Physica B: Condensed Matter 567 (2019) 138–141

Contents lists available at ScienceDirect

Physica B: Condensed Matter

journal homepage: www.elsevier.com/locate/physb

Effects of relaxation and pre-history in the course of plastic twisting

Yu. D. Zavorotnev[a,*], L.S. Metlov[a], A. Yu. Zakharov[b], O. Yu. Popova[c]

[a] Donetsk Institute for Physics and Engineering, 72, R. Luxemburg St., Donetsk, 83114, Ukraine
[b] Yaroslav-the-Wise Novgorod State University, 41, B. St.-Petersburgskaya St., Veliky Novgorod, 173003, Russia
[c] Donetsk National Technical University, 2, Shybankova Square, Pokrovsk, Donetsk region, 85300, Ukraine

ARTICLE INFO

Keywords:
Phase transition
Order parameter
Thermodynamic potential
Plastic twisting
The landau-khalatnikov equation

ABSTRACT

The effect of temporal delay and relaxation on the structural order parameter (OP) in the course of plastic deformation by twisting is theoretically analyzed. It is shown that an anomalous behavior of the OP modulus takes place. The analysis is based on the Landau-Khalatnikov equation.

1. Introduction

At the moment, the severe plastic deformation (SPD) is applied to the materials of different nature, namely, polycrystalline metals [1–3], shape memory alloys [4–6], alloys characterized by phase transitions and stratifications [7,8], amorphous and semi-crystalline alloys [9–11], polymers [12–14]. At the same time, the processes of generation and annihilation of the defects within the material [15–17] can be accompanied by modifications of phase and component composition, magnetic and structural ordering. The classical theory of phase transitions is based on the idea that there exist ideally symmetric crystals. The effects of the structural defects that are inevitably present in real objects are neglected or taken into account in the lowest approximation [18].

At the same time, SPD enhances the density of the structural defects to the level when their effect cannot be neglected. They distort the symmetry of the phases on both sides of a phase transition and modify the energy physics of the material [19]. In particular, interactions of the symmetry order parameters and the densities of structural defects in the course of processing by twisting under pressure are of great interest [20].

Abrasion processing of inter-metallic compound of Fe_3Al [21] supplemented by volume processing by SPD [22] has demonstrated complex non-monotonic behavior of the parameters in the course of treatment including a decrease in the structural order parameter down to almost zero value and a succeeding increase resulting in a stable value capture (see Fig. 2 in Ref. [22]). This behavior can be determined by a joint effect of a temporal delay and relaxation in the course of twisting. The present work reports the study of possible mechanisms of the anomalies.

2. Theory

When a plastic deformation of any type is applied, four zones can be separated. The first zone is characterized by elastic behavior only. Plastic deformation becomes substantial within the second one. The third zone is an area of prevailing plastic deformation. The fourth zone associated with a fracture, we do not consider here. It should be noted that a conventional criterion of the separation of the first zone and the second one is absent. This fact is determined by substantial effect of plasticity on the behavior of the material even under small deformation.

All the of aforesaid is also related to plastic deformation of twisting about a crystal axis. The further analysis is based on the explicit dependence of the modulus of twisting moment M on the number of revolutions N. To establish the dependence, generally, the description of the evolution of structural defects [15,23,24] and their effect on the plastic yield stress of the twisting moment is required. The problem becomes more complex, so simplifying assumptions should be made. Namely, at high N, the system achieves constant stationary values. Thus, the modulus of the twisting moment M depends on the number of revolutions N as a function characterized by a horizontal asymptote

$$M = \alpha_1 \tanh(\alpha_2 N) \quad (1)$$

where α_1 and α_2 are phenomenological constants. The choice is based on the fact of constant M within the third zone because the twisting moment is determined by the elastic component of deformation only.

