Formation of deformation substructures in FCC crystals under the influence of point defect fluxes

M V Matveev[1], O V Selivanikova[1] and D N Cherepanov[2]
[1] Department of Nuclear Power Plants, Tomsk Polytechnic University, 30, Lenina ave., Tomsk, 634050, Russia
[2] Department of Higher Mathematics, Tomsk State University of Architecture and Building, 2, Solyanaya sq., Tomsk, 634003, Russia

E-mail: ohgres@yahoo.com

Abstract. The article deals with substructural transformations in FCC crystals under the influence of point defect fluxes. Different relationships between accumulation of point defects in crystal and substructure transformations, in particular during the process of fragmented dislocation structure formation have been received.

1. Introduction

The most productive approach to the study of staging of metal and alloys plastic deformation is to identify substructural transformations and related hardening mechanisms [1]. In mathematical modeling of plastic deformation the occurrence of individual elements of every substructure at all stages of deformation is expected, wherein the substructural transformation means element accumulation of a new substructure to such significant quantities that these elements become predominant among all others.

2. Overall dislocation density

Figure 1 shows calculations of dependencies of different types of dislocation densities on the deformation degree in a model with dynamic generation of point defects. For comparison, there are experimental data of dislocation densities, obtained by the method of electron microscopy by different authors. Triangles correspond to dislocation density, calculated according to formula $\rho = 7.8 \cdot 10^6 \tau^2$ (E. Gottler, 1973, [2]) based on the hardening curve of a copper single crystal oriented in the [100] direction, deformable at room temperature and at constant rate of shear deformation $a = 10^4$ s^{-1}. Snowflakes correspond to dislocation density, calculated using formula $\rho = 7.8 \cdot 10^6 \tau^2$, based on hardening curve of a copper single crystal oriented in the [001] direction, deformable at $T = 293$ K and at constant speed of shear deformation $a = 10^4$ s^{-1}.

   Other dataare taken from [3], which gives and overview of the experimental data for dislocation density obtained by different methods. Bright circles are obtained from the data on energy, accumulated in a copper single crystal (D. Roennpagel, Ch. Schwtnk, 1978). Dark circles are the data on electron microscopy of the copper single crystal (E. Gottler 1973). Bright squares are the data on the X-ray analysis of the copper single crystal (T. Ungár, H. Mughrabi, D. Roennpagel, M. Wilkens, 1984). Bright diamonds are the data on the X-ray analysis of the copper polycrystal, obtained by the authors of [3].
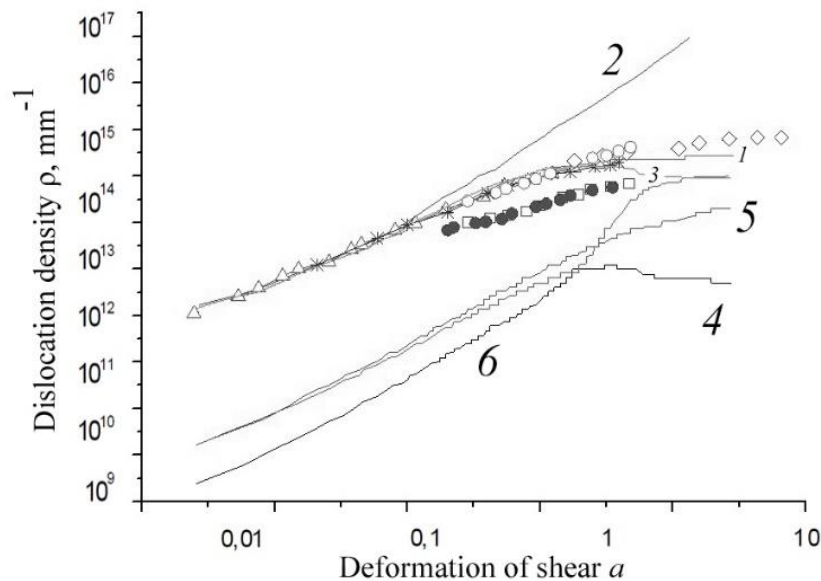
Figure1. Dependence of dislocation density on the deformation degree.

