Differential Equations in Modelling Motion of Dislocations†

Jiří Šremr

Institute of Mathematics, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic

E-mail: `sremr@fme.vutbr.cz`

Most of the technologically important materials are crystals, where atoms are arranged in a periodic lattice of a defined symmetry (cubic, hexagonal, orthorhombic, etc.). It is known that a plastic deformation of body-centred cubic metals is governed by the thermally activated motion of *screw dislocations*. Dislocations are line defects in crystals, that are caused by the finite rate of solidification because the atoms do not have sufficient time to take perfect lattice positions. Each dislocation is characterized by the so-called *Burgers vector* $\vec{b}$ and the tangential vector $\vec{u}$. We distinguish two basic types of dislocation segments: *edge* segment ($\vec{b} \perp \vec{u}$) and *screw* segment ($\vec{b} \parallel \vec{u}$), see Figure 1.

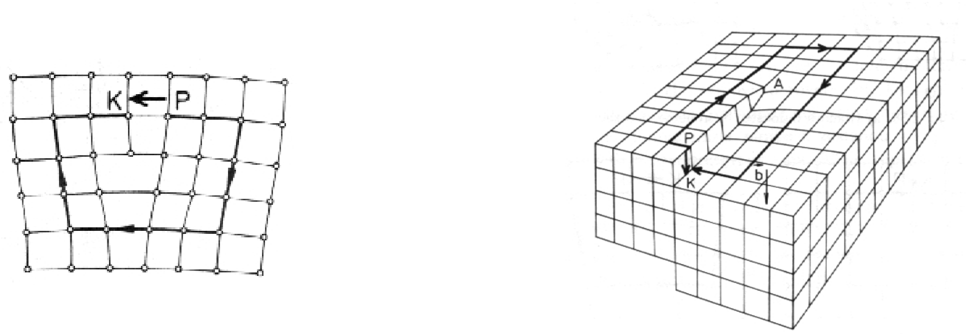

Figure 1. Edge and screw dislocations in a simple cubic lattice

If none of these conditions is satisfied, we speak about a *mixed* segment.

In this thesis, we consider the so-called $1/2\langle 111\rangle$ screw dislocation in a body-centred cubic lattice. In that case, the tangential vector $\vec{u}$ of the dislocation line has the direction of a body diagonal of the cubes. We choose a slip plane as shown in Figure 2 and introduce an appropriate coordinate system. The motion of screw dislocations in a slip plane is thermally activated – they move due to the applied load and this motion is aided by thermal fluctuations. The dislocation first moves by the applied shear stress τ as a straight line from $y = 0$ to $y = y_0$, where the value of y_0 is given by the relation $\Gamma'(y_0) = \tau b$ (see Figure 3).

Here Γ denotes the so-called Peierls barrier representing lattice friction that acts against moving the dislocation. From the straight *initiated shape*, the dislocation vibrates due to the finite thermal energy and reaches its *activated shape* (see Figure 3). This activated shape of the dislocation determines the the activation enthalpy for the motion of the dislocation under the applied stress τ.

In the paper [1], the following relation is derived for the enthalpy corresponding to the shape of the dislocation $y = y(x)$:

$$H_\tau(y) = \int\limits_{-\infty}^{+\infty} \Big[\Gamma(y(x))\sqrt{1 + [y'(x)]^2} - \Gamma(y_0) - \tau b(y(x) - y_0)\Big]\,\mathrm{d}x.$$

†The problem was suggested by Roman Gröger from the Institute of Physics of Materials of the Czech Academy of Sciences (e-mail: `groger@ipm.cz`).