Suppose that the second-order phase transition results in formation of a highly-symmetrical state characterized by vector order parameter q and non-zero Lifshits invariants. Non-equilibrium thermodynamic potential is written as

* Corresponding author.
E-mail address: zavorotnev.yurii@mail.ru (Y.D. Zavorotnev).

https://doi.org/10.1016/j.physb.2018.12.019
Received 7 December 2018; Accepted 13 December 2018
Available online 14 December 2018

$$\Phi = \frac{b_1}{2}q^2(N) + \frac{b_2}{4}q^4(N) + \frac{b_3}{6}q^6(N) + \gamma_1 M^s\left(q_x\frac{\partial q_y}{\partial z} - q_y\frac{\partial q_x}{\partial z}\right) + \gamma_2 M^r\left(\left(\frac{\partial q_x}{\partial z}\right)^2 + \left(\frac{\partial q_y}{\partial z}\right)^2\right) + q^2(N)\frac{1}{\Delta N}\int_{N-\Delta N}^{N} A(x)q^2(x)dx + \Phi_{el} \quad (2)$$

where γ_i *(i = 1, 2)*, b_i *(i = 1, 2, 3)* are phenomenological constants, Φ_{el} is the potential of elastic interaction related to the elastic tensor. The terms that include derivatives describe spiral structure generated as a result of twisting. The next to last term in (2) accounts for the prehistory, factor *A(x)* determines the law of distribution of interaction in the past. In particular, the law can describe the preceding states totally or partially as well as the rate of decrease in the interaction (exponential, elliptical, linear etc.). After the equilibrium values of the elastic tensor components are found as functions of *q(N)* and the obtained results are substituted in (2), we get a non-equilibrium thermodynamic potential without term Φ_{el} that is analogous to (2). As a result, the expansion coefficients will depend on the components of the elastic tensor and the twisting moment, in turn. When expanding the coefficient of the fourth degree of the structural OP into a series in square twisting moment, in the first approximation, the new coefficient at the fourth degree has the form $(1 + BM^2)b_2$, where B is a phenomenological coefficient. The related Euler equation that determines the minimum of the functional (2) is a second-order differential equation with the solutions written as follows if the terms including the first-order derivatives are taken into account

$$q_x = q\cos(kz), \quad q_y = q\sin(kz) \quad (3)$$

where k is the modulus of propagation vector. After substituting (3) into (2), differentiation with respect to k results in

$$k = -\frac{M^{s-r}\gamma_1}{2\gamma_2} \quad (4)$$

According to estimations reported in Ref. [25], *s–r = 4*. In the present work, *s = 6*, *r* = 2.

Account of deformation implies that the system passes to a non-equilibrium state as a result of a process. Transition to the equilibrium state is due to a relaxation in some time period. Thus, under instantaneous relaxation, the solution of the state equation will be formed by the equilibrium states. At the finite relaxation time and fast external action, the states are non-equilibrium and the modulus of the structural OP is modified. The delay of the equilibrium state can be described by the Landau-Khalatnikov equation

$$\frac{\partial q}{\partial t} = -\gamma(q)\frac{\delta\Phi}{\delta q} \quad (5)$$

where $\gamma(q)$ characterizes the rate of the system relaxation to the equilibrium state, $\frac{\delta\Phi}{\delta q}$ is the functional derivative, t is time. Generally $\gamma(q)$ is temperature dependent, but we neglect this fact. According to the definition of functional Φ (2), with account of constant modulus of an irreducible OP along the axis of twist at fixed time and the number of revolutions, equation (5) is written in the form

$$\frac{\partial q}{\partial t} = -\gamma(q)q(N)\{b_1 q(N) + b_2 q^3(N) + b_3 q^5(N) + \gamma_1 M^s k + \gamma_2 M^r k^2 + \frac{2}{\Delta N}\int_{N-\Delta N}^{N} A(x)q^2(x)dx\} \quad (6)$$

where $N = N(t)$. Further, we suppose that the rate of twisting is small enough and the adiabaticity condition is not valid.

We analyze three variants of time dependence of the number of revolutions here: $N_1 \sim t$, $N_2 \sim t^2$, $N_3 \sim \sqrt{t}$. The dependences imply steady rotation, rotation with positive and negative acceleration, respectively. Equation (6) was solved numerically using the MatLab package. It should be noted that the selection of the phenomenological coefficients in (2) is determined by the analyzed compound. In the present work, the values are selected to provide existence of real solutions of state equation (6).

3. Results and discussion

When analyzing state equation (6), we suppose that $\gamma(q)$ is a constant.

1) Without of prehistory account. The results of theoretical analysis of time dependence $q(t)$ at varied twisting conditions are presented in Fig. 1. The dash-dotted line is the linear dependence $N_1 \sim t$, the dashed line is the square dependence $N_2 \sim t^2$ and the dotted line marks the rotation with negative acceleration $N_3 \sim \sqrt{t}$. For the sake of comparison, solid line illustrates $q(N)$ without relaxation (the system is in the equilibrium state at any twisting moment) at $N \sim t$ (steady rotation).

