

A Review on Accommodation Processes in Non-Equilibrium Grain Boundaries

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Abstract. The grain boundaries in ultrafine-grained materials, including nanostructured ones, are in a specific non-equilibrium state, which is associated with extrinsic grain boundary dislocations trapped during plastic deformation. This grain boundary state plays a significant role in the stability and evolution of many mechanical and physical properties of nanocrystalline materials. In the present review, accommodation of different components of non-equilibrium grain boundary structure resulting in a formation of a more equilibrium structure and associated with a decrease in the internal stresses is analyzed. These are spreading of lattice dislocations trapped by grain boundaries, relaxation of disordered dislocation walls, relaxation of ensembles of sessile and glissile extrinsic grain boundary dislocations. The main advantages and limitations of the models describing accommodation processes are overviewed. Application of the obtained results to nanomaterials is discussed.

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REFERENCES

[1] R.P. Feynman, *There's plenty of room at the bottom: an invitation to enter a new field of physics*, In: *Handbook of nanoscience, engineering and technology*, (Boca Raton: CRC Press, 2002), pp. 1-9

- [2] H. Gleiter, *Nanocrystalline Materials*, Prog Mater Sci, 1989, vol. 33, no. 4, pp. 223-315. [https://doi.org/10.1016/0079-6425\(89\)90001-7](https://doi.org/10.1016/0079-6425(89)90001-7).
- [3] [H. Gleiter, *Nanostructured materials: Basic concepts and microstructure*, Acta Mater 48\(1\) \(2000\) 1-29.](#)
- [4] A.A. Nazarov and R.R. Mulyukov, In: *Handbook of Nanoscience, Engineering, and Technology* (Boca Raton, CRC Press, 2003).
- [5] R.Z. Valiev and I.V. Aleksandrov, *Bulk Nanostructural SPD Materials with Advanced Properties, Nanostructures: Synthesis, Functional Properties and Applications* (Moscow, Akademkniga, 2007).
- [6] T. Daniel Thangadurai, N. Manjubaashini, Sabu Thomas and H.J. Maria, *Nanostructured Materials* (Springer, 2020).
- [7] [R.Z. Valiev, R.K. Islamgaliev and I.V. Alexandrov, *Bulk nanostructured materials from severe plastic deformation*, Prog Mater Sci, 2000, vol. 45, no. 2, pp. 103-189.](#)
- [8] [A.A. Nazarov, A.E. Romanov and R.Z. Valiev, *On the structure, stress-fields and energy of nonequilibrium grain-boundaries*, Acta Metall et Mater, 1993, vol. 41, no. 4, pp. 1033-1040.](#)
- [9] [S. Van Petegem, F. Dalla Torre, D. Segers and H. Van Swygenhoven, *Free volume in nanostructured Ni*, Scripta Mater, 2003, vol. 48, no. 1, pp. 17-22.](#)
- [10] [S.R. Agnew, B.R. Elliott, C.J. Youngdahl, K.J. Hemker and J.R. Weertman, *Microstructure and mechanical behavior of nanocrystalline metals*, Mat Sci Eng a-Struct, 2000, vol. 285, no. 1-2, pp. 391-396.](#)
- [11] [P.G. Sanders, J.A. