Dislocation-diffusion mechanism of high-temperature healing of the cracks in crystals under loading

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The regularities of disc-like voids (cracks) healing in polycrystalline copper samples under conditions of uniaxial compression at 600°C were experimentally studied. The theory of crack healing by diffusion-dislocation mechanism was developed. Comparing the experimental data with the theoretical dependences has shown their complete correspondence, which is supported by agreement of the experimental Peierls threshold stress with literature data. The work is an important step for solving the general problem on mechanisms of stress relaxation near various stress concentrators in crystals.

Экспериментально изучены закономерности процесса залечивания дискообразных полостей (трещин) в поликристалле меди при температуре 600°C в условиях одноосного сжатия. Построена теория диффузионно-дислокационного механизма залечивания. Сопоставление экспериментальных данных с теоретическими зависимостями показало их полное взаимное соответствие, что подтверждается также совпадением значения величины порогового напряжения Пайерлса, полученного в эксперименте, с литературными данными. Работа является важным шагом в решении общей задачи о механизмах релаксации напряжений в кристаллах вблизи различного рода концентраторов напряжений.

1. Introduction

It has been established earlier that an external mechanical loading applied to crystals containing pores (isomer interstices) or fractures (disc-like voids) causes reducing the defect volume, i.e. results in healing the defects [1–3]. It was shown, if the loading was applied at room temperature and the stress obtained was less than yield point of the crystalline substance, the healing process for such type of defects would be realized by the dislocation mechanism. In this case, the "emptiness" from the defect bulk is transferred with prismatic dislocation loops into the sample bulk. This process is over when the reverse stress created by the formed dislocation assemblage and acting over the defect surface becomes equal to the value of stress caused by the external loading. In this case, the dislocation sources are found to be locked and substance transport ceases. On this stage in the "crystal-defect" system a quasi-equilibrium state is established, that is kept up by a certain loading level. Further, the defect healing process can be reactivated if the conditions for unblocking the dislocation sources will be created. Such conditions can be realized when the external loading acts at an increased temperature. In this case, either diffusion merging the dislocation loops positioned in the assemble end or transferring them into the crystal bulk by thermo-fluctuation movement promotes the dislocation sources unblocking and, respectively, can renew the defect healing process. This mechanism of substance transport during the defect healing in crystals was termed as "dislocation-diffusion" one [3]. In this work we present the results of theoretical and experimental studying the cracks healing process under conditions of external stress acting onto the crystal at increased temperatures, i.e., when the dislocation-diffusion mechanism of substance transport is the most probable. As an investigation object copper coarse-grain polycrystalline sample containing artificially created disc-like voids (cracks) was used. Mechanical stress was applied to the sample using uniaxial loading scheme. The averaged over the sample stress value was always lower than the yield point of the studied crystal under applied loadings.

2. Regularities of crack healing process by dislocation-diffusion mechanism (theory)

It is known, that even when the stress created by external loading is lower than the crystal yield point, local stresses exceeding the threshold value occur around the crack top due to the "concentrator" factor [2–4]. Relaxation of the stresses results in formation of plasticity zone. The stress on external boundary zone is equal to the threshold stress corresponding to dislocation sliding σ_p (Peierls threshold). Using an approximate description of stress field σ near the vertex of disc-like crack with a_0 radius (the case of plane stress state [4]), it is easy to obtain an expression for the plasticity zone radius, which is given by the length l_{dis} of dislocation assemble: $l_{dis} = (\sigma/\sigma_p)^2 a_0$. As it was already mentioned the dislocation assemble formed at high temperature is not stationary, but it is in dynamical equilibrium, i.e. how many dislocation loops disappear — so many new loops appear near the crack vertex. Therefore, the crack healing kinetics in such regime should be determined by the rate of merging (disappearing) of dislocation loops, which is described in general case by the following expression [5]:

$$\frac{dR_l}{dt} = -\frac{2\pi}{b\ln(8R_l/b)}\left\{\frac{Gb[\ln(R_l/b) + g]D_V C_V \omega}{4\pi(1-\nu)R_l kT} + D_i \Delta C_i\right\}, \quad (1)$$

where D_V, D_i — diffusion coefficients of vacancies and interstices, respectively; T — temperature; G — shear modulus; ν — Poisson coefficient; k — Boltzmann constant; ω — atomic volume; b — Burgers vector; R_l — dislocation loop radius; ΔC_i — supersaturation of crystalline lattice by interstitials far from the loop; C_V — vacancy equilibrium concentration far from the loop; $g \approx 2–3$ coefficient takes into consideration the dislocation nucleus energy. The first summand in (1) takes account of the vacancy flow away from the loop contour, which is due to its curvature; the second one takes into account the interstitial flow directed to the loop, which is caused by supersaturation by interstitials. Both the flows cause reducing the loop radius. For obtaining the expression (1), it was postulated that the outflow power is not limited for vacancies emitted by dislocation loops including the dislocations with Burgers vector with edge component.