From the mathematical viewpoint, the minimum of function $q(t)$ is determined by competition of the fourth-order terms and the first-order derivatives in thermodynamic potential (2). At small values of $N \sim t$ (the first zone), the coefficient of the fourth degree of the OP prevails and the modulus of $q(t)$ is reduced. Within the second zone, the terms associated with the first-order derivatives become substantial and the contribution of plastic deformation is large. This fact results in an increase in the modulus of the structural OP. Within the third zone, the twisting moment and the potential are constant, so the OP is independent of the number of revolutions.

From the viewpoint of physics, a stable state of a crystal is characterized by some energy minimum. At high temperature, the global minimum is of highly symmetrical state. At the temperature drop, an additional minimum arises that is associated with a state of low symmetry. Under further temperature decrease, the low-symmetry phase is of lower energy. If the system is located below the temperature of transition in the area of lability, where two minima coexist, and the twisting deformation is applied, the elastic component enhances the energy of the system. As a result, the minima of high- and low-symmetry phases start convergence and the reverse transition to a high-symmetry state becomes favorable. Thus, the modulus of the OP is reduced.

Further, increase if N reduces a contribution of the elastic component according to (1). A spiral structure becomes the most favorable state of the system.

As a result, the energy of the crystal decrease and the modulus of the OP rises. In the steady mode, the contribution of the elastic component stays constant, being accompanie by a fixed energy of the system and the modulus of the OP becomes independent of the number of revolutions. As shown in Fig. 1, an account of possible relaxation results in an increase in the modulus of the structural OP and a shift of the minimum of $q(t)$ towards later moments.

The lowest shift is generated by the linear dependence $N_1 \sim t$, the highest one is related to $N_3 \sim \sqrt{t}$. One should note unusual behavior of

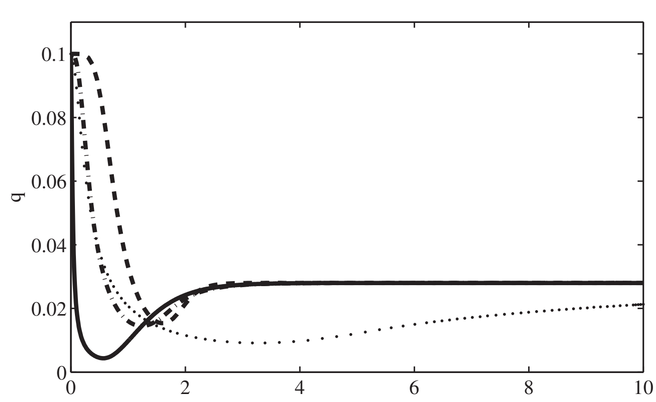

Fig. 1. Rotation without an account of prehistory.

the dotted line (exponential distribution) characterized by a plateau at minor values. This fact is determined by low twisting rate in this area, so the energy of the sample stays almost the same. The ratio of the energies in the highly-symmetrical and low-symmetrical phases is stable, resulting in local stability of the structural order parameter. In the last two cases, the twisting rate in the vicinity of zero time is higher. The equalization of the energies of highly-symmetrical and low-symmetrical states proceeds faster and the value of $q(t)$ is reduced faster, too. The case of $N_3 \sim \sqrt{t}$ is of the highest rate and a reduction of $q(t)$ is faster, consequently.

2) In view of prehistory

a) We consider the case of $N_1 \sim t$ (rotation at a constant angular velocity). From the viewpoint of Physics, due regard to the prehistory means that there exist areas with the frozen preceding values of the twisting moment within the crystal. The size of the areas and their interaction with the current state may vary. The areas evolve and their size is fast reduced. From the viewpoint of Mathematics, the relation of these area and the current state can be described by a distribution function.
In Fig. 2, the results of theoretical calculations inclusive of four distribution laws of prehistory are presented. The solid, dotted, dash-dotted and dotted lines mark rectangular ($\Delta N < N$), exponential, elliptical ($\Delta N < N$) and linearly descending ($\Delta N < N$) distribution law, respectively. A sharp change of the monotonous solid line in the vicinity of $t \sim 5{,}5$ arises due to the fact that preceding states become not involved to the prehistory and their contribution is of the same intensity. With respect to this fact, in the third zone, $q(t)$ demonstrate substantial convergent oscillations in the vicinity of the minimum of the non-equilibrium potential that is an evidence of gradual approaching the equilibrium. The first peak is determined by a sharp rejection of sharply changeable initial states. The next minimum arises as a result of the rejection of the states in the vicinity of $t \sim 5{,}5$. An analogous feature is less pronounced in the rest of cases because the rejections occur at small parameter of distribution $A(x)$. The anomaly is almost invisible at the exponential distribution law. An increase in the relaxation constant results in smoothing of $q(t)$ within the third zone (Fig. 3). We should also note abrupt decrease in the modulus of the OP at small time values.

