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On role of mass-transfer crowdion mechanism in local relaxation processes

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Character of relaxation processes has been analyzed in crystalline materials near stress local concentrators of various types (a crack in copper under its healing by uniaxial compression; a rigid (corundum) inclusion in a KCl single crystal; a hole in a KCl single crystal due to pulse optical breakdown of the single crystal by ruby laser radiation). It was shown that in the first two cases (crack and rigid inclusion), the main mechanism resulting in relaxation of about 50% stress was the dislocation-diffusion one. According to this mechanism, excess vacancies and interstitials occur at intersections of screw dislocations; as a result, rapid crowdion (interstitial) mass transfer is switched on completing the relaxation process. In the case of laser breakdown, the crowdion mass transfer mechanism is principal. The diffusion-and-dislocation mechanism steps in at the final stage of the process and provides near 5% of the full necessary mass transfer amount.
Keywords: dislocations; crowdions; interstitial atoms; diffusion; concentration of stress; relaxation processes.

Приведен анализ характера релаксационных процессов в кристаллических материалах в окрестности локальных концентраторов напряжений разных типов (трещина в меди при ее залечивании одноосным сжатием; жесткое (корунд) инородное включение в монокристалле KCl; полость в монокристалле KCl, полученная в результате импульсного оптического пробоя монокристалла излучением рубинового лазера). Показано, что в первых двух случаях (трещина, жесткое включение) ведущим механизмом массопереноса, приводящим к снятию до 50 % напряжений, является дислокационно-диффузионный механизм. Согласно этому механизму, на пересечениях винтовых дислокаций появляются избыточные вакансии и межузельные атомы, благодаря чему включается быстрый краудионный (межузельный) массоперенос, завершая релаксационный процесс. В случае лазерного пробоя ведущим является механизм краудионного массопереноса. Диффузионно-дислокационный механизм подключается на заключительной стадии процесса, обеспечивая порядка 5 % полной величины необходимого массопереноса.
Ключевые слова: дислокации; краудионы; межузельные атомы; диффузия; концентрация напряжений; релаксационные процессы.

Приведено аналіз характеру релаксаційних процесів в кристалічних матеріалах навколо локальних концентраторів напружень різних типів (тріщина в міді при її заліковуванні одноосним стисненням; жорстке (корунд) чужорідне включення в монокристалі KCl; порожнина в монокристалі KCl, отримана в результаті імпульсного оптичного пробою монокристала випромінюванням рубінового лазера). Показано, що в перших двох випадках (тріщина, жорстке включення) провідним механізмом масопереносу, що приводить до зняття до 50% напружень, є дислокаційно-дифузійний механізм. Згідно цьому механізму, на перетинах гвинтових дислокацій з'являються надлишкові вакансії і міжвузельні атоми, завдяки чому включається швидкий краудіонний (міжвузельний) масоперенос, завершуючи релаксаційний процес. У разі лазерного пробою ведучим є механізм краудіонного масопереносу. Дифузійно-дислокаційний механізм підключається на завершальній стадії процесу, забезпечуючи порядка 5 % повної величини необхідного масопереносу.
Ключові слова: дислокації; краудіони; міжвузельні атоми; дифузія; концентрація напружень; релаксаційні процеси.

Introduction

Real solid crystalline bodies as physical systems always possess some excess thermodynamic potential in comparison with equilibrium ones due to presence of crystalline lattice defects. These defects as foreign inclusions, pores, grain boundaries, dislocations, vacancies, interstitials (intrinsic and foreign) may be either artificially created with some specific aim (for example, for dispersion strengthening of a material) or production outgoings. Various defects are introduced into material in technologies of diffusion welding, powder metallurgy, dispersion strengthening, etc. [1, 2, 3].

Under analyzing specific situations, one should take into account not only requirements to products under exploitation conditions but also the fact that near any defect being a stress concentrator of external loading, relaxation processes take place which in one way or another reduce both efficiency and service life of the product. These relaxation processes are necessary to study in order to get a possibility to control them and to estimate real capabilities of specific technologies and quality of materials produced with them.

Experimental Results and Discussion

Based on our previous works [4, 8 – 10] where kinetics of relaxation processes near specific local stress concentrators like cracks, foreign inclusions and pores was considered, we form the intention to accent the main peculiarities of relaxation processes and to specify the transfer mechanisms leading to relieving or damping stress state. Additionally, it is necessary to estimate the role of each of the mechanisms under specific conditions.

