Numerical Simulation of Dislocation Dynamics

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Introduction The aim of this contribution is to present the current state of our research in the field of numerical simulation of dislocations moving in crystalline materials. The simulation is based on recent theory treating dislocation curves and dipolar loops interacting by means of forces of elastic nature and hindered by the lattice friction. The motion and interaction of one dislocation curve and one dipolar loop placed in 3D space is considered. Equations of motion for a parametrically described dislocation curve are discretized by the flowing finite volume method in space. The interaction force is computed for each dipolar loop and along the discretized curve. The resulting system of ordinary differential equations is solved by a higher order time solver.

Physical background Plastic deformation of crystalline solids is a result of the motion of dislocations. The theory of dislocations is described in number of text books, e.g. [8]. Here we recall only the basic mobile properties of dislocations and the nature of their mutual interactions.

A dislocation is a line defect of the crystal lattice. Along the dislocation line the regular crystallographic arrangement of atoms is disturbed. The dislocation line is represented by a closed curve or a curve ending at the surface of the crystal. At low homologous temperatures the dislocations can move only along crystallographic planes (the slip planes) with the highest density of atoms. The motion results in mutual slipping of the neighboring parts of the crystal along the slip planes. The slip displacement carried by a single dislocation, called Burgers vector, is equal to one of the vectors connecting the neighboring atoms.

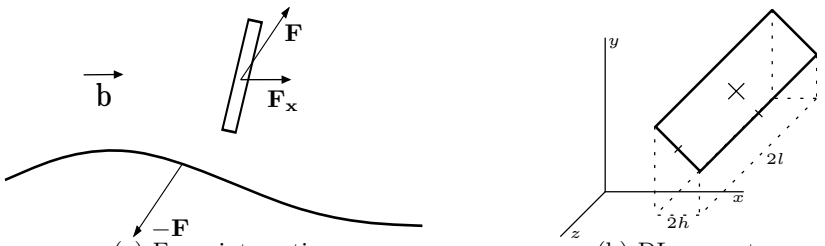
The displacement field of atoms from their regular crystallographic positions around a dislocation line can be treated (except the close vicinity of the line) as elastic stress and strain fields. On the other hand, a stress field exerts a force on a dislocation. The combination of these two effects causes the elastic interaction among dislocations.

One of the most distinguished features of plastic deformation at the microscale is a great overproduction of dislocations during a deformation process. Only a small fraction of generated dislocations is needed to carry plastic deformation, the rest is stored in the crystal. The deformed crystals supersaturated with dislocations tend to decrease the internal energy by mutual screening of their elastic fields. If dislocations possess a sufficient maneuverability provided by easy cross-slip (solids with wavy slip) the leading mechanism is an individual screening. The dislocations are stored in the form of dipoles which are transformed to prismatic dislocation dipolar loops of the prevailing edge character or such loops are directly formed (the experimental evidence is summarized in [9]).

The glide dislocations and the dislocation loops have much different characteristic length scales and mobile properties:
– While the segments of glide dislocations extend over distances of micrometers, the size of the prismatic dipolar loops is of the order of 10 nm.
– The glide dislocations are moved by the shear stress resolved in the slip plane, while the loops are drifted by stress gradients and/or swept by the glide dislocations. The loops being prismatic they can move along the direction parallel to the direction of their Burgers vector only.
– During deformation, the glide dislocations become curved. The local curvature of the glide dislocations seems to be one of the leading factors controlling the pattering [11, 12]. The loops can be approximately treated as rigid objects.

Due to the above mentioned complexity the formation of dislocation structures as a consequence of the interactions among dislocations is still an open problem. In this paper we will be concerned with a particular case: a dislocation curve interacting with a dipolar loop.

Dislocation Curve and Dipolar Loop We consider a plane dislocation segment with fixed ends; the segment represented by a plane curve can bow in a slip plane which is identified with the xz-plane of the coordinate system, i.e. $y = 0$. If the dislocation segment approaches a loop, the curve can pass by or the curve and the loop start to move together or the curve is stopped by the loop [13].



(a) Force interaction (b) DL geometry

Fig. 1. Dislocation dynamics problem geometry: (**a**) Dislocation curve and dipolar loop interaction; (**b**) Dipolar loop geometry

As the loop is allowed to move along the direction parallel to its Burgers vector **b** only (see Fig. 1a) just the force component in that direction causes the loop motion. Additionally, the lattice friction acts against the motion. The detailed condition for the dislocation curve and the loop is specified in Sect. .

