori* probability makes the equation valid for single crystals only. For the polycrystalline condition, we may adapt the equation with additional approximation as has been done by Leighly, *et al.*

2. RELATION BETWEEN RECRYSTALLIZED GRAIN SIZE AND PRIOR DEFORMATION

The number of nuclei that actually form from ΔN potential nuclei will depend on the rate of formation of the nuclei and the rate of growth of those nuclei that have previously formed. Following Leighly, *et al.*, we may assume that the number of recrystallization nuclei N_r per unit volume is proportional to ΔN; *i.e.*, $N_r = \alpha \cdot \Delta N$, the constant of proportionality α being essentially independent of temperature. If we consider the recrystallized grains which fill up unit volume of the material to be cubical in shape, we shall have N_r cubes after recrystallization. This means that the recrystallized grain size G_r is $G_r = N_r^{-\frac{1}{3}}$. Since $N_r = \alpha \cdot \Delta N$, the relation between the logarithm of the grain size and the stored energy from equation (7) becomes

$$\ln G_r = -\tfrac{1}{3} \ln(\alpha NK) + (Nq_s - W_s)/3NkT \tag{9}$$

In order that equation (9) may be put into a form suitable for comparison with experimental data, it is required that the stored energy be related to the prior deformation. It is known that the energy stored per unit volume of metal, by plastic deformation, cannot be calculated as a definite fraction of the total mechanical work expended in producing the plastic deformation. If W_a is the total work expended in deforming a unit volume of metal, say under simple onedimensional compression, then the energy stored in the metal during cold working can be written in the form:

$$W_s = W_d - (Q + W_{el}) \tag{10}$$

where Q is the heat evolved in the process and W_{el} is the elastic energy recovered when the load is removed. A relation between W_s and the strain ν cannot be obtained from theoretical considerations at present, but we can conceive of a way in which stored energy varies as the deformation is gradually increased, and can arrive at a relation which may be justified from indirect experimental observations. We do know that the energy stored in metals increases rapidly with deformation, when the deformation is small, but the rate of increase of stored energy with deformation decreases when the deformation is large. Further, the stored energy tends toward a saturation value at very large deformations. Since a greater quantity of work is stored at large deformations, the simplest way to reconcile these facts is to assume that the rate of increase of stored energy with increase of deformation at any moment is inversely proportional to the amount of stored energy existing at that particular moment. Thus,

$$\frac{dW_s}{d\nu} = \frac{k}{W_s} \tag{11}$$

where k is a constant of proportionality depending on the nature of the deformed metal, and ν is the strain; for simple compression it is the fractional reduction in height. Integration of equation (11) gives

$$\tfrac{1}{2} W_s^2 = k\nu + \delta \tag{12}$$

where δ is an integration constant. To evaluate the constants k and δ we assume, in accordance with experimental observations, that the metal starts storing energy only after a critical deformation ν_c and that W_s tends to a maximum value W_0 as ν approaches unity. Then, $\delta = -k\nu_c$ and $k = \tfrac{1}{2}W_0^2/(1 - \nu_c)$. Hence,

$$W_s = W_0 \left(\frac{\nu - \nu_c}{1 - \nu_c}\right)^{\frac{1}{2}} \tag{13}$$

We are now in a position to substitute W_s obtained from equation (13) directly into equation (9). Some fraction of W_s will be recovered preceding nucleation, but this is extremely small and does not materially affect our equation. The term Nq_s in equation (9) represents the energy of deformation that will be stored if all the cells in the volume element had received the same energy q_s. Since q_s is the energy level required for nuclei to form, we can therefore consider $Nq_s \approx W_0$ and then,

$$\begin{aligned} \ln G_r &= -\left[\ln \{(aNK)^{\frac{1}{2}}\, e^{-W_0/3NkT}\}\right] - \frac{W_0}{3NkT} \cdot \left(\frac{\nu - \nu_c}{1 - \nu_c}\right)^{\frac{1}{2}} \\ &= -\ln m - n\left(\frac{\nu - \nu_c}{1 - \nu_c}\right)^{\frac{1}{2}} \end{aligned} \tag{14}$$

where

$$m = (\alpha NK)^{\frac{1}{3}} e^{-W_0/3NkT}$$

and

$$n = W_0/3\, NkT$$

The quantities m and n can be considered as constants for a given metal for a given temperature and time of anneal.

Equation (14) predicts a variation in recrystallized grain size with prior deformation. That such a relation does exist was first pointed out by Walker.[3] He found that the recrystallized grain size in cold rolled cartridge brass can be expressed by the relation

$$\log G_r = - a\,(100\nu)^{\frac{1}{2}} - b \tag{15}$$

where ν is the fractional cold deformation prior to recrystallization, and the constant b is a function of the annealed grain size prior to final cold deformation. This equation refers to polycrystalline metal. Equation (14) agrees with the experimental observations of Walker and this agreement indicates that the basic assumptions made in deriving the equation are valid.

Equation (14) refers to single crystals where every cell has an equal chance

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ERRATA

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Equation 13 on page 182 *should read* as:—

$$W_s = W_0 \left(\frac{\nu - \nu_c}{1 - \nu_c}\right)^{\frac{1}{2}}$$

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energy (Fig. 1). Thus stored energy is found to be proportional to the square-root of the deformation, and equation (12) which has been derived from physical arguments is seen to be verified experimentally.

