IJDIAS International Journal of Discoveries and Innovations in Applied Sciences

| e-ISSN: 2792-3983 | www.openaccessjournals.eu | Volume: 1 Issue: 6

Micromechanics of Solids

Bozorov Nosirjon Sodiqovich

Senior lecturer of the Kokand State Pedagogical Institute, candidate of physical and Mathematical Sciences

Annotation:

An effective approach to connecting between scales is to use molecular dynamics (MD) modeling to extract parameters from a small system consisting of one or more dislocations, and then use the parameters to construct a coarse-grained phenomenological description at the next higher scale. Guided by this philosophy, we study plastic flow in a microscale polycrystal consisting of several thousand atoms, a system suitable for studying the interaction between dislocations and grains.

Keywords: dynamics of underlying dislocations, constant load, direct transformation

Such localized spots are also visible in cut polycrystals. In terms of particle motion, such a quadrupole displacement pattern corresponds to the appearance of an unstable saddle point. One stable and the other unstable axes pass through such a point, and the particles move respectively to a point along these axes and from it. While it is not clear for amorphous materials how such singular points are created within the system, in polycrystalline material the generation of such saddle structures can be explained using the dynamics of underlying dislocations, as we will explain later. A similar pattern of the saddle can be obtained by the movement of dislocation in a stressed single crystal, near the beginning of plasticity.

In simple viscous liquids, the velocity profile is linear between two moving plates. However, in solids (amorphous/crystalline) this is not the case. In a polycrystalline solid, the presence of grains leads to a highly inhomogeneous flow field. The grain resists movement until the accumulated deformation crosses its elastic limit, when it either rotates relative to neighboring grains or breaks up into smaller grains.

At isolated points with high activity, the movement of particles demonstrates a four-pole pattern, essentially a saddle pattern, in the field of particle displacement. We show that such a picture arises when two oppositely "charged" edge dislocations approach each other laterally. The saddle disappears after the dislocation annihilation (see additional film M1). A similar pattern of velocities, which appears as a saddle only on a scale exceeding the minimum approach distance between two oppositely "charged" dislocations, was reported by Moretti et al., Near the beginning of plasticity in a single crystal subjected to uniaxial, quasi-static stress In their system pairs of dislocations originated at a distance from each other, and they went to the boundary without forming a special point, unlike our case, when pairs of dislocations approach arbitrarily close and eventually annihilate.

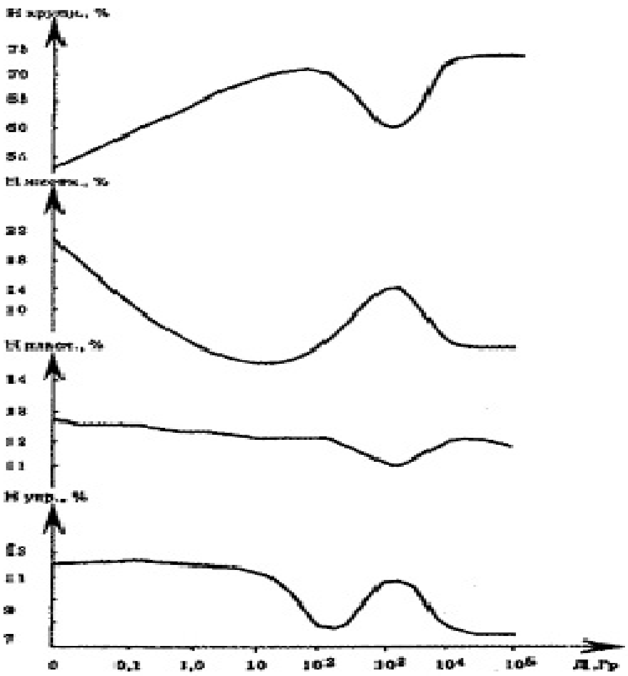
Thus, we have shown that the plastic flow in shifted polycrystals exhibits a strong spatio-temporal heterogeneity, which manifests itself as three different modes in the distribution of particle displacement. Here, the presence of grains of different sizes makes the movement more heterogeneous compared to amorphous solids. In addition, elementary plastic events of the flow field can be explained in terms of the basic dislocation dynamics. We assume that such a heterogeneous flow field could be experimentally observed in cut-off colloids. The collective movement of particles forming strings or demonstrating cellular diffusion has already been observed 22 at the grain boundaries of colloidal polycrystals in particle tracking experiments.