The position of the loop is represented by 3 coordinates of its center. There are two types of dipolar loops: a *vacancy dipolar loop* and an *interstitial dipolar loop*; each type in two stable configurations [10] (see Fig. 2).

In vacancy loops a strip of atoms in regular crystallographic positions is missing. On the other hand; in interstitial loops an extra strip of atoms is added. For that reason the vacancy and interstitial loops produce different stress fields. The Burgers vectors of vacancy and interstitial loops have opposite directions. This fact we incorporate into our model by using negative value for the x-axis component of the Burgers vector for interstitial loop.

We denote the dipolar loop types and stable configurations by V_1, V_2 for the vacancy loop, and I_1, I_2 for the interstitial loop, respectively (see Fig. 2). In the mathematical

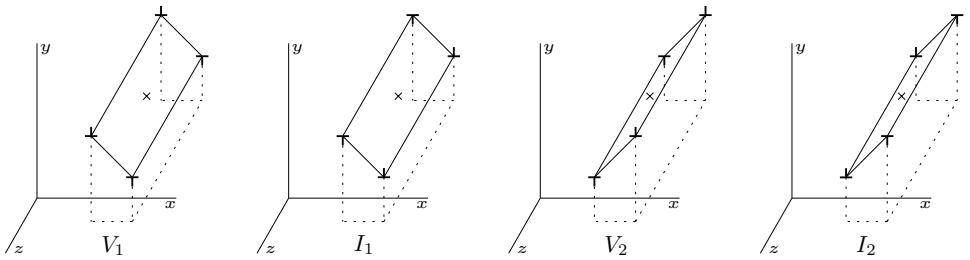


Fig. 2. Types and stable configurations of a dipolar loop. Longer sides of dipolar loop are parallel to the z-axis and lie in different layers of the atomic lattice

model we represent the dipolar loop as a small rectangle with two longer sides parallel to the z-axis and two shorter sides parallel either to $[1,1,0]$ or $[1,-1,0]$ depending on the type of loop. The dimensions of dipolar loop are $2l$ and $2\sqrt{2}h$, respectively, see Fig. 1b.

Stress Field of Dipolar Loop Each type of dipolar loop produces a stress field. The formula for this field will be needed in the numerical simulation of the dislocation dynamics. In this work we use the stress field σ_{ij} presented by Kroupa et al [6, 7] (using Einstein's symbolic rule for sums):

$$\begin{aligned}\sigma_{ij} = -\frac{\mu}{4\pi(1-\nu)} \iint\limits_A \frac{1}{\varrho^3} \Bigg\{ & \left[\frac{3(1-2\nu)}{\varrho^2} b_k \varrho_k \nu_n \varrho_n + (4\nu-1) b_k \nu_k\right] \delta_{ij} \\ & + (1-2\nu)\left(b_i\nu_j + b_j\nu_i\right) + \frac{3\nu}{\varrho^2}\left[b_k\varrho_k(\nu_i\varrho_j + \nu_j\varrho_i) + \nu_k\varrho_k(b_i\varrho_j + b_j\varrho_i)\right] \\ & + \frac{3(1-2\nu)}{\varrho^2} b_k\nu_k\varrho_i\varrho_j - \frac{15}{\varrho^4} b_k\varrho_k\nu_n\varrho_n\varrho_i\varrho_j \Bigg\} \mathrm{d}A \ . \end{aligned} \tag{1}$$

In (1) we introduce following symbols ($i,j,k,n \in \{1,2,3\}$):

- σ_{ij} $\sigma_{ij} = \sigma_{ij}(x,y,z)$ — components of the stress field tensor, depending on the position in space
- μ shear modulus
- ν Poisson's ratio
- A area of the dipolar loop, with $\mathrm{d}A = 2h\sqrt{2}\mathrm{d}t$
- b_i, b_j, b_k components of the Burgers vector
- $\varrho_i, \varrho_j, \varrho_k, \varrho_n$ components of the relative position vector, $\varrho_1 = x, \varrho_2 = y, \varrho_3 = z$
- ϱ relative distance from the dipolar loop, $\varrho = \sqrt{\varrho_1^2 + \varrho_2^2 + \varrho_3^2}$
- $\nu_i, \nu_j, \nu_k, \nu_n$ components of the dipolar loop normal vector
- δ_{ij} Kronecker symbol

The normal unit vector ν is chosen to be $\frac{1}{\sqrt{2}}[1,1,0]$ for dipolar loops of type V_1 and I_1, and $\nu = \frac{1}{\sqrt{2}}[1,-1,0]$ for dipolar loops of type V_2 and I_2.