b) Time dependence of the number of revolution is quadratic $N_2 \sim t^2$ (rotation with constant acceleration). In Fig. 4, the results of theoretical experiment are presented as in Item 2a at four distribution laws and small relaxation constant. As compared to Fig. 2, the maxima become more explicit when passing to the third zone except the case of the constant distribution law. The width of the maxima is smaller and they are higher of that in case 2a. This effect is determined by a higher rotation velocity in the present zone as compared to the linear case. An increase in the relaxation constant results in smoothing of $q(t)$ within the third zone similar to that in case 2a.

c) Suppose $N_3 \sim \sqrt{t}$ (rotation with deceleration). In Fig. 5, the results of theoretical experiment with four distribution laws of the prehistory at small relaxation constant are presented. Comparison of Figs. 2–5 shows that at small time values, the behavior of the modulus of the structural OP does not depend on the twisting character and the distribution law of the prehistory. This fact is associated with the prevailing effect of the fourth-order term of the thermodynamic potential (2) within this time range. The comparison of the last three figures demonstrates that due regard to the prehistory results in a faster decrease in $q(t)$ at the initial time moments and a vanishing plateau if $N_2 \sim t^2$. An increase in the relaxation constant is followed by vanishing maximum of $q(t)$ at the boundary of the second zone and the third one in this case. The related dependence becomes monotonic ascending after the minimum.

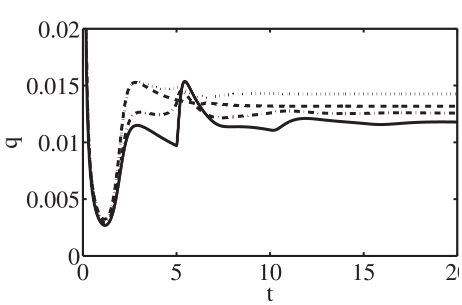

Fig. 2. Steady rotation. Small value of the parameter of system relaxation.

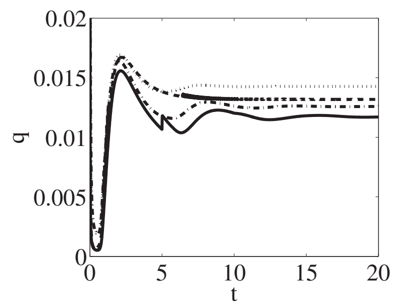

Fig. 3. Uniform rotation. Great value of the relaxation parameter.

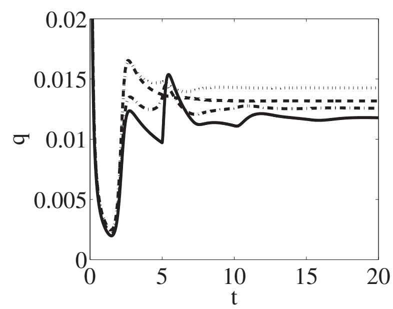

Fig. 4. Steady rotation.

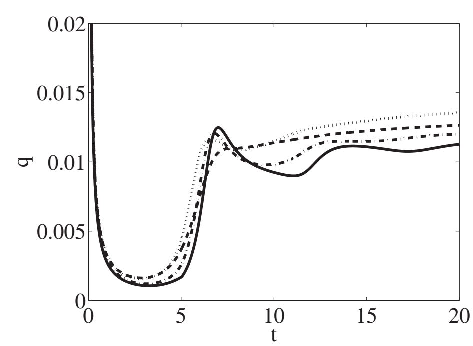

Fig. 5. Rotation with negative acceleration.

4. Conclusions

1) Account for the prehistory results in emergence of a local maximum at the boundary of the second zone and the third one.
2) Account of the time delay affects the rate of decrease in $q(t)$ within the first zone.
3) The rate of time evolution of the rotation function affects the behavior of $q(t)$ within the third zone.