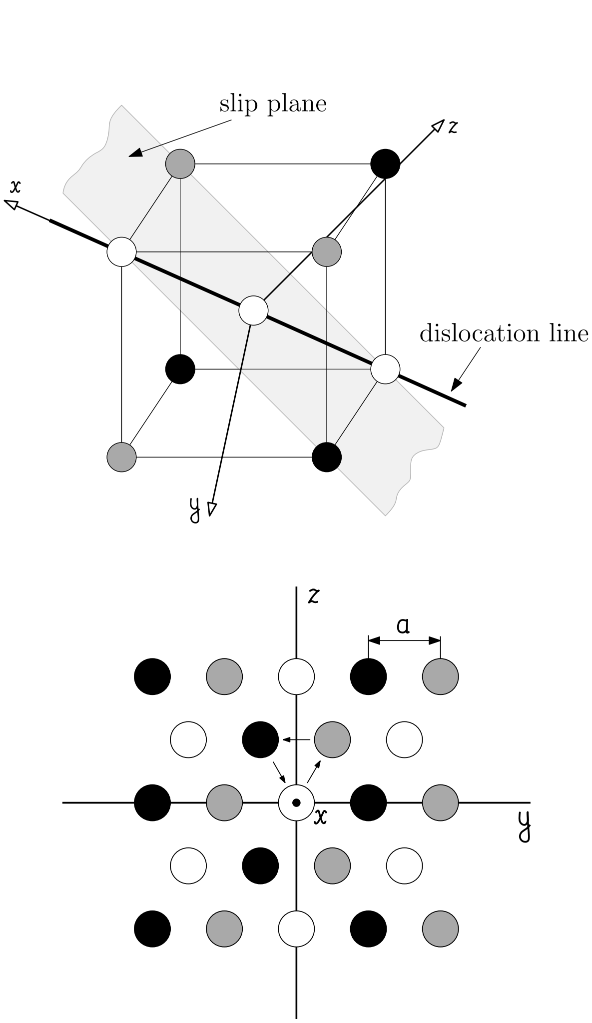

Figure 2. Coordinate system

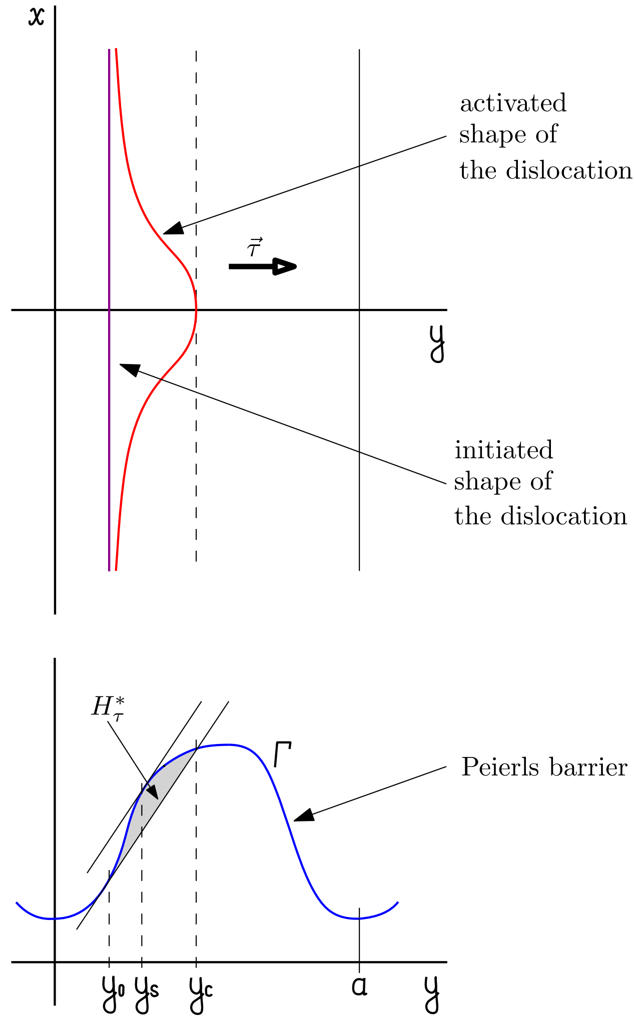

Figure 3. Peierls barrier

The first term under the integral sign corresponds to the energy of a curved dislocation, the second term deals with the energy of the straight dislocation, and the third term represents the work done by the stress τ on changing the shape from y_0 to y. We are looking for the shape of the dislocation $y = y(x)$ with fixed ends $y(\pm\infty) = y_0$, that corresponds to the minimum of the enthalpy H_τ. Such a shape of the dislocation is called *activated shape* and, as was mentioned above, it determines the value H_τ^* of the activation enthalpy for the motion of the dislocation under the given shear stress τ. Applying the Euler-Lagrange equation to the described variational problem leads to the boundary value problem

$$\frac{\Gamma(y)y''}{\sqrt{1+[y']^2}} = \Gamma'(y) - \tau b\sqrt{1+[y']^2}\,, \tag{1}$$

$$\lim_{x\to-\infty} y(x) = y_0, \quad \lim_{x\to-\infty} y(x) = y_0. \tag{2}$$

Hence, the *activated shape* of the dislocation can be mathematically described as a non-constant solution to the boundary value problem (1), (2). Recall that, in equation (1), τ is the share stress, b stands for the magnitude of the Burgers vector, and Γ denotes the Peierls barrier (see Figure 3).

Motivated by the shape of the Peierls barrier Γ discussed in [1], we introduce the assumption

$$\left.\begin{array}{c}\Gamma\in C^2(\mathbb{R};\,]0,+\infty[\,) \text{ is an } a\text{-periodic function,}\\ \text{there exists } \ 0<y_0<y_c<a \ \text{ such that}\\ \Gamma'(y_0)=\tau b, \quad \Gamma'(y_c)<\tau b,\\ \Gamma(y)>\Gamma(y_0)+\tau b(y-y_0) \ \text{ for } \ y\in[0,y_c[\,\setminus\{y_0\},\\ \Gamma(y)<\Gamma(y_0)+\tau b(y-y_0) \ \text{ for } \ y\in\,]y_c,a],\end{array}\right\} \tag{A_1}$$

which allows one to prove the following theorem.