In [4] healing of a disc-shaped plane crack with size 2*a* and thickness *c* was studied. Under uniaxial compression perpendicular to the crack occurrence plane, a dislocation-diffusion mechanism of healing was assumed, i.e. generation of prismatic dislocation loops with their subsequent diffusion dissolution. The kinetic equation [4] for dissolution of dislocation loops contains two components; one of them depends on loading and crack size, and another is defined by the value of lattice supersaturation by interstitials:

$$1-\left(\frac{a}{a_0'}\right)^2=\left(\alpha\gamma+\alpha\beta D_V \Delta C_i\right)\frac{\sigma^3\left(t-t_0\right)}{\sigma_p^2}, \quad (1)$$

where α, β, γ are experimental constants [4]; a, a_0' are, respectively, current and initial (under loading) radii of the crack; D_V is vacancy diffusion coefficient; $D = D_V C_V^0$, D is self-diffusion coefficient of copper atoms (at T = 873 K D = 3.1·10^{-17} m^2/s); C_V^0 is vacancy equilibrium concentration at a given temperature T; σ is stress created by external loading; t, t_0 are, respectively, current time and the time for formation of a quasi-stationary dislocation assemble in the crack tip after loading (in our case t_0 = 5 minutes); σ_p is Peierls threshold; $\Delta C_i = C_i - C_i^0$ is supersaturation of lattice by interstitials; C_i, C_i^0 are, respectively, real and equilibrium concentrations of interstitials at T temperature.

Naturally, Eq. (1) contains the external load value and Peierls threshold (for details, see [4]). Generally speaking, the level of lattice supersaturation by interstitials is unknown a priori, and we can not take it into account in the process under study without additional considerations. If interstitial atoms are allowed to migrate reliably in crowdion configuration, we can not really evaluate also the contribution of crowdions into cracks healing so far. Let us turn to specific estimations. It has been found that if dislocation loop dissolution flow due to interstitial atoms migration is neglected, i.e. the second summand in parentheses of Eq.(1) is assumed zero, after experimental data treatment we obtain understated Peierls threshold $\sigma_p \approx 0.4 \cdot 10^5$ N/m^2. On the other hand, using the known from independent sources Peierls threshold we can evaluate the second summand in parentheses of Eq. (1).

If, for example, the typical Peierls threshold $\sigma_p \approx 10^5$ N/m^2 is taken, the second summand in (1) is found to be twice as large as the first one. That means, in this situation under high-temperature healing of cracks in loaded copper, the interstitial (crowdion) mechanism of transfer acts. A specific physical model of such transfer of atoms is in that vacancies occurring within atomic close-packed rows move quickly along the close-packed rows forming crowdion configurations and “take away hollow” from the crack, so the crack is filled by atoms. Such configurations are called anti-crowdion ones in [5]. All theoretical concepts developed in [5] for crowdions are found to be fully applied to anti-crowdions.

A physical model for appearance of lattice supersaturation by interstitials under plastic deformation was proposed by Hirth and Lothe [6]. The supersaturation is related with intersections of screw dislocation loops. Here vacancies and interstitial atoms are generated. But concentration of interstitial atoms is always predominates due to their high mobility [6].

If these considerations are taken, we can believe that experiments done in [4] and results of their treatment prove justifiability of assumption on participation of interstitial migration (crowdions) in the process under study.

Found participation of interstitial (crowdion) mass-transfer for cracks healing in copper samples under uniaxial compression perpendicular to the plane of crack bedding is principal also because this allows correct planning the regimes of technology operations for crack getting out in the production cycle.

Similar situation appears also in other cases like this, for example, during relaxation of stresses near foreign inclusions in the matrix. In literature there are described many different cases on reaction of the system near various inclusions under changing external conditions [7]. Usually, dislocation and diffusion mechanisms of mass-transfer were discussed which were really observed (crowdions did not mentioned practically).