As to interstitials supersaturation and their possible participation in the crack healing process, it is necessary to note the following. One of possible sources which can provide noticeable supersaturation is the interstitial generation as a result of intersection of dislocations moving under plastic deformation [6, 7]. In the places of dislocation intersections, steps appear which movement is accompanied by generation of interstitials or vacancies. This is related to the fact that the steps are forced to move in a non-conservative manner in the stress field if they are not in the sliding planes of moving dislocations, this causes the dislocation inhibition and, respectively, results in generation of the mentioned point defects. Schematically, this mechanism of defect generation is shown in Fig. 1. The type and quantity of point defects, N, occurring as a result of intersection of moving dislocations, is defined by the relation

$$N = \frac{\left[\mathbf{L}_1\left(\mathbf{m}_1 \times \mathbf{L}_2\right)\right]\left[\mathbf{b}_1\left(\mathbf{l}_1 \times \mathbf{b}_2\right)\right]}{\omega\left|\mathbf{L}_1\left(\mathbf{m}_1 \times \mathbf{L}_2\right)\right|}, \quad (2)$$

where $\mathbf{L}_1$, $\mathbf{L}_2$ — unit vectors along the dislocation line; ω — atomic volume; $\mathbf{m}_1$ — a unit vector along the direction of dislocation movement; $\mathbf{l}_1$ — vector of dislocation displacement after intersection; $\mathbf{b}_1$, $\mathbf{b}_2$ — Burgers vectors of intersected dislocations [7]. The positive sign of N indicates generation of interstitials, negative — vacancies.

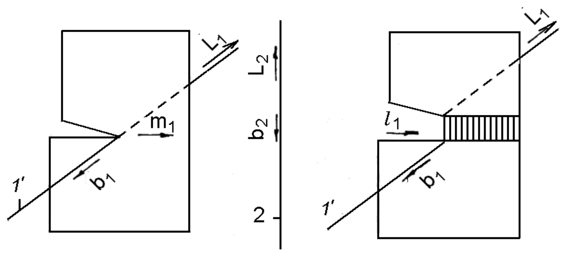

Fig. 1. Scheme of a step formation at intersection of screw dislocations. a — dislocation initial position; b — after intersection with dislocation 2.

If both of the intersected dislocations are right-handed ones or both are left-handed ones, interstitials occur; if one is right-handed, and another — left-handed, vacancies occur. In the simplest case of high symmetry crystals, where $\mathbf{L}_1 \perp \mathbf{l}_1$; $\mathbf{m}_1 \| \mathbf{l}_1$, and $|\mathbf{b}_1| = |\mathbf{b}_2|$, an evident result follows from (2): $N = |\mathbf{l}_1|/|\mathbf{b}_1|$, which shows that the quantity of occurred point defects is proportional to the path passed by dislocations. Thus, participation of both types of point defects in the process studied is equiprobable in our specific case of copper crystal.

Kinetic equation describing time dependence of the crack size variation $a(t)$ can be obtained, if the "void" flow removed from the crack volume dV_{cr}/dt to equal to the "void" flow related with the dislocation assemble, surrounding the crack mouth: dV_{dis}/dt. Assuming the crack volume with radius (a) and height (c), and the void volume removed by a single prismatic dislocation loop with radius R_l and "height" b, — are the volumes of respective cylinders, for the mentioned void flows the following expressions can be written:

$$\frac{dV_{cr}}{dt} = 2\pi ac\frac{da}{dt}, \tag{3}$$

$$\frac{dV_{dis}}{dt} = 2\pi R_l b N_{dis}\frac{dR_l}{dt}, \tag{4}$$

where N_{dis} — the number of prismatic dislocation loops with radius R_l in the dislocation assemble. From the condition of equality of the reverse stress acting on the crack surface due to the dislocation assemble:

$$\sigma_{tur} = \frac{GN_{dis}b}{2\pi(1-\nu)l_{dis}} \tag{5}$$

to the stress caused by the external loading, σ:

$$\left(\sigma_{xy}\right)_{\max}\Big|_{L=c/2} \approx \sigma\sqrt{\frac{a_0}{c}}, \tag{6}$$

the expression for N_{dis} is following:

$$N_{dis} = \frac{2\pi(1-\nu)a_0^{3/2}\sigma^3}{Gbc^{1/2}\sigma_p^2}. \tag{7}$$

Equaling (3) with (4) and taking in account (1) and (7), and in view of the fact that in the first summand of (1) the values [ln (R_l/b)+ g)] and ln$(8R_l/b)$ are of the same order and can be reduced, we obtain the following differential equation:

$$a\frac{da}{dt} = \frac{\pi a_0^{3/2}\sigma^3}{c^{3/2}\sigma_p^2}\left(\frac{D\omega}{kT} + \frac{4\pi(1-\nu)R_lD_i\Delta C_i}{Gb\ln(8R_l/b)}\right).$$

Here $D = D_v\, C_v$ — atomic self-diffusion coefficient. This equation is solved simply under the starting condition: $a = a_0'$ at $t = t_0$, where a_0' and t_0 — are, respectively, crack length and time spend for the dislocation assemble formation. In fact, the t_0 time determines the beginning of the crack healing process in the regime of dislocation- diffusion mechanism. The required solution is as follows:

$$1 - \left(\frac{a}{a_0'}\right)^2 = \tag{8}$$

$$= \frac{2}{(a_0')^2}\frac{\pi a_0^{3/2}\sigma^3}{c^{3/2}\sigma_p^2}\left(\frac{D\omega}{kT} + \frac{4\pi(1-\nu)R_lD_i\Delta C_i}{Gb\ln(8R_l/b)}\right)(t-t_0).$$

This kinetic equation can be directly applied for analysis of experimental results. If the developed notions about the dislocation-diffusion mechanism of crack healing are right, then, firstly, the dependence $\{1-(a/a_0')^2\}$ — $(t-t_0)$ should be described by a linear function. Secondly, the dependence $\{1-(a/a_0')^2\}$ — σ^3 should have the similar character at the fixed exposures of the sample under loading.

3. Experiment results and discussion

Experimental investigations were carried out on the samples of coarse-grained copper, in which structure thin disc-like voids simulating cracks were created artificially. These samples were prepared by diffusion welding of two polished one-half parts, in one of which cavities were made. After

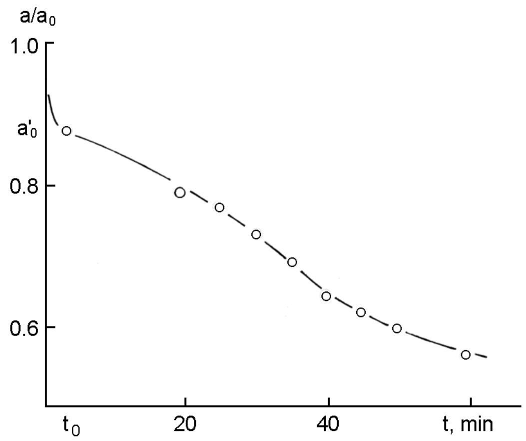

Fig. 2. Dependence of (a/a_0) versus t.

welding and normalization annealing for 40 min at the temperature 800°C, voids (cracks) of $\sim 3{\cdot}10^{-2}$ cm radius and $\sim 4{\cdot}10^{-4}$ height positioned at distances excluding their influence on one another were formed in the sample.

Experiments on the crack healing were carried out at the temperature 600°C. The loading value was chosen so that in the whole sample, stress does not exceed the yield point. At the chosen temperature, the total deformation of the samples did not exceed 3 %. The crack radiuses were measured by metallography on the fractograms in the planes of the crack location, and on the metallographic sections, prepared in the perpendicular plane. The experimental dependence $a(t)$ is given in Fig. 2. It is seen that the dependence is non-monotonic in the beginning stage. This is explained simply by the fact that in the healing process beginning (after the sample loading) at any temperature there is the first stage when the crack size reduces from an initial (a_0) to (a_0') value during a short time period, t_0. This portion corresponds to the dislocation mechanism of healing, when a quasi-stationary dislocation assemble forms near the crack mouth. Further the healing can take place only under condition of a combined mechanism of substance transfer. In Fig. 3, the experimental data as $\{1 - (a/a_0')^2\}$ — versus $(t - t_0)$ dependence at $t > t_0$ are presented. According to (8) this dependence is described well by a linear function. However, application of (8) does not allow separating the contributions into the dislocation loops disappearing both under influence of the pressure due to their curvature and of the pressure caused by supersaturating the crystalline lattice by interstitial atoms. The