Dipolar Loop and Dislocation Curve Interaction The interaction force per unit length of dislocation line is given by the Peach-Koehler equation, which written for the i-th component reads:

$$f_i = \varepsilon_{ijk}\sigma_{jm}b_m s_k \ , \tag{2}$$

where we denote:

f_i i-th component of the interaction force per the unit length of the dislocation line
ε_{ijk} Levi-Civita symbol
σ_{jm} components of the stress field tensor at the dislocation position
b_m components of the Burgers vector
s_k components of unit vector $\mathbf{s}$ which has the direction of the dislocation line

Mathematical Model The dynamics of the system of a dislocation curve and a dipolar loop is governed by a system of two equations describing their motion. The motion law for the dislocation curve is represented by the well-known mean curvature flow equation (see e.g. [4, 1, 3])

$$B\nu = \kappa + F \tag{3}$$

where ν is the normal velocity of evolving curve, κ its curvature, B (drag coefficient) is a constant given by material and F represents external driving force.

The moving dislocation curve Γ_t can be parameterized by a smooth time dependent vector function $\mathbf{X} : I \times S \to R^2$, i.e., at any time t it is given as the Image$(\mathbf{X}(.,t)) = \{\mathbf{X}(u,t), u \in S\}$ where S is a fixed parametrization interval and I is a time interval. For a smooth curve $|\mathbf{X}_u| > 0$ and for unit arc-length parametrization s, $ds = |\mathbf{X}_u|du$. Then $\mathbf{X}_s$ and $\mathbf{X}_s^\perp$ represent unit tangent and normal vectors, respectively. Using Frenet's formulae, the evolution equation (3) can be rewritten to the form of intrinsic diffusion equation [4, 1, 3, 5]

$$B\mathbf{X}_t = \mathbf{X}_{ss} + F\mathbf{X}_s^\perp \tag{4}$$

for the position vector $\mathbf{X}$. If we denote by $X^x(t,s)$ and $X^z(t,s)$ the components of the dislocation curve position vector in the xz-plane, then $\mathbf{X}_s^\perp = [X_s^z, -X_s^x]$. The equation (4) will be solved numerically to model a complicated dislocation curve dynamics.

Now we must explain exactly what is covered by the term F in (4). We know that F incorporates the interaction between the dislocation curve and the dipolar loop. To get detailed knowledge of F, we must go back to the Peach-Koehler equation (2). Assuming the dislocation curve can move only in the xz-plane and the dipolar loop can glide along the x-axis, we need to put f_x and f_z from the Peach-Koehler equation into the governing equations. Denoting the Burgers vectors of the dislocation curve and the dipolar loop $\mathbf{b}_{curve} = [b_{curve}, 0, 0]$ and $\mathbf{b} = [b, 0, 0]$, respectively, we get

$$f_x = \sigma_{xy} b_{curve} s_z \ , \quad f_z = -\sigma_{xy} b_{curve} s_x \ , \tag{5}$$

where $\sigma_{xy} = \sigma_{12}$, and s_x, s_z are the components of the dislocation curve's tangential vector, which can be also written as

$$[s_x, s_y, s_z] = \mathbf{X}_s^\perp = [X_s^z, 0, -X_s^x] \ . \tag{6}$$

Thus, the term $F = \sigma_{ext} b_{curve} + \sigma_{xy} b_{curve}$ covers the stress of the dipolar loop exerted on the dislocation curve, as well as any external stresses which may the material be exposed to. To be more precise, in order to obtain force vector acting at given position of the dislocation curve, one needs to multiply F and the dislocation curve's normal vector $\mathbf{X}_s^\perp$ at that position. We also explicitly write the dependence of F on the dislocation curve Γ_t because the curve position is required for the evaluation of its relative position to the dipolar loop. The obtained relative position is then used in the evaluation of σ_{xy}.