Curve 1 is in good agreement with the experimental data. There is satisfactory quantitative and qualitative agreement with the experimentally observed character of changes in total dislocation density $\rho = \rho_m + \rho_d + \rho_{\pm}$ with the order of shear deformation.

Curve 2 in Figure1 is a dependence of total dislocation density on the deformation degree, calculated on the assumption that the process of dislocation annihilation and transformation is absent. This condition in case of a small deformation degree practically has no effect on calculated curve $\rho(a)$, which is evident from a comparison of curves 1 and 2, in case of high deformation degrees leads to a significant discrepancy in the experimental data: there is an unlimited increase in dislocation density with the further increase in the deformation degree. This suggests that both mechanisms play a significant role in the process of dislocation annihilation: a mechanism of screw dislocation annihilation, due to cross-slip, and a mechanism of edge dislocation annihilation due to climbing. The absence of one of these mechanisms leads to an infinite increase in the dislocation density.

3. Modeling results for components of overall dislocation density

Calculated curves 3, 4, 5, b in Figure 1 reflect the nature of the change in the dislocation density deformation: shearforming ρ_m (curve 3), in dynamic dipole configurations $\rho_d = \rho_d^v + \rho_d^i$ vacancy ρ_d^v and interstitial ρ_d^i types (curve 4 and 5, respectively), in dislocation walls $\rho_W = N_W \cdot d_W^{-1}$ (curve b). Figure 1 shows that the main contribution to the overall dislocation density (curve 1) cause shearforming dislocations (curve 3), which density is comparable in order of power with overall dislocation density (comparing curves 1 and 3). Dislocation density in dynamic dipole configurations of vacancy (curve 4) and interstitial (curve 5) types as well as density in walls (curve 6) contribute more in case of a higher deformation degree.

Figure 2 shows the calculated dependenciesof dislocation densities on the deformation degree: in a dipole configuration of vacancy and interstitial types (Figure 2a, b), during shearforming (Figure 2c), in dislocation walls (Figure 2d).

The presented results suggest that in the initial stages of deformation a non-disoriented cellular substructure is formed, which elements are dislocation dipoles formed by dislocation in the dynamic dipole configuration, dislocation scraps, and shearforming dislocations. Available individual