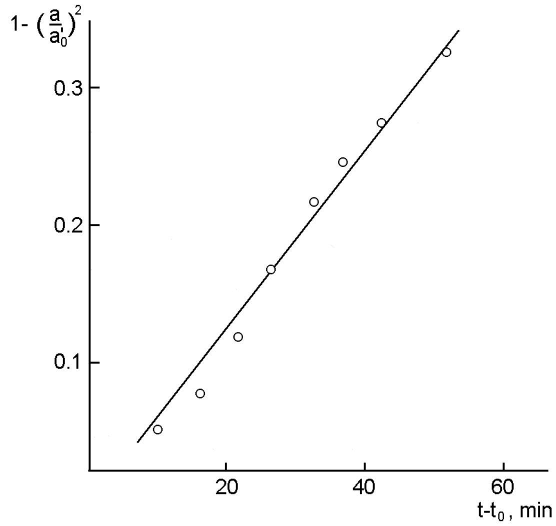

Fig. 3. Dependence of $\{1 - (a/a_0')^2\}$ versus $(t - t_0)$.

energy of interstitial atom formation is high (~4 eV), consequently, their concentration in the crystalline lattice can be supposed to be low. Therefore, the estimations given below were done without taking their role into account. In this case, from (8) it follows:

$$1 - \left(\frac{a}{a_0'}\right)^2 = \frac{\beta}{(a_0')^2}(t - t_0), \qquad (9)$$

$$\beta = \frac{2\pi a_0^{3/2}\sigma^3 D\omega}{c^{3/2}\sigma_p^2 \; kT}.$$

Substituting the $D = 3.45{\cdot}10^{-17}$ m^2/s as the self-diffusion coefficient in copper at $T = 600$°C [8, 9], the constants values $\omega = 1.18{\cdot}10^{-29}$ m^3, $kT = 1.205{\cdot}10^{-20}$ J, and taking into $\sigma^3 = 120{\cdot}10^{18}$ (N/m^2)^3, $a_0 = 3{\cdot}10^{-4}$ m, $c = 4{\cdot}10^{-6}$ m, $a_0' = 0.88a_0$, the value of Peierls barrier $\sigma_p = 0.34{\cdot}10^5$ N/m^2 was estimated from the slope angle of the curves shown in Fig. 3. For comparison, we have got another independent estimation of σ_p at higher temperature, but under conditions when only the dislocation mechanism of healing acts. For this purpose the experiments were carried out at $T = 600$°C, in which the value (a_0'/a_0) was measured as well under various loadings σ, however, the exposure (t_0) under loading was fixed short enough only to form a quasi-stationary dislocation assemble near the crack vertex. Comparing the crack volume variation as its radius changing from a_0 to a_0', with the volume of the "void" removed by all the dislocation

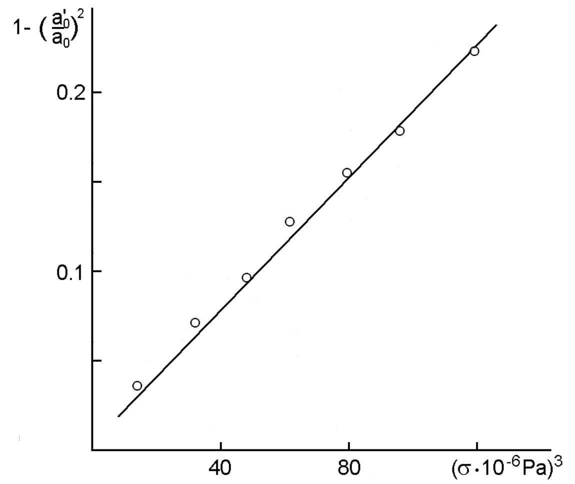

Fig. 4. Dependence of $\{1 - (a/a_0)^2\}$ versus σ^3 at $(t - t_0)$ =0.

