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ORIGINAL ARTICLE

Discrete model of dislocations in fractional nonlocal elasticity

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Abstract Discrete models of dislocations in fractional nonlocal materials are suggested. The proposed models are based on fractional-order differences instead of finite differences of integer orders that are usually used. The fractional differences allow us to describe long-range interactions in materials. In continuous limit the suggested discrete models give continuum models of dislocations in nonlocal continua. Fractional generalization of the Frenkel–Kontorova model by using long-range interactions is suggested. We also propose a fractional generalization of interacting atomic chains (IAC) model of dislocations by considering long-range interacting chains.
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1. Introduction

Dislocations in materials can be described by a microscopic approach based on discrete models and by a macroscopic approach based on continuum models. Continuum description of dislocations can be derived as a limit of lattice model, where the length scales of infinitesimal continuum elements are much greater than inter-particle distances in the lattice. The elasticity theory of nonlocal continuum was initiated by the papers of Eringen (1972). Models of nonlocal elasticity are based on the assumption that the forces between material points are a long-range type, thus reflecting the long-range character of inter-atomic forces (Eringen, 2002; Rogula, 1983). As it was shown in Tarasov (2006a,b, 2011, 2014, 2015) (see also Tarasov, 2013, 2014a,b) the differential equations with fractional derivatives of non-integer orders (Samko et al., 1993; Kilbas et al., 2006; Yang, 2012) can be derived from equation for lattice particles with long-range interactions by continuous limit, where the distance between the lattice particles tends to zero. A direct connection between lattice with long-range interaction and nonlocal continuum has been proved by using the special transform operation (Tarasov, 2006a,b, 2011). The discrete models for fractional nonlocal elasticity and the correspondent continuum equations have been suggested in Tarasov (2013, 2014a,b,c). In this paper, we apply this approach to formulate discrete models for dislocations in fractional nonlocal continua. The proposed models are based on fractional-order differences of Grünwald–Letnikov type. These differences, which are represented by infinite series, allow us to describe long-range interactions in chains and lattices. The suggested discrete models with long-range interaction give fractional differential equations of continuum dislocations in continuous limit.

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2. Fractional Frenkel–Kontorova model of dislocation

Let us consider the equations for displacements u_i in the form

$$M\frac{d^2u_i(t)}{dt^2} = K(\alpha)\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(1+\alpha)}{2\Gamma(m+1)\Gamma(1+\alpha-m)}(u_{i+m}(t)+u_{i-m}(t)) - \frac{U\pi}{b}\sin\left(\frac{2\pi u_i}{b}\right), \quad (1)$$

where b is the Burgers vector, M is the particle mass, U is the energy per unit area of the cut plane, α is the order of lattice nonlocality, $K(\alpha)$ is the constant of long-range interactions that depends on the Bravais vector a, respectively. For a cut at the positive x-axis, the field $u(x) = u_+(x) - u_-(x)$ is the relative displacement (the disregistry) across the cut plane. In Volterra dislocation, $u(x)$ is the step function $b\theta(x)$, equal to b for $x > 0$ and zero otherwise. The term with sine at the right hand side of (1) is the force acting on the atoms as a result of having rigidly displaced the upper half of crystal a distance u over the lower half.

Eq. (1) can be considered as a fractional generalization of the Frenkel–Kontorova model, where the nonlocality is considered by long-range interactions. For $\alpha = 2$, Eq. (1) give the well-known equations of the Frenkel–Kontorova model

$$M\frac{d^2u_i}{dt^2} = K(2)(u_{i+1} - 2u_i + u_{i-1}) - \frac{U\pi}{b}\sin\left(\frac{2\pi u_i}{b}\right). \quad (2)$$

Discrete Eq. (2) have been suggested by Frenkel and Kontorova in 1938 to describe a model of interconnected harmonic springs in a periodic potential, which may be created by a fixed substrate (Frenkel and Kontorova, 1939; Nabarro, 1967; Braun and Kivshar, 2004). Dislocations are described by kink solutions of these equations (Nabarro, 1967), but the distortion $(u_{i+1} - u_i)$ decays exponentially far from the dislocation core, not as $1/i$ as the elastic far field of a true dislocation does. This unrealistic exponential decay remains in some related microscopic models.