In [8] relaxation processes and transfer mechanisms were studied in a KCl single crystal with immersed into it corundum (Al_2O_3) balls at melting temperature (model experiment). During cooling of the system from melting temperature, as a result of different expansion coefficients of the crystal and the ball, dislocations appear in the KCl single-crystal as in much softer material; some of them are dissolved by diffusion, whereas some new appear again and

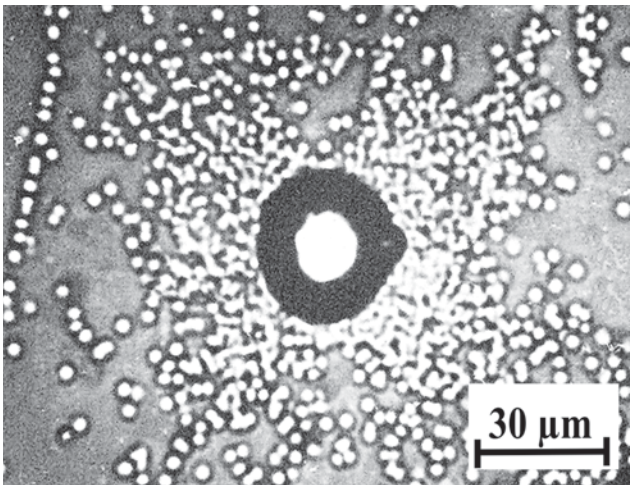

Fig. 1. Typical dislocation structure in KCl single crystal cooled from melting T_m to room T_{room} temperature around a corundum ball of 30 μm diameter (cooling constant æ = 1.05×10^{-3}s^{-1}).

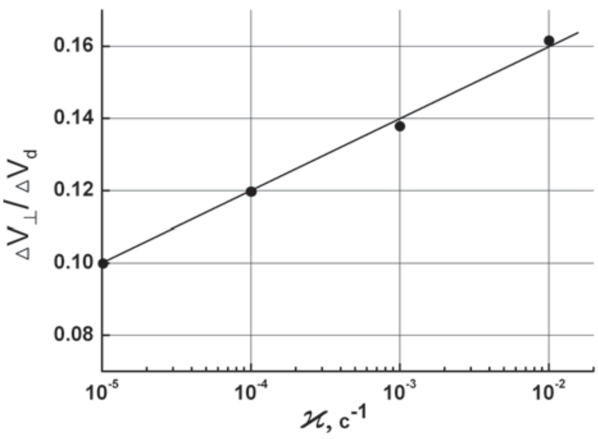

Fig.2. Relative portion of full misfit ($\Delta V_\perp/\Delta V_d$) versus cooling constant æ in KCl single crystals cooled from melting temperature T_m to room value T_{room}.

again due to continuing cooling. As a result, under cooling to room temperature, a certain amount of undissolved dislocations accumulate in the crystal (see Fig. 1). Under cooling, temperature varies by the exponential law ($T = T_m e^{-æ t}$) from melting point T_m to room T_{room} = 293 K. In experiments, the cooling constant æ takes the following values: 3.0×10^{-5}s, 1.05×10^{-4}s, 1.05×10^{-3}s, and 1×10^{-2}s.

Quantitative treatment of dislocation structures (like given in Fig.1) obtained at different cooling temperatures near balls of different size was carried out in order to reveal the cooling rate dependence of the relative portion of full volume misfit of dislocation loops ($\Delta V_\perp/\Delta V_d$) remained in the crystal after cooling. The value ΔV_d is the misfit between void and ball volumes at room temperature. According to calculations, the value ($\Delta V_\perp/\Delta V_d$) does not depend on ball size, but depends on cooling rate (Fig.2).

As the cooling rate increases, larger misfit value is "frozen" in dislocation loops as it was expected. But it is important that only (10 – 15) % of the misfit is found to be "frozen" in the remaining dislocation loops. In [8], sufficiently accurate calculations of the misfit value were fulfilled. From these it follows that quantitatively the misfit value in dissolved and unobservable dislocation loops is also rather small, not more (20 – 30) % dependently on the cooling rate.

Thus, in "frozen" and dissolved dislocation loops there is less than a half of substance taken out of the stressed area. Because after cooling the stresses in the crystal near an inclusion were insignificant according to photo-elastic method estimations, we can consider that more than a half of full misfit was taken out from the stressed area by the crowdion (interstitial) transfer.