The stress σ_{xy} is given by (1), but we can simplify this formula for our specific situation – Burgers vector has only one non-zero component and the dipolar loop is a

rectangle which has one of the two possible configurations. Under the assumption that the dipolar loop parameter h is very small, we can use Taylor expansion in (1) and integrate it to obtain an algebraic formula for the stress:

$$\begin{aligned}\sigma_{xy}(x,y,z) = -\frac{\mu h b}{2\pi(1-\nu)}\Bigg\{ &\left[\frac{l-z}{\varrho_-} + \frac{l+z}{\varrho_+}\right]\left[\frac{x \pm y}{(x^2+y^2)^2}\left(\pm x + y - 8\frac{x^2 y}{x^2+y^2}\right)\right] \\ &+ \left[\frac{l-z}{{\varrho_-}^3} + \frac{l+z}{{\varrho_+}^3}\right]\left[\pm\nu + \frac{xy}{(x^2+y^2)^2}\left(y^2 - 3x^2 \mp 4xy\right)\right] \\ &+ \left[\frac{l-z}{{\varrho_-}^5} + \frac{l+z}{{\varrho_+}^5}\right]\left[-\frac{3x^2 y(x \pm y)}{x^2+y^2}\right]\Bigg\},\end{aligned} \tag{7}$$

where

$$\varrho_- = \sqrt{x^2+y^2+(l-z)^2}\,, \quad \varrho_+ = \sqrt{x^2+y^2+(l+z)^2}\,. \tag{8}$$

With the upper sign in (7) we get the stress formula for the dipolar loops V_1 and I_1, while with the lower sign we get the formula for V_2 and I_2 dipolar loops.

In order to obtain the equation governing the motion of the dipolar loop we have to sum all the stress contributions of the dislocation curve. It is enough to consider only the contributions in the x-axis direction because it is the only direction the dipolar loop is allowed to glide in.

The stress contribution of the dislocation curve can be obtained according to the action-reaction principle by simple reversing the sign of f_x in (5) and integrating along the dislocation curve:

$$F_x^c = \int_{\Gamma_t} \sigma_{xy} b_{curve} n_x \mathrm{d}s\,, \tag{9}$$

where n_x is the x-axis component of the dislocation curve element normal vector. Note it can be replaced using the derivatives of $\mathbf{X}$ with respect to the parametrization s since it holds $n_x = X_s^z$. Besides F_x^c there is one other kind of force — the friction force F_0 which is a constant given by the material and which acts against the gliding of the dipolar loop. Giving all the above information together, we come to the equation governing the gliding of the dipolar loop:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{1}{BP} F_{x,total}(\Gamma_t, x(t))\,, \tag{10}$$

where $x(t)$ is the x-axis position of the dipolar loop, $P = 4(l+\sqrt{2}h)$ is the perimeter of the dipolar loop, and

$$F_{x,total}(\Gamma_t, x(t)) = \begin{cases} F_x^c - F_0 \text{ if } F_x^c > F_0 \\ 0 \qquad\quad \text{if } |F_x^c| < F_0 \\ F_x^c + F_0 \text{ if } F_x^c < -F_0\,. \end{cases} \tag{11}$$

The complete dislocation dynamics problem for one dislocation curve and one dipolar loop then follows when we put (4) and (10) together with initial and boundary conditions.

Numerical Scheme For discretization of the problem described earlier, we use the flowing finite volume method [5] in space and the method of lines [2] in time. Discrete solution is represented by a moving polygon given, at any time t, by plane points $\mathbf{X}_i, i = 0, ..., M$. The values $\mathbf{X}_0$ and $\mathbf{X}_M$ are prescribed in case of fixed ends of the curve. The

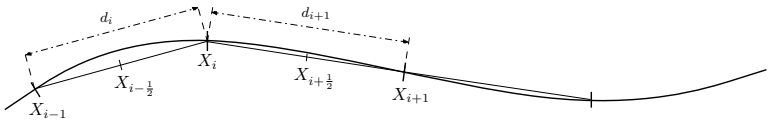


Fig. 3. Piecewise linear approximation of the dislocation curve.

segments $[\mathbf{X}_{i-1}, \mathbf{X}_i]$ are called flowing finite volumes. We construct also dual volumes $\mathcal{V}_i = \left[\mathbf{X}_{i-\frac{1}{2}}, \mathbf{X}_i\right] \cup \left[\mathbf{X}_i, \mathbf{X}_{i+\frac{1}{2}}\right]$, $i = 1, .., M-1$, where $\mathbf{X}_{i-\frac{1}{2}} = \frac{\mathbf{X}_{i-1}+\mathbf{X}_i}{2}$ (see Fig. 3). Integrating evolution equation (4) in dual volume $\mathcal{V}_i$ we obtain

$$\int_{\mathcal{V}_i} B\frac{\partial \mathbf{X}}{\partial t}\mathrm{d}s = \int_{\mathcal{V}_i} \frac{\partial^2 \mathbf{X}}{\partial s^2}\mathrm{d}s + \int_{\mathcal{V}_i} F\left(\frac{\partial \mathbf{X}}{\partial s}\right)^{\perp}\mathrm{d}s. \tag{12}$$