Other discrete models of dislocations such as a model of moving screw dislocations in terms of sliding chains (Suzuki, 1967) and the Landau–Kovalev–Kondratiuk model of interacting atomic chains (IAC) for edge dislocations (Landau et al., 1993) change the Frenkel–Kontorova model to get an algebraic decay of the distortion far from dislocation cores. They are all related to the Frenkel–Kontorova model of idealized springs on a periodic substrate and are related to discretization of linear elasticity by finite differences. We suggest new discrete models based on differences of non-integer orders instead of finite differences of integer orders that are usually used. These differences allow us to describe dislocations in the fractional nonlocal continua. As fractional differences we use the Grünwald–Letnikov differences of fractional orders (see Section 20 of Samko et al. (1993)). Continuum analogs of the fractional-order difference operators of the Grünwald–Letnikov type are the fractional derivatives of Grünwald–Letnikov type (Tarasov, 2014).

Fractional-order difference operator, which is used in Eq. (1), is transformed by the continuous limit operation into the fractional derivative of Grünwald–Letnikov type with respect to coordinate. The continuum fractional derivatives of the Grünwald–Letnikov type ${}^{GL}\mathbb{D}^{\alpha,\pm}_{C}$ are defined by

$${}^{GL}\mathbb{D}^{\alpha,\pm}_{C} = \frac{1}{2}\left({}^{GL}D^{\alpha}_{x_j,+} \pm {}^{GL}D^{\alpha}_{x_j,-}\right), \quad (3)$$

which contain the Grünwald–Letnikov fractional derivatives ${}^{GL}D^{\alpha}_{x,\pm}$ with respect to space coordinate x that can be written as

$${}^{GL}D^{\alpha}_{x,\pm}u(x,t) = \lim_{a\to 0+}\frac{1}{|a|^{\alpha}}\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(\alpha+1)}{\Gamma(m+1)\Gamma(\alpha-m+1)}u(x\mp ma,t), \quad (\alpha > 0). \quad (4)$$

In the continuous limit $a \to 0$, equations of motion (1) give the continuum equation for displacement fiels $u(x,t)$ in the form

$$\frac{\partial^2 u(x,t)}{\partial t^2} = A(\alpha){}^{GL}\mathbb{D}^{\alpha,+}_{C}u(x,t) - \frac{U\pi}{b}\sin\left(\frac{2\pi u(x,t)}{b}\right), \quad (5)$$

where $A(\alpha) = K(\alpha)a^{\alpha}/M$. For $\alpha = 2$, we have ${}^{GL}\mathbb{D}^{\alpha,+}_{C} = \partial^2/\partial x^2$.

Note that the Grünwald–Letnikov fractional derivatives (4) coincide with the Marchaud fractional derivatives (see Section 20.3 in Samko et al. (1993)) for the functions from the space $L_r(\mathbb{R})$, where $1 \leqslant r < \infty$ (see Theorem 20.4 in Samko et al. (1993)). Moreover both the Grünwald–Letnikov and Marchaud derivatives have the same domain of definition. The Marchaud fractional derivative is defined by the equation

$${}^{M}D^{\alpha,\pm}_{x}u(x,t) = \frac{1}{a(\alpha,s)}\int_0^{\infty}\frac{\Delta^{s,\pm}_{z}u(x,t)}{z^{\alpha+1}}dz, \quad (0 < \alpha < s), \quad (6)$$

where $\Delta^{s,\pm}_{z}$ are the finite differences of integer order s,

$$\Delta^{s,\pm}_{z}u(x,t) = \sum_{k=0}^{s}\frac{(-1)^k s!}{(s-k)!k!}u(x-kz,t), \quad (7)$$

and $a(\alpha,s)$ is defined by

$$a(\alpha,s) = \frac{s}{\alpha}\int_0^1\frac{(1-\xi)^{s-1}}{(\ln(1/\xi))^{\alpha}}d\xi. \quad (8)$$