dislocation walls and dislocating clusters are also rearranged to form the dipole configuration with the closest dislocation of the opposite sign.
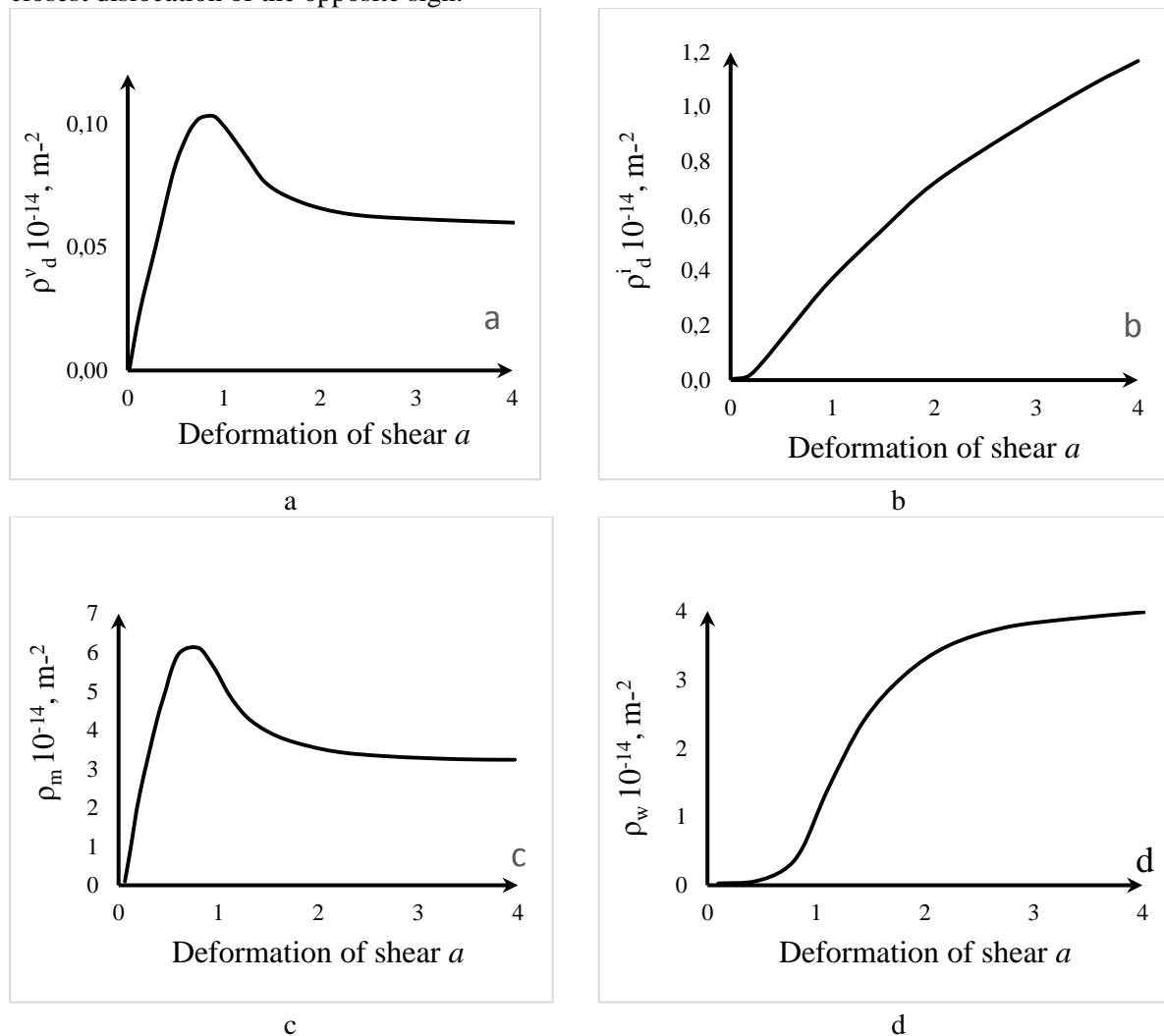

a

b

c

d

Figure 2. Dependencies of dislocation density in a dipole configuration of the vacancy type (a), dislocation density in a dipole configuration of the interstitial type (b), shearforming dislocation density (c), dislocation density in walls (d) depending on the deformation degree.

The greater the deformation is, the greater number of dislocation becomes integrated into dislocation walls, and dislocations together with dislocation clusters form excess dislocation density on the boundaries of shear zones. The boundaries of the fragments formed from dislocation walls, which are sprouting through the volume of a crystal as a result of absorption of shearforming dislocation, meet and form bodies, which shape is close to the convex polyhedron thatconnects in the junctures.

Figure 3a provides calculated and experimental data (Δ) [4] for the excess dislocation density. The excess growth of the dislocation density is directly related to the increase in the angle of disorientation, because it is inherent in the formula for the continuous disoriented angle.

Figure 3b provides calculated data for generated (curve 1), destroyed (curve 2) and accumulated (curve 3) densities of dislocation walls. At the initial stage the density of accumulated walls (curve 3) is greater than the density of the destroyed ones (curve 2), but in the late deformation stages the density of the destroyed walls is significantly higher than the density of the accumulated ones. The