Theorem 1. *Let $a,b,\tau>0$ and the function Γ satisfy assumption (A_1). Then problem $(1),(2)$ has a unique (up to a translation) non-constant solution.*

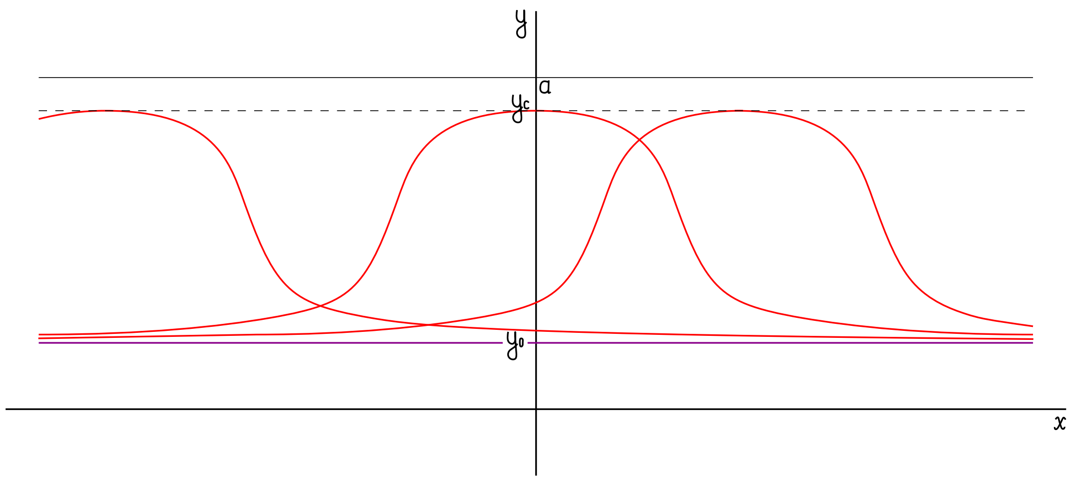

Figure 4. Solutions to problem $(1),(2)$ – activated shape of the dislocation

Remark 2. It follows from the proof of Theorem 1 that each solution to problem $(1),(2)$ is a solution to the Cauchy problem

$$\frac{\Gamma(y)y''}{\sqrt{1+[y']^2}}=\Gamma'(y)-\tau b\sqrt{1+[y']^2}\,; \quad y(0)=\alpha_1, \ \ y'(0)=\alpha_2$$

for some $\alpha_1\in\,]y_0,y_c]$, $k\in\{1,2\}$, and $\alpha_2=(-1)^k\sqrt{[\frac{\Gamma(\alpha_1)}{\Gamma(y_0)+\tau b(\alpha_1-y_0)}]^2-1}\,$.

From the mathematical point of view, it is interesting task to investigate a shape of each solution to equation (1). Assume that, in addition to (A_1), the Peierls barrier Γ satisfies the following condition

$$\text{there exists a unique } \ y_s\in\,]y_0,y_0+a[\ \text{ such that } \ \Gamma'(y_s)=\tau b. \tag{A_2}$$

Then we can derive qualitative properties of all solutions to equation (1) and describe the phase portrait of (1) in detail, see Figures 5 and 6 on below.

References

[1] J. E. Dora and S. Rajnak, Nucleation of king pairs and the Peierls' mechanism of plastic deformation. *Trans. AIME* **230** (1964), 1052–1064.