3. Fractional long-range interacting atomic chains model of dislocation

The interacting atomic chains (IAC) model of edge dislocations considers displacement vectors with a single non-zero component $(u_{i,j}(t),0,0)$ in two space dimensions (Landau et al., 1993). We can propose a generalization of this model to describe dislocations in materials with power-law nonlocality. The main idea is to consider a model of long-range interacting atomic chains. As a model of long-range interacting atomic chains (LLIAC) we can consider discrete model that is described by equations

$$\frac{d^2u_{i,j}}{dt^2} + \gamma\frac{du_{i,j}}{dt} = K_x(\alpha)\sum_{m=0}^{\infty}\frac{(-1)^m\Gamma(1+\alpha)}{2\Gamma(m+1)\Gamma(1+\alpha-m)} \times (u_{i+m,j}(t) + u_{i-m,j}(t)) + K_y(\beta)\left(\sin\left(\sum_{n=0}^{\infty}\frac{(-1)^n\Gamma(1+\beta)}{\Gamma(n+1)\Gamma(1+\beta-n)}u_{i,j+n}(t)\right) + \sin\left(\sum_{n=0}^{\infty}\frac{(-1)^n\Gamma(1+\beta)}{\Gamma(n+1)\Gamma(1+\beta-n)}u_{i,j-n}(t)\right)\right), \quad (9)$$

where, for simplicity, the atomic masses and the interatomic distances are assumed to be equal to unity. Here γ is the dimensionless friction coefficient, and the dimensionless parameter $K_y(\beta)$ characterizes the amplitude of long-range interaction between atom chains.

For $\alpha = 2$ and $\beta = 1$, using the properties of the Grünwald–Letnikov differences, Eq. (9) give well-known equations of interacting atomic chains (IAC), which are suggested in Landau et al. (1993), in the form

$$\frac{d^2 u_{i,j}}{dt^2} + \gamma \frac{du_{i,j}}{dt} = K_x(2)(u_{i+1} - 2u_i + u_{i-1}) - K_y(1)\big(\sin(u_{i,j} - u_{i,j+1}) + \sin(u_{i,j} - u_{i,j-1})\big). \quad (10)$$

In the continuous limit $a \to 0$, equations of motion (9) give the continuum equation for displacement field $u(x, y, t)$ in the form

$$\frac{\partial^2 u(x,y,t)}{\partial t^2} + \gamma \frac{\partial u(x,y,t)}{\partial t} = A_x(\alpha)\, {}^{GL}\mathbb{D}^{\alpha,+}_{C} u(x,y,t) + A_y(\beta)\, {}^{GL}\mathbb{D}^{\beta,+}_{C} u(x,y,t). \quad (11)$$

where $A_x(\alpha) = K_x(\alpha) a_x^{\alpha}$, and $A_y(\alpha) = 2K_y(\beta) a_y^{\beta}$. It should be noted that ${}^{GL}\mathbb{D}^{\beta,+}_{C}$ is nonlocal operator for $\beta = 1$ that cannot be represented as derivative of integer order (Tarasov, 2014). For $\alpha = \beta = 2$, Eq. (11) gives the equation of continuum model in the from

$$\frac{\partial^2 u}{\partial t^2} + \gamma \frac{\partial u}{\partial t} = A_x(2) \frac{\partial^2 u}{\partial x^2} + A_y(2) \frac{\partial^2 u}{\partial y^2} = A_x(2) \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y_*^2} \right) = A_x(2) \Delta u, \quad (12)$$

where the coordinate y has been rescaled as $y_* = (A_x(2)/A_y(2))^{-1/2} y$. The static continuum case satisfies the harmonic equation $\Delta u = 0$.

Discrete models of dislocations for gradient elasticity theory can be based on the lattice models suggested in Tarasov (2014, 2015).

In paper Ariza and Ortiz (2005) (see also Ramasubramaniam et al., 2007), an approach based on finite elements discretization of elasticity by using algebraic topology is proposed. We assume that a discretization of fractional gradient elasticity also can be realized.

Note that kink-like solutions for equations of chain of coupled oscillators with the long-range power-law interactions have been considered in Korabel et al. (2007).

More complete discrete models can be obtained by taking into account anisotropic linear nonlocal elasticity far from defect cores and dislocation glide. A way to get this can be based on a fractional generalization of models suggested in Carpio and Bonilla (2005) and Bonilla et al. (2007). In this paper the gradient of the displacement vector in the strain tensor is redefined as a nonlinear periodic function of the corresponding finite differences that restores the translation invariance of the crystal and allows sliding of atomic chains as a dislocation moves.

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References

Ariza, M.P., Ortiz, M., 2005. Discrete crystal elasticity and discrete dislocations in crystals. Arch. Ration. Mech. Anal. 178, 149–226 (78 pages).

Bonilla, L.L., Carpio, A., Plans, I., 2007. Dislocations in cubic crystals described by discrete models. Phys. A. 376, 361–377, arxiv:0805.1221.