density of generated dislocation walls ten times greater than current density (curve 3), whichindicates high intensity process of the dislocation walls destruction.
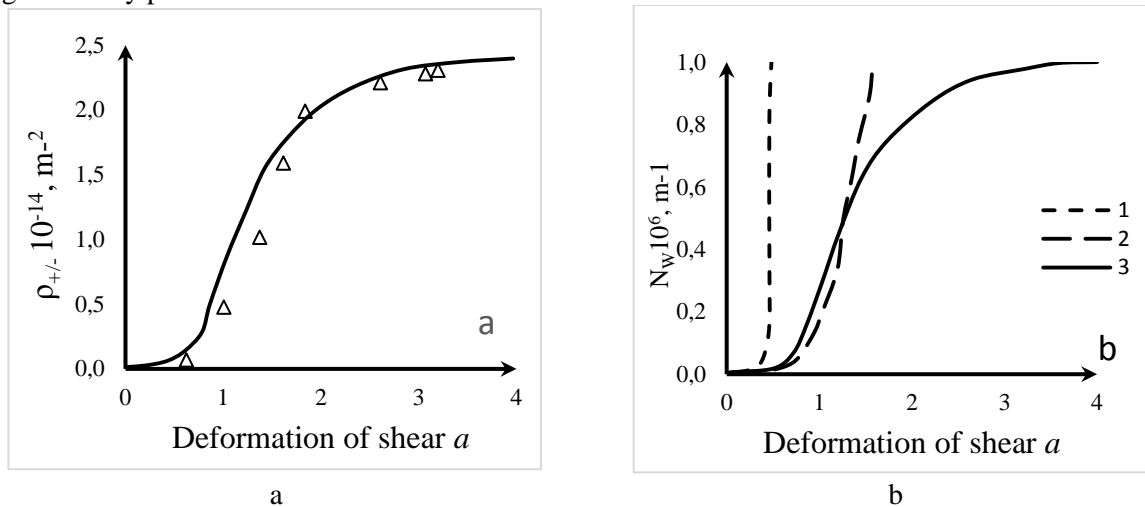

a   b

Figure 3. Dependence of excess dislocation density (a), generated densities (1) and destroyed dislocation walls (2), and current density (3) (b) on the deformation degree.

The intensity of dislocation absorption by walls is significantly higher than the annihilation intensity of dislocations due to the deposition of point defects (Figure 3b). Both of them contributein intensity of decreasing of shearforming dislocation density, that the density at the deep deformations becomes less than the dislocation density in walls.

Figure 4 shows the dependences of generated density (curve 1), annihilated (curve 2) and accumulated (curve 3) shearforming dislocations on the deformation degree.
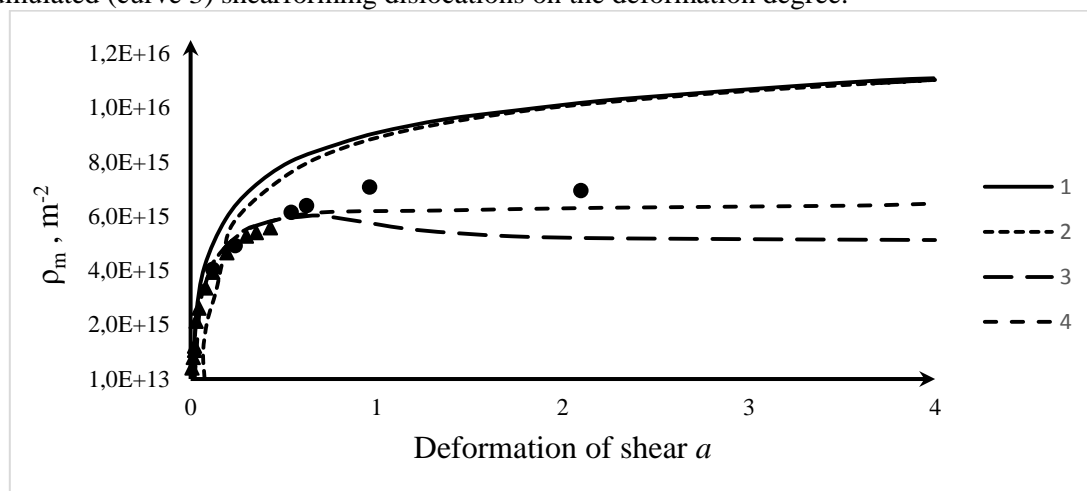

Figure 4. Dependences of generated (1), annihilated (2) and accumulated (3) shearforming dislocation densities, and total dislocation density (4) on the deformation degree.