Then we simply get

$$B\frac{d_i + d_{i+1}}{2}\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}t} = \left[\frac{\partial \mathbf{X}}{\partial s}\right]_{\mathbf{X}_{i-\frac{1}{2}}}^{\mathbf{X}_{i+\frac{1}{2}}} + F_i\left[\mathbf{X}^{\perp}\right]_{\mathbf{X}_{i-\frac{1}{2}}}^{\mathbf{X}_{i+\frac{1}{2}}} \tag{13}$$

where

$$d_i = |\mathbf{X}_i - \mathbf{X}_{i-1}| = \sqrt{(X_i^x - X_{i-1}^x)^2 + (X_i^z - X_{i-1}^z)^2} \tag{14}$$

and F_i is a constant approximation of F in dual volume $\mathcal{V}_i$, $F_i = \sigma_{xy}(\mathbf{R_i})b_{curve}$, where $\mathbf{R_i} = \mathbf{X}_i - [x(t), y, z]$ is the relative positional vector of $\mathbf{X}_i$ and the dipolar loop center. If we replace the terms on the right-hand side by finite differences and averaged values, respectively, we end up with the system of ordinary differential equations

$$B\frac{\mathrm{d}\mathbf{X}_i}{\mathrm{d}t} = \frac{2}{d_i + d_{i+1}}\left(\frac{\mathbf{X}_{i+1} - \mathbf{X}_i}{d_{i+1}} - \frac{\mathbf{X}_i - \mathbf{X}_{i-1}}{d_i}\right) + \frac{2}{d_i + d_{i+1}}F_i\frac{\mathbf{X}_{i+1}^{\perp} - \mathbf{X}_{i-1}^{\perp}}{2}\ , \quad i = 1, \ldots, M-1\ . \tag{15}$$

In discretization of the governing equation (9) for the dipolar loop we sum contributions of every curve segment to obtain

$$F_x^c = \sum_{i=0}^{M-1} \sigma_{xy}\left(X_{i+\frac{1}{2}}^x - x(t), -y, X_{i+\frac{1}{2}}^z - z\right) b_{curve}\left(X_{i+1}^z - X_i^z\right)\ , \tag{16}$$

where $[x(t), y, z]$ is the center of the dipolar loop at time t. Next, we use formula (11) applied to discrete F_x^c defined above and get

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{1}{BP}F_{x,total}(\mathbf{X}_0, \ldots, \mathbf{X}_M, x). \tag{17}$$

The complete discrete problem consists of (15) and (17) with accompanying initial and boundary conditions.

Results of Numerical Experiments We made several numerical simulations in which we used different settings. For the basic physical parameters we used values which were experimentally measured for nickel crystals at room temperature [10]: average length and width of the dipolar loop $l = 60$ nm, $h = 4$ nm, Burgers vector $b = 0.26$ nm, shear

modulus $\mu = 80$ GPa, and Poisson's ratio $\nu = 0.33$. When not specified otherwise, we used drag coefficient $B = 10^{-5}$ Pa s.

In the simulations we were changing not only the type and initial position of the dipolar loop, but also the initial shape of the dislocation curve and the value of friction force. We observed following facts (not all of them can be demostrated here):

- For the dislocation curve with fixed ends the curvature acts against the external stress. Therefore, there exists some equilibrium shape the dislocation curve tends to.
- When no external stress is applied, the dislocation curve of any initial shape tends to the straight line (potential energy minimization). Adding dipolar loop, an oscillating motion (Fig. 4) of the dipolar loop as well as the dislocation curve can occur.
- The direction in which the dipolar loop leaves the dislocation curve's interaction region depends on the type of the dipolar loop. Simply, V_2 shifts to the left where V_1 shifts to the right.