Braun, O.M., Kivshar, Yu.S., 2004. The Frenkel–Kontorova Model: Concepts, Methods, and Applications. Springer, New York.

Carpio, A., Bonilla, L.L., 2005. Discrete models of dislocations and their motion in cubic crystals. Phys. Rev. B. 71 (13), 134105, arxiv:cond-mat/0503020.

Eringen, A.C., 1972. Nonlocal polar elastic continua. Int. J. Eng. Sci. 10 (1), 1–16.

Eringen, A.C., 2002. Nonlocal Continuum Field Theories. Springer, New York.

Frenkel, J., Kontorova, T., 1939. On the theory of plastic deformation and twinning. J. Phys. Moscow. (Izvestiya Akademii Nauk USSR. Ser. Fizika) 1, 137–149.

Kilbas, A.A., Srivastava, H.M., Trujillo, J.J., 2006. Theory and Applications of Fractional Differential Equations. Elsevier, Amsterdam.

Korabel, N., Zaslavsky, G.M., Tarasov, V.E., 2007. Coupled oscillators with power-law interaction and their fractional dynamics analogues. Commun. Nonlinear Sci. Numer. Simulat. 12 (8), 14051417, arxiv:math-ph/0603074.

Landau, A.I., Kovalev, A.S., Kondratyuk, A.D., 1993. Model of interacting atomic chains and its application to the description of the crowdion in an anisotropic crystal. Phys. Status Solidi B. 179 (2), 373–381.

Nabarro, F.R.N., 1967. Theory of Crystal Dislocations. Oxford University Press, Oxford.

Ramasubramaniam, A., Ariza, M.P., Ortiz, M., 2007. A discrete mechanics approach to dislocation dynamics in BCC crystals. J. Mech. Phys. Solids 55 (3), 615–647.

Rogula, D., 1983. Nonlocal Theory of Material Media. Springer-Verlag, New York.

Samko, S.G., Kilbas, A.A., Marichev, O.I., 1993. Integrals and Derivatives of Fractional Order and Applications (Nauka i Tehnika, Minsk, 1987); and Fractional Integrals and Derivatives Theory and Applications. Gordon and Breach, New York.

Suzuki, H., 1967. Motion of dislocations in body-centered cubic crystals. In: Rosenfield, A.R., Hahn, G.T., Bement, A.L., Jaffee, R.I. (Eds.), Dislocation Dynamics. MacGraw Hill, New York, pp. 679–700.

Tarasov, V.E., 2006a. Map of discrete system into continuous. J. Math. Phys. 47 (9), 092901, arxiv:0711.2612.

Tarasov, V.E., 2006b. Continuous limit of discrete systems with long-range interaction. J. Phys. A. 39 (48), 14895–14910, arxiv:0711.0826.

Tarasov, V.E., 2011. Fractional Dynamics: Applications of Fractional Calculus to Dynamics of Particles, Fields and Media. Springer, New York.

Tarasov, V.E., 2013. Lattice model with power-law spatial dispersion for fractional elasticity. Central Eur. J. Phys. 11 (11), 1580–1588, arxiv:1501.01201.

Tarasov, V.E., 2014. General lattice model of gradient elasticity. Mod. Phys. Lett. B. 28 (7), 1450054 (17 pages) arxiv:1501.01435.

Tarasov, V.E., 2014. Toward lattice fractional vector calculus. J. Phys. A. 47 (35), 355204 (51 pages).

Tarasov, V.E., 2014a. Lattice model of fractional gradient and integral elasticity: Long-range interaction of Grünwald–Letnikov–Riesz type. Mech. Mater. 70 (1), 106–114, arxiv:1502.06268.

Tarasov, V.E., 2014b. Fractional gradient elasticity from spatial dispersion law. ISRN Condens. Matter Phys. 2014, 794097, arxiv:1306.2572.

Tarasov, V.E., 2014c. Lattice with long-range interaction of power-law type for fractional non-local elasticity. Int. J. Solids Struct. 51 (15-16), 2900–2907, arxiv:1502.05492.

Tarasov, V.E., 2015. Lattice model with nearest-neighbor and next-nearest-neighbor interactions for gradient elasticity. Discont. Nonlinear. Complex. 4 (1), 11–23, arxiv:1503.03633.

Tarasov, V.E., 2015. Lattice fractional calculus. Appl. Math. Comput. 257, 12–33.

Yang, X.-J., 2012. Advanced Local Fractional Calculus and its Applications. World Science, New York.