For comparison, there is a dependence of total dislocation density on the deformation degree (curve 4). Curve 3 is calculated considering the annihilation of both screw and edge dislocations, as well as the mechanism of the dislocation walls relaxation growth. Points show the experimental data for single (Δ) and polycrystalline copper ($\circ$) according to [1, 2].

Figure 5, a shows the dependence of the density of generated dislocation wallson concentrations that gone to point defect sinks. Monovacancies – curve 1, divacancies – curve 2, interstitial atoms – curve 3.
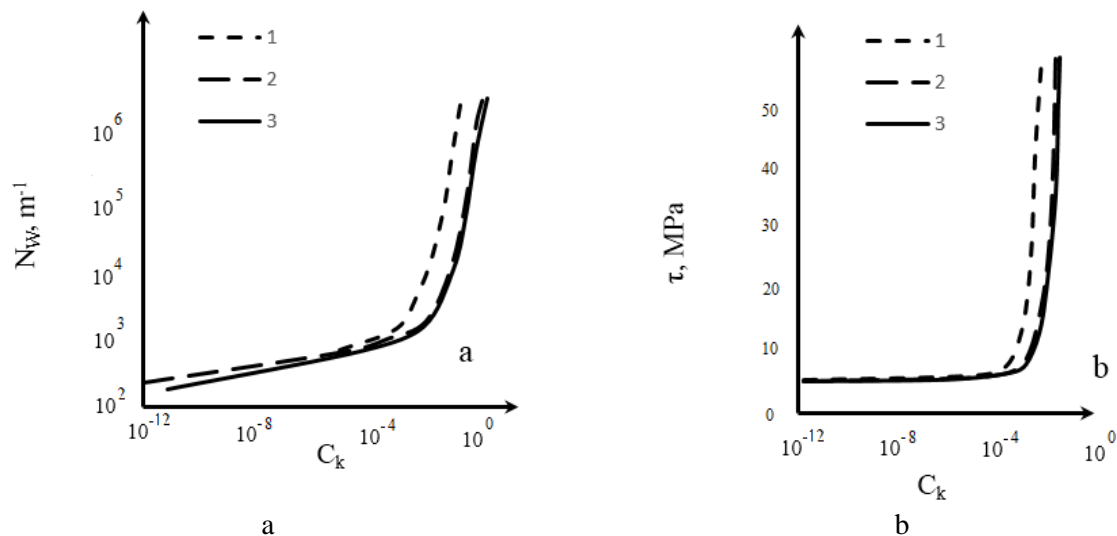
Figure 5. Dependences of the density of generated dislocation walls (a) and creep stress (b) on the concentrations that gone to point defect sinks. Monovacancies – curve 1, divacancies – curve 2, interstitial atoms – curve 3.

There is also a direct link between the formation of the fragmented structure and the departure of point defects on sinks. This direct relationship is revealed only in the simulation, and has not been explicitly incorporated in the model. It is evident that the more intensive deposition of point defects on dislocations, gives the more intensivefragmentation.

Conclusion

In conclusion, it should be mentioned that modelling allows discovering the relationships between accumulation of point defects in crystal and substructure transformations, particular during the process of fragmented dislocation structure formation. The overwhelming majority of the generated defects involved in relaxation processes, was associated with the substructure transformation.

The process of the disoriented structure formation is a significant factor in the balance of deformation defects. A significant part of interstitial atoms is involved in the process of dynamic formation of dislocation wall germs. Annihilation processes play the main role in accumulation of interstitial atoms.

High values of the point defects concentration in the absence of their annihilation mechanisms allows suggesting that formation of amorphous deformation structures is possible in suppressed diffusion (in case of plastic effects at low temperatures of high-speed deformations).

Therefore, on the one hand, point defects absorption by dislocations prevents anamorphization process, and on the other hand, a major role of impact of point defect fluxes of high intensity on dislocations in dislocation substructure evolution becomes clear. Considering the connections between structure elements, that are carried out by point defects, is particularly important in the analysis of the nanostructure formation processes under the influence of deep deformations.

References
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