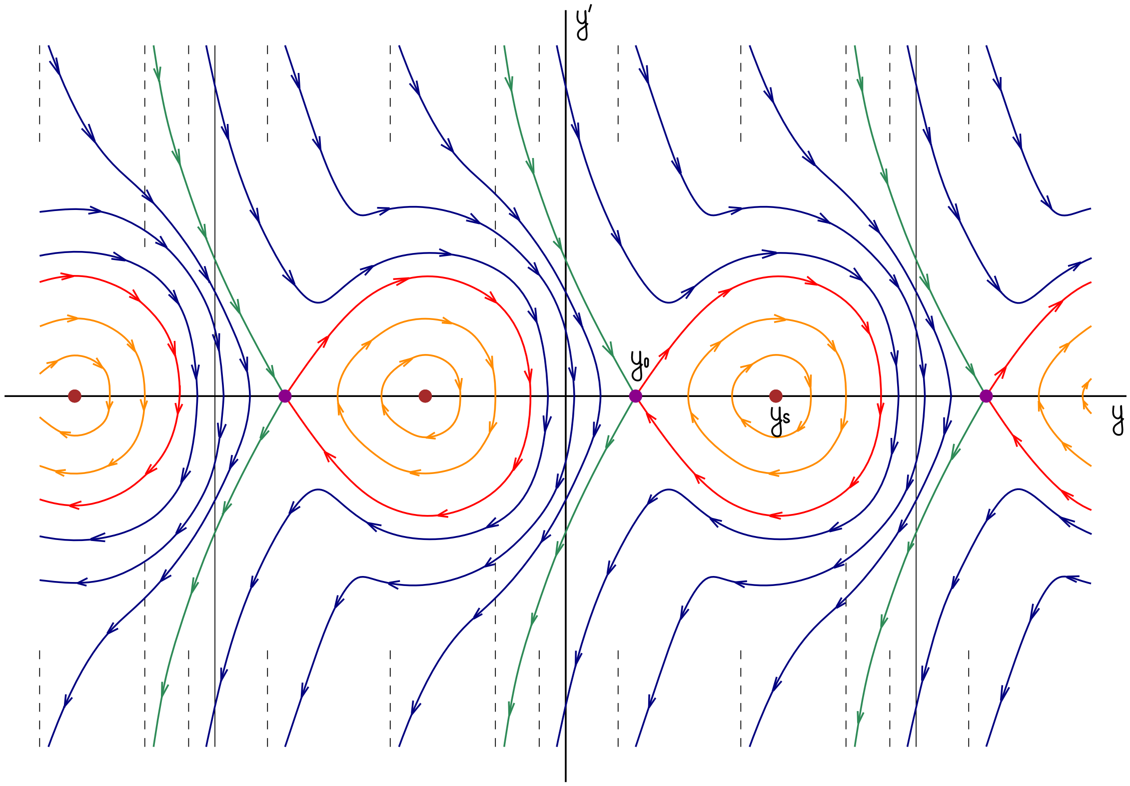

Figure 5. Phase portrait of equation (1)

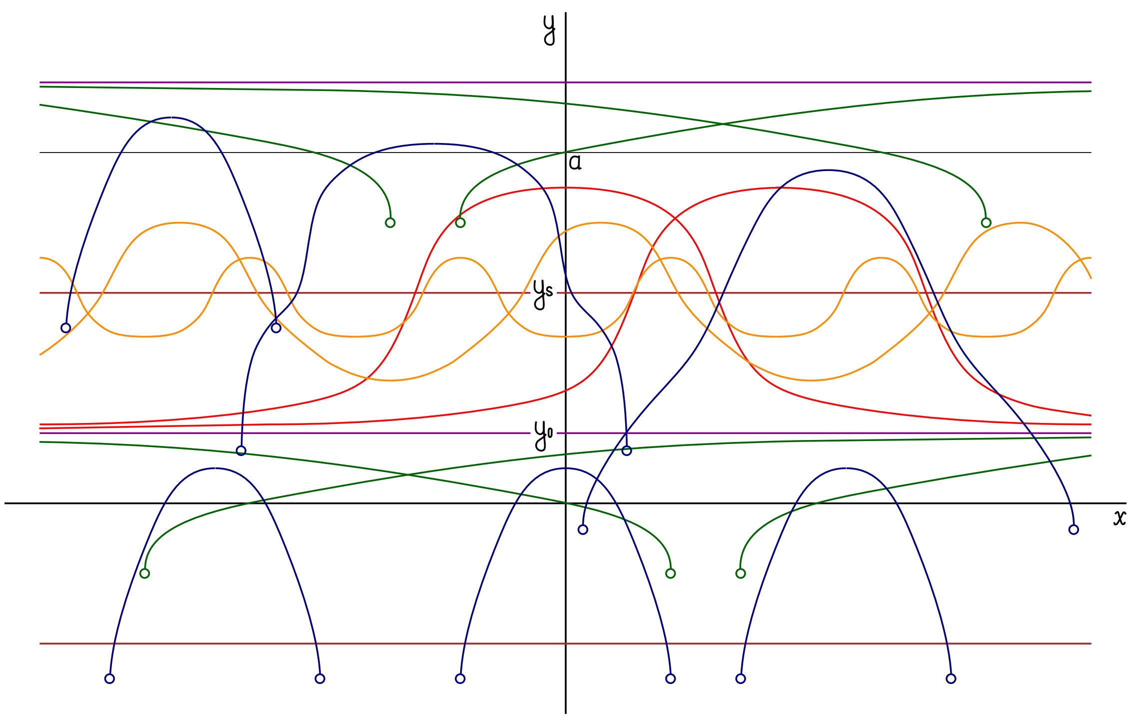

Figure 6. Graphs of various solutions to equation (1), colours of solutions correspond to colours of orbits in Fig. 5