Another type of stress concentrators was discussed in [9]. These are voids remaining in the ion single crystal after focused laser beam transmission accompanied by so called laser optical breakdown. This phenomenon is being under study for a long time, and a lot of works was devoted to it. Different mechanisms of local optical breakdown (formation of a crystal local destruction) under transmission of laser radiation as well as emission spectra, formation of a plasma clot, kinetics of the breakdown, etc. were considered. In a number of our works, mechanisms of taking out of substance from the breakdown zone and void formation are discussed. The main attention was concentrated at studying the dislocation mechanism as the most rapid for taking out of substance from the breakdown zone.

Quantitative treatment of investigation results and first of all the treatment of dislocation structures around the breakdown zone [9] allowed us to realize that the registered quantity of dislocation loops observed in the cleavage plane intersecting the formed void might explain only about (4 – 5) % of substance taken out of the breakdown zone.

In this connection, we have studied large amount of literature data on this point, analyzed rates of energy losses under transmission of laser radiation through single crystals and developed the mechanism of void pulse formation – the model of a local thermal explosion [10]. According to this model, melting, evaporation and heating of the radiation absorption zone to plasma state take place so rapidly that atoms of the overheated area stay put. Therefore, this process is an explosion with estimated duration less than 10^{-6} s. High pressure occurs and a shock wave forms which, according to explosion theory, initially has the supersonic speed. On the crest of the wave, atoms of overheated substance are taken out with the supersonic speed. This is possible if the atoms form crowdion configurations because only crowdions are able to move with the supersonic speed [11].

According to results of microfilming of the breakdown zone using nano-second resolution [12], at the initial time, removal of substance and void formation (almost 80% of its size) occur so rapidly that atoms would have the supersonic speed to move to a distance close to observed size of the heated zone. Dislocations and dislocation mass-transfer are observed practically at the final stage after crystallization of the substance.

Conclusions

Thus, analysis of particular but typical cases of relaxation processes by dislocation-diffusion mechanism near stress concentrators in various materials (metals and nonmetals) was proposed. It has been shown that if interstitial atoms and vacancies are generated at dislocation lines intersections, the mass-transfer process is accompanied by joining the crowdion (interstitial) mechanism. In the cases where generation of interstitial atoms is not related with plastic deformation but takes place as a result of local pulse impact onto the crystal (thermal explosion under laser optical breakdown), the crowdion mass-transfer becomes principal.

Under healing of a crack, emptiness – vacancy-by-vacancy – is removed from its volume by generation and movement of vacancy dislocation loops and crowdion configurations of vacancy type.

In the cases of thermo-elastic stress relaxation near a rigid inclusion in the crystal or of a local thermal explosion, atoms are taken out from the defect zone by generation and movement of interstitial prismatic dislocation loops and the flow of interstitial atoms (crowdions).

References

1. V.V. Skorokhod. *Powder Metallurgy*, **9/10**, 42 (2014).
2. I.M. Neklyudov, V.N. Voyevodin, I.N. Laptev, A.A. Parkhomenko. *Problems of Atomic Science and Technology,* **2 (90)**, 21 (2014).
3. R.A. Andrievski. *Phys. Usp*., **57**, 945 (2014).
4. M.A.Volosyuk, A.V. Volosyuk, N.Ya. Rokhmanov. *Functional Materials*, **22**, 51 (2015).
5. J.Hirth, J.Lothe. Theory of dislocations, McGraw-Hill, New York (1968), 600 p.
6. V.D. Natsik, E.I. Nazarenko, *Low Temperature Physics,* **26**, 283 (2000).
7. V.G. Kononenko. *Metallofizika*, **7**, 71 (1985) *[in Russian].*
8. V.G. Kononenko, V.V. Bogdanov, A.N. Turenko, M.A. Volosyuk, A.V. Volosyuk. *Problems of Atomic Science and Technology*, **4 (104)**, 15 (2016).
9. Yu.I. Boyko, M.A. Volosyuk. *Bulletin of Kharkov National University named by V.N. Karazin, ser. «Fizyka»,* **1020**, 42 (2012) *[in Russian].*
10. V.G. Kononenko, M.A. Volosyuk, A.V. Volosyuk. *Problems of Atomic Science and Technology*, **5 (99)**, 15 (2015).
11. A.M. Kosevich, A.S. Kovalev. *Solid State Comm.*, **12**, 763 (1973). A.V. Gorbunov, M.Yu. Maksimuk. *Phys. solid state*, **36** (5), 1416 (1994).