Equation (14) differs from the equation derived by Leighly, *et al.* The equation derived by these authors can be written in the form

$$ln\, G_r = ln\, a + b/W_s \tag{16}$$

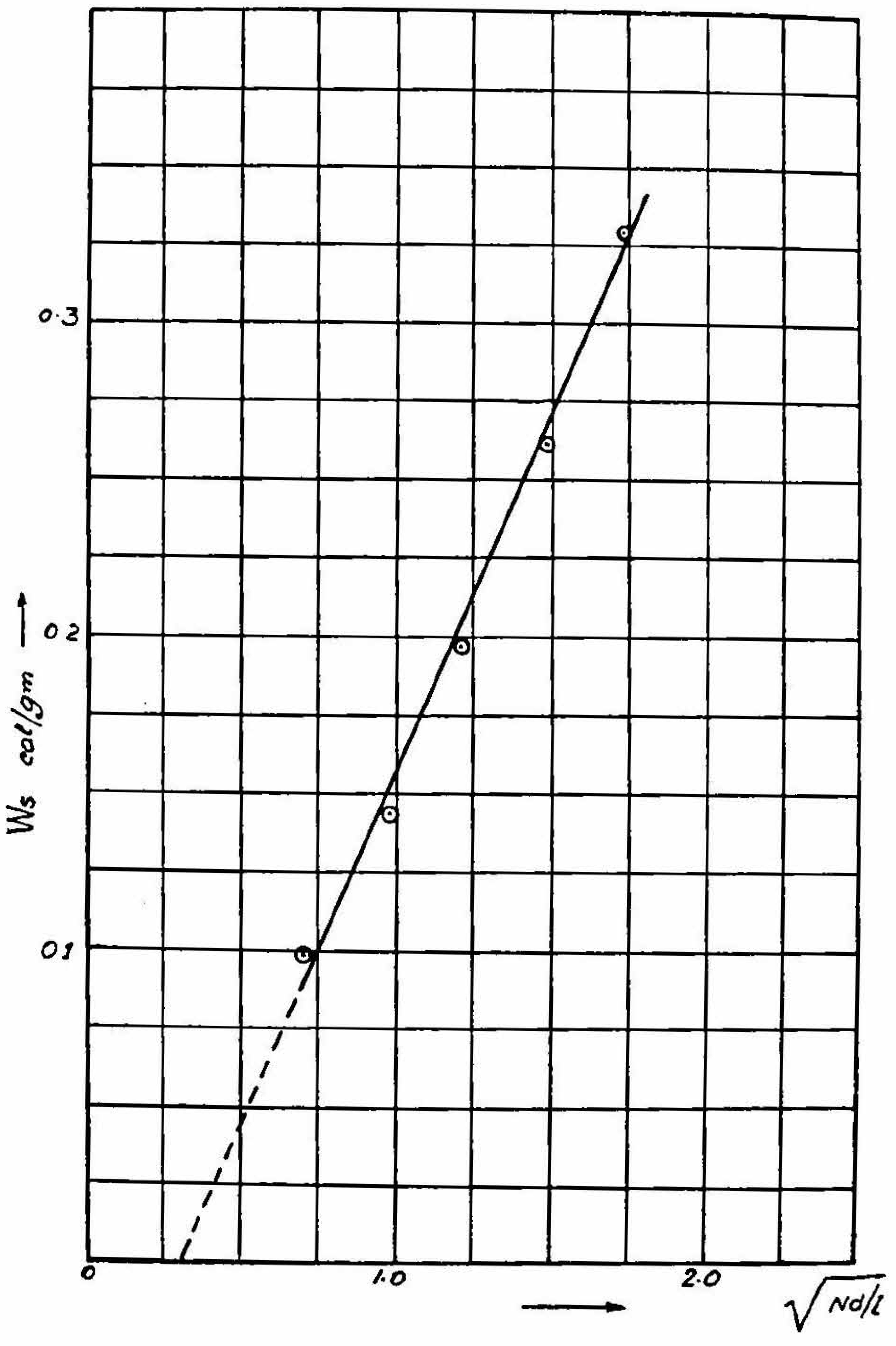

FIG. 1. Variation of stored energy W_s with square-root of the shear strain (expressed in terms of the dimensionless twist Nd/1, N being the number of turns, d the diameter of the specimen and l the length) for electrolytic copper. (Data obtained from Clarebrough, *et al.*, Reference 5).

where W_s is the total stored energy in unit volume of the metal prior to recrystallization, where G_r is the recrystallized grain size, and where *a* and *b* are experimentally determined constants. For a polycrystalline metal, *a* is a function of initial grain size existing in the metal prior to cold deformation. By assuming that the stored energy is a definite fraction of the total mechanical work done in deforming the metal, the final equation obtained is:

$$ln\, G_r = B + P\left(\frac{1-\nu}{\nu}\right) \tag{17}$$

where ν is the strain.

Equation (17) is not correct because it predicts a linear relationship between the logarithm of the recrystallized grain size and the reciprocal of the deformation, which is not found experimentally. Leighly, *et al.*, tried to overcome this difficulty by considering B and P as fitting parameters instead of constants, but such a procedure lacks theoretical significance.

The error in the treatment of these authors lies in two basic assumptions made. First, they have assumed the modulus of energy distribution β in the fundamental equation of statistical mechanics as equal to $1/\bar{\epsilon}$, where $\bar{\epsilon}$ is the average energy per cell. No valid argument for this assumption has been given. As is known, the average energy per cell is given by the equation

$$\bar{\epsilon} = \frac{W}{N} = \frac{\Sigma \epsilon_N e^{-\beta\epsilon_N}}{\Sigma\, e^{-\beta\epsilon_N}} \tag{18}$$

This is a transcendental equation in β, and the solution is not $\beta = 1/\bar{\epsilon}$. From other arguments the value of β, for any statistical system, is always found equal to the thermal modulus $1/kT$, and this cannot be replaced arbitrarily by any other function. Second, they have assumed the stored energy to be a definite fraction of the work expended in deformation, which is also an incorrect assumption.

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