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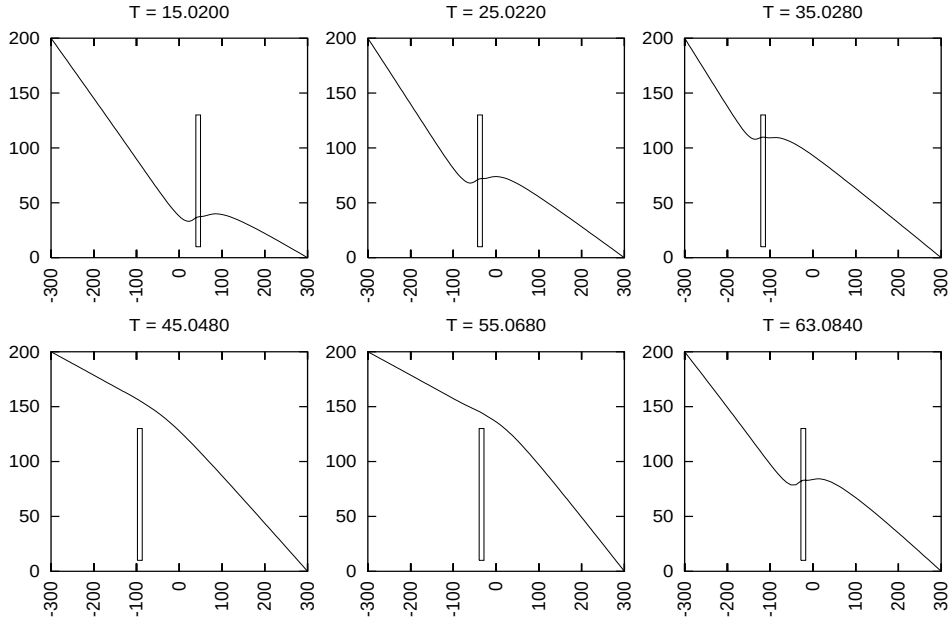

Fig. 4. Dipolar loop oscillations. Dipolar loop of type V_1 starts to glide to the left of the dislocation curve (timelevels $T = 15.02$, $T = 25.022$, $T = 35.028$). Then it reverses as the attractive force of the dislocation curve gains the control over the system for some time ($T = 45.048$, $T = 55.068$). Second reversing occurs before $T = 63.084$

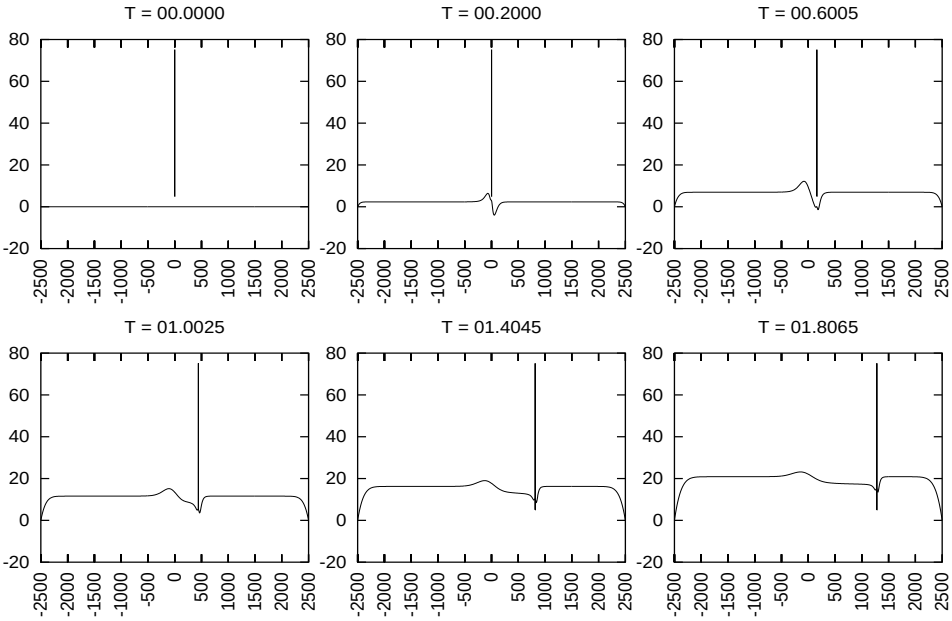

Fig. 5. Dipolar loop swept by the curve; on the other hand, the curve is distorted by the stress field of the loop. In this test there were used: $\mu = 80$ GPa, $\nu = 0.33$, $B = 10^{-4}$ Pa s, $b = 0.707$ nm, $l = 35$ nm, $h = \sqrt{2}$ nm, $F_0 = 4$ MPa m, applied stress $\sigma_a = -1.155$ MPa. Initial position of dipolar loop was $[0, 40, -30]$. The subsequent stages are shown for increasing time T