Quasi-viscous deformation mode in nonequilibrium nanocrystalline structures

I I Sukhanov¹,², D S Zaytsev², I A Ditenberg¹,²,³ and A N Tyumentsev¹,²,³

¹Institute of Strength Physics and Materials Science SB RAS, Tomsk, 634055, Russia
²National Research Tomsk State University, Tomsk, 634050, Russia
³Siberian Physical-Technical Institute, Tomsk, 634050, Russia

E-mail: suhanii@mail.ru

Abstract. Based on the analysis of the elastic-stressed state of partial disclinations of nanodipoles the rate of the quasi-viscous deformation mode in nanocrystalline structures is estimated. It’s shown that velocity of movement of point defects (V) and nanodipole propagation (L_d) within the quasi-viscous deformation mechanism, depending on the activation energy of the migration of point defects (vacancies, interstitial atoms) and deformation temperature, can reach high values close to the speed of sound in metals.

1. Introduction
At present, the study of non-equilibrium states is obtained considerable interest, in particular, at the description of processes of nanostructured materials formation, the features of their plastic deformation and destruction. These states largely determine the unique complex of physicomechanical properties of such materials (low-temperature and high-speed superplasticity, the phenomenon of anomalous mass transfer, etc.). In [1, 2], after intense plastic deformation on Bridgman anvils on a wide class of metallic materials (pure Ni, V-based alloys, Mo-Re solid solution, etc.), nanobands of deformation localization were discovered with the crystal lattice reoriented with dimensions (width) from several to several tens of nanometers. In this case the carriers of the rotational mode of deformation are various compensated disclination configurations, including dipoles of partial disclinations. In contrast to the traditional collective dislocation models, the motion of these defects can be described within the quasi-viscous mechanism of plastic deformation by fluxes of nonequilibrium point defects.

In this work, based on the analysis of the elastic-stressed state of partial disclination nanodipoles, the rates of the quasi-viscous deformation mode depending on the type (vacancies and interstitial atoms) of these defects are estimated.

2. Experimental materials and procedures
The calculation of the stress fields and nanodipole energies was conducted in the software Maple 17 using the partial wedge disclination stress tensor with the direction of the defect lines along the z axis, which has the form [3, 4]:

\[ \sigma^{(e)x}_{ij} = D \omega \theta^{(e)x}_{ij}, \] (1)
where \( D = G/[2\pi(1 - \nu)] \), \( r^2 = x^2 + y^2 \), \( G \) – shear modulus, \( \nu \) – Poisson’s ratio, \( \omega \) – Frank’s vector (power of disclinations).

Based on the experimental data, the moduli of pure nickel were used as elastic moduli of the continuum in which the analysis of elastically stressed states was performed. To simplify the calculation, only wedge disclinations were considered. The visualization of stress fields and gradients of these fields was made using the graphical tools of the Maple 17 package.

### 3. Results and discussion

The above mentioned nanobands of reorientation with sizes from several to several tens of nanometers are characterized by a high (hundreds of degrees per micrometer) elastic curvature of the crystal lattice. Plastic accommodation of such structural states is associated with significant mass transfer effects. The effects of anomalous mass transfer can be realized within the quasi-viscous deformation mechanism (Figure 1) \cite{1, 2}. The reorientation of the crystal lattice in the nanoband is realized by quasi-viscous mass transfer from the OPQ compression regions in the ORS extension region by non-equilibrium fluxes (generated during plastic deformation) point defects in fields of high local pressure gradients. For small values of the crystal lattice reorientation \( (\phi \approx 1^\circ) \) the expressions for the average velocity of point defects \( (V) \) in the \( x \) direction and the average velocity of nanodipole propagation \( (\dot{L}) \) within this model have the form \cite{1, 2}:

\[
D \approx \nu r^2 \exp \left( \frac{-E_m}{kT} \right),
\]

\[
V \approx \frac{D}{kT} \Omega \frac{\partial P}{\partial x},
\]

\[
\dot{L} \approx \frac{2cD \Omega \partial P}{kT \phi \partial x}
\]

Here \( \nu \approx 10^{13} \text{ s}^{-1} \) – Debye frequency and \( r \approx 3 \times 10^{-10} \text{ m} \) – length of an elementary jump of a point defect, \( c \) – concentration of nonequilibrium point defects; \( D \) – their diffusion coefficient; \( k \) – Boltzmann constant; \( T \) – deformation temperature; \( \Omega \) – atom volume (vacancies); \( \phi \) – angle of reorientation of the nanobands; \( \partial P/\partial x \) – pressure gradient in the direction of mass transfer.

Integral averaging of pressure gradients for a nanodipole of partial disclinations with size \( l \) has the form:

\[
\frac{\partial P}{\partial x} = \frac{1}{l} \int_{-\delta}^{\delta} \left( \frac{\partial P}{\partial x} \right) dx
\]

Here, the parameter \( \delta \approx 0.3 \text{ nm} \) characterizes the size of the singular regions of the stress fields near the lines of disclination type defects. The maximum values of the pressure gradients are reached in the plane of the nanodipole of partial disclinations and were \( \frac{\partial P}{\partial x} \approx 0.015 \text{ E nm}^{-1} \) (\( E \) – Young’s modulus). Due to the high localization of stress fields, the above-mentioned values decrease to \( \frac{\partial P}{\partial x} \approx 0.003 \text{ E nm}^{-1} \) as the distance from this plane increases.
Figure 1. (a) – pressure change $P = (\sigma_{11} + \sigma_{22} + \sigma_{33})/3$ in the direction of its maximum gradient in the dipole plane (curve 1) and at distances of 1 nm (curve 2) and 3 nm (curve 3) from this plane. (b) – scheme of reorientation of the crystal lattice by diffusion streams of point defects in the process of movement of the partial disclinations dipole.