Acknowledgement

One of the authors (A.Yu. Zakharov) is grateful to the Ministry of Education and Science of Russian Federation for the financial support within the framework of the project part of the Government Assignment (Grant No. 3.3572.2017).

References

[1] R.Z. Valiev, Nanostruct. Mater. 6 (1995) 73–82.
[2] Z. Horita, M. Furukawa, M. Nemoto, T.G. Langdon, Mater. Sci. Technol. 16 (2000) 1239–1245.
[3] T.G. Langdon, Rev. Adv. Mater. Sci. 13 (2006) 6–14.
[4] V.G. Pushin, R.Z. Valiev, Y.T. Zhu, D.V. Gunderov, N.I. Kourov, T.E. Kuntsevich, A.N. Uksusnikov, L.I. Yurchenko, Mater. Trans. 47 (2006) 694–697.
[5] N.I. Kourov, V.G. Pushin, A.V. Korolev, V.V. Marchenkov, E.B. Marchenkova, V.A. Kazantsev, H.W. Weber, Phys. Solid State 53 (2011) 91–99.
[6] M. Shimono, K. Tsuchiya, H. Onodera, Mater. Trans. 54 (2013) 1575–1579.
[7] Yu. N. Gornostyrev, I.K. Razumov, A.Ye. Yermakov, J. Mater. Sci. 39 (2004) 5003–5009.
[8] I.K. Razumov, Yu. N. Gornostyrev, A.Ye. Yermakov, Rev. Adv. Mater. Sci. 18 (2008) 757–763.
[9] R.V. Sundeev, A.M. Glezer, A.P. Menushenkov, A.V. Shalimova, O.V. Chernysheva, N.V. Umnova, Mater. Des. 135 (2017) 77–83.
[10] A.M. Glezer, L.S. Metlov, R.V. Sundeev, A.V. Shalimov, JETP Lett. (Engl. Transl.) 105 (2017) 332–334.
[11] R.V. Sundeev, A.V. Shalimova, A.M. Glezer, E.A. Pechina, M.V. Gorshenkov, G.I. Nosova, Mater. Sci. Eng. 679 (2017) 1–6.
[12] A. Phillips, P. Zhu, G. Edward, Macromolecules 39 (2006) 5796–5803.
[13] T. Wang, S. Tang, J. Chen. J. Appl. Poly. Sci. 122 (2011) 2146–2158.
[14] V.A. Beloshenko, A.V. Voznyak, Yu. V. Voznyak, L.A. Novokshonova, V.G. Grinyov, V.G. Krasheninnikov, Int. J. Poly. Sci. (2016) 85642451.
[15] L.S. Metlov, Phys. Rev. E90 (2014) 022124(8).
[16] M.P. Kashchenko, A.G. Semenovih, V.G. Chashchina, J. Phys. IV France 112 (2003) 147–150.
[17] M.P. Kashchenko, V.J. Chashchina, Lett. Mater. 5 (1) (2015) 82–89.
[18] In book: T. Castan, E. Vivas, L. Minosa, A. Planes, A. Saxena, Magnetism and structures in functional materials, in: A. Planes, L. Minosa, A. Saxena (Eds.), Springer Series in Material Science, vol. 79, Springer-Verlag, Berlin-Heldelberg, 2005.
[19] L.S. Metlov, Bull. Lugansk Nat. Univ. 5 (11) (2018) 88–90 (in Russian).
[20] Yu. D. Zavorotnev, A. Yu. Zakharov, L.S. Metlov, Phys. Solid State 59 (2017) 2290–2295.
[21] J. Ren, D. Li, P. Xu, J. Mater. Eng. Perform. 23 (2014) 308–314.
[22] A.M. Glezer, I.A. Timshin, I.V. Shchetinin, et al., J. Alloy. Comp. 744 (2018) 791–796.
[23] E.I. Teitel, L.S. Metlov, D.V. Gunderov, A.V. Korznikov, Phys. Met. Metallogr. 113 (2012) 1162–1168.
[24] A.V. Khomenko, Ya. A. Lyashenko, L.S. Metlov, Metallofizika i noveishie tekhnologii 30 (2008) 859–872.
[25] Yu. D. Zavorotnev, E.H. Pashinskaya, V.N. Varyukhin, O. Yu. Popova, JMMM 349 (2014) 244–248.