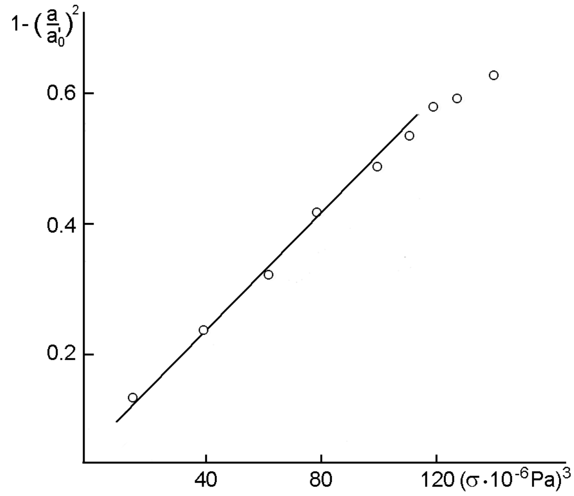

Fig. 5. Dependence of $\{1 - (a/a_0')^2\}$ versus σ^3 at $(t - t_0)$ =30 min.

loop s (in assumption of $R_l \approx c/2$), and using the (5)—(7) relationships, we obtain an expression describing the dependence $\{1 - (a_0'/a_0)^2\}$ versus σ in the following form:

$$1-(a_0'/a_0)^2 = B\sigma^3, \text{ where } B = \frac{2\pi(1-\nu)c^{1/2}}{a_0^{1/2}G\sigma_p^2}. \quad (10)$$

The results of the experimental data treatment according to this relationship are shown in Fig. 4. The dependence obtained, as it was expected in accordance with (10), was found to be close to linear function, and σ_p value obtained from the straight line slope angle is characterized by $\sigma_p = 0.75 \cdot 10^5$ N/m^2. This value σ_p is more reliable than $\sigma_p = 0.34 \cdot 10^5$ N/m^2 obtained under conditions of simultaneous acting the both mechanisms of mass transfer — the dislocation, and the dislocation-diffusion ones. For the purpose to obtain information about Peierls threshold, σ_p, on the stage when only the dislocation-diffusion mechanism acts, an addition series of experiments was carried out. In these experiments the dependence characterizing the crack relative size variation on loading only at 30-th minute of healing (a_{30}) after forming the quasi-stationary dislocation assemble was measured. Like earlier, in assumption of determining role of only linear tension in the dislocation loops disappearing, for σ_p estimation we used the equation (9). In Fig. 5 the results of treating the experimental data in coordinates $\{1 - (a_{30}/a_0')^2\}$ versus σ^3 at $t - t_0 = 30$ min are shown. As it is seen from the figure this dependence is also well described by the near-to-linear function. The values of Peierls threshold obtained both from the straight line slope angle in Fig. 5 and from equation (9) were found to be equal to $\sigma_p \approx 0.2 \cdot 10^5$ N/m^2.

Thus, all three estimations of Peierls threshold obtained at the temperature 600°C for different stages of the crack healing process in independent experiments were found to be rather similar. These threshold stress values agree with data available for copper crystals [10]. Hence, the fulfilled experimental investigations support the rightness of the developed theoretical concept concerning the mechanisms of substance transfer in different stages of the crack healing process in crystals.

4. Conclusions

Thus, in present work the regularities describing the process of disc-like voids (cracks) healing in polycrystalline copper samples at higher temperature under uniaxial compressive loading were studied.

Assuming the determinative contribution of the dislocation-diffusion mechanism of substance transfer for crack healing under these conditions, theoretical concept of the process was developed.

Comparison of the experimental data with the theoretical dependences has shown their complete correspondence. This is supported also by coincidence of the experimental value of Peierls threshold stress with literature data. This fact indicates rightness of the proposed physical description of the process studied.

The work is an important step for resolving the general problem on the mechanisms of stress relaxation near various defects as stress concentrators in crystals.

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Дислокаційно-дифузійний механізм високотемпературного заліковування тріщин в кристалах під навантаженням

Ю.И.Бойко, М.А.Волосюк, В.Г.Кононенко

Експериментально вивчено закономірності процесу заліковування дископодібних порожнин (тріщин) у полікристалі міді при температурі 600°C в умовах одновісного стиснення. Побудовано теорію дислокаційно-дифузійного механізму заліковування. Зіставлення експериментальних даних з теоретичними залежностями показало їх повну взаємну відповідність, що підтверджується також збігом значення величини порогової напруги Пайерлса, що отримана в експерименті, з літературними даними. Робота є важливим кроком у рішенні загальної задачі про механізми релаксації напружень в кристалах поблизу різного роду концентраторів напруги.