As can be seen from relations (3), (4) and (5) the rate of plastic deformation in addition to the elastic-stressed state of the continuum medium is largely determined by the diffusion properties (diffusion activation energy $E^m_\text{m}$) and the concentration of point defects. In the case of mass transfer by fluxes of non-equilibrium vacancies ($E^m_\nu = 0.6$ eV) at their concentrations $c_\nu \approx 10^{-4}$ for nanodipoles and local pressure gradients presented in Figure 1 (a) the velocity of movement of point defects $V$ and movement of the nanodipole of partial disclinations $\dot{L}$ in depending on the temperature of deformation was estimated (Table 1). The characteristic values of the velocity of a quasi-viscous deformation mode for this type of point defects lie in the interval $V = 0.3 \times 10^{-6}...3.2$ m/s.

Table 1. The speeds of movement of point defects ($V$) and the propagation of a nanodipole of partial disclinations ($\dot{L}$), depending on the activation energy of point defects and deformation temperature.

| Vacancies $E^m_\nu = 0.6$ eV | \( T \) (K) | 293 | 473 | 673 | 873 | 1073 |
|-------------------------------|------------|-----|-----|-----|-----|-----|
| V (nm/s)                      | 371.5      | 1.92 \times 10^6 | 1.07 \times 10^8 | 8.81 \times 10^8 | 3.17 \times 10^9 |
| \( \dot{L} \) (nm/s)         | 4.26       | 2.2 \times 10^6  | 1.22 \times 10^6 | 1.01 \times 10^7 | 3.63 \times 10^7 |

| Interstitial atoms $E^m_\text{m} = 0.1$ eV | \( V \) (nm/s) | 1.45 \times 10^{11} | 4.057 \times 10^{11} | 5.9 \times 10^{11} | 6.75 \times 10^{11} | 7.03 \times 10^{11} |
|--------------------------------------------|-----------|-------------------|--------------------|------------------|-------------------|-------------------|
| \( \dot{L} \) (nm/s)                      | 1.67 \times 10^9 | 4.65 \times 10^9 | 6.76 \times 10^9 | 7.73 \times 10^9 | 8.06 \times 10^9 |       |

$c_\nu \approx 10^{-4}$; $\partial P/ \partial x \approx 0.015 E$ nm$^{-1}$.

Another type of flux carrier of point defects involved in plastic deformation is interstitial atoms, the activation energy of diffusion of which is significantly lower than the similar energy for vacancies ($E^m_\text{m} = 0.1$ eV). It was demonstrated that in the low-temperature region in this case the values of $V$ and $\dot{L}$ are tens of times higher than those for vacancies (Figure 2). Despite the fact that the interstitial atoms correspond to a weaker temperature dependence of the velocity of point defects motion, the magnitude of the rate of plastic deformation is about hundreds of meters per second. In [5, 6], the method of molecular dynamics was used to estimate the generation and accumulation of point defects (vacancies, bi-vacancies, and interstitial atoms) in single crystals with fcc structure taking into account the interactions between ensembles of point defects and a dislocation ensemble during plastic deformation. It was shown that at the stages of developed plastic deformation, the concentration of generated point defects in the absence of annihilation mechanisms on dislocations can reach very large values of $c = 10^7$.
With such values of concentration, the magnitude of the velocity of the quasi-viscous mode reaches the value of the speed of sound in metals already at temperatures of local heating of the shear zones of metallic samples that are deformed on Bridgman anvils $T \geq 473$ K. The question of the limitation of the propagation speed of nanobands within the quasi-viscous deformation mechanism still remains open and requires further analysis.

![Figure 2](image_url)  
**Figure 2.** The rate of the quasi-viscous deformation mode, depending on the activation energy of vacancy migration and the strain temperature.

The presented rates of the quasi-viscous deformation mode are approximate and do not take into account a number of many factors and conditions of deformation. Among them: an increase in the concentration of nonequilibrium point defects, in particular, when they are generated by cores of moving disclinations; change in the relative contribution of pair vacancies; non-equilibrium boundaries of nanograins and partial disclinations as potential sources of point defects, etc.

4. Conclusion

It is shown that a quasi-viscous mechanism of deformation by fluxes of non-equilibrium point defects can be realized on the example of pure Ni. Based on the analysis of the elastic-stressed state of a partial disclination nanodipole, theoretical estimates were made of the velocity of the movement of point defects $V$ and the motion of the nanodipole of partial disclinations $L$. It has been demonstrated that, within the quasi-viscous deformation mechanism, depending on the activation energy of migration of point defects (vacancies, interstitial atoms) and deformation temperature, the velocity of the quasi-viscosity deformation mode can reach high values close to the speed of sound in metals.

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