A non-serial microhardness meter of the UPM-1 type was used, which allows recording the kinetics of indentation, exposure and extraction of the diamond indenter in the coordinates "load-depth of penetration".

Measurements of the micromechanical properties of minerals were carried out on the initial, non-irradiated and irradiated by accelerated electrons samples. Radiation doses varied in the range from 0 to 10 Gy. From 10 to 20 hardness tests were performed on each mineral with registration of the full cycle of indentation, exposure and extraction of the indenter in the coordinates "load-depth". The maximum load on the indenter reached 100 kN.

The plasticity of galena, which characterizes the tendency of the mineral to deform plastically under constant load, changes slightly, decreasing from 12.6% to 11.1% at a dose of 102 Gy, and then increases to 11.7%. The rigid component of hardness associated with the ability of the mineral to harden under the action of a loaded indenter, changes very sharply in the dose range of 10-102 Gy, decreasing from 20.4% in the initial samples to 6-9% in non-irradiated ones. The fragility of galena under irradiation increases from 54% to 69-72%.

Analysis of the results of statistical processing of samples shows that for galena, fluctuations in hardness values are observed with an increase in the radiation dose, and the maximum hardness value is an unradiated sample. The initial galena is also characterized by maximum elasticity, plasticity, rigidity. Irradiation causes a drop in hardness, a decrease in elasticity, stiffness, plasticity and leads to an increase in brittleness.



The effect of irradiation on the brittleness, rigidity, plasticity, elasticity of galena

A further increase in the dose to 105 Gy leads to radiolysis of individual lead sulfide molecules. The decrease in the hardness of the mineral associated with this phenomenon continues until the increase in the radiation dose reaches a certain value, after which the processes of formation of the crystal structure of a new metallic phase begin to prevail. This is evidenced by the fact that starting from a dose of 103 Gy, an increase in the hardness of galena is observed. An increase in the radiation dose of 105 Gy contributes not only to the further destruction of the crystal structure of the sulfide, but also to the disordering of the newly formed structure of the radiolysis phase of the metal.

ISSN 2792-3983 (online), Published under Volume: 1 Issue: 6 in November-2021

The De value is comparable to an instantaneous deformation jump corresponding to the same stress jump. A similar phenomenon is observed with soft step loading in the super elasticity mode. With soft step unloading in the super elasticity mode, there is a decrease in deformations over time at constant temperature and stress. There is a phenomenon of stress relaxation after monotonous loading of a titanium nick elide sample in the mode of martens tic inelasticity and subsequent isothermal exposure at a fixed value of total deformations. Immediately after fixing the deformations, the stresses decrease at a high rate, but over time the relaxation rate drops to indistinguishable values over a time period of about 1 hour.

The most important property of direct thermoelastic transformation is its multivariance, which consists in the fact that a highly symmetric cell of the austenitic phase can pass into a low-symmetric cell of the martensitic phase in several different directions. There are 12 such directions for titanium nickelide. If we take into account the disorientation of various grains of polycrystalline alloy with shape memory, then there is a fairly dense set of different directions of direct transformation at the micro level. As a result, it turns out that the single term "martensite" means a whole set of structural states having the same elementary cell, but differing in the degree of orientation of low-symmetric martensitic elements.

Both the process of nucleation and the process of development of martensitic mesoelements contribute to the accumulation of deformations of direct transformation. This thesis is confirmed by experimental data related to the phenomenon of oriented transformation [1], which consists in the fact that after the removal of the acting stresses, the deformations of the direct martensitic transformation continue to accumulate "towards" the previously acting stresses while continuing the direct transformation in the absence of macroscopic stresses, and the rate of deformation growth is significantly lower than for the case when the stresses continue to act. If only the process of nucleation of martensitic mesoelements contributed to the deformation of direct transformation, then the growth of deformations after stress relief would stop. If the contribution to the deformation was given only by the process of mesoelement development, then after stress relief, the growth of deformations would continue at the same rate.

The simplest ones can be considered disconnected boundary value problems, in the formulation of which the effect of acting stresses on the phase transition process and dissipative terms in the energy balance equation are neglected. As a result, the temperature regime can be determined from an analogue of the thermal conductivity equation with an effective heat capacity depending on temperature. After that, the dependence of the phase composition parameter on coordinates and time is determined, then the stress—strain state is determined.

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ISSN 2792-3983 (online), Published under Volume: 1 Issue: 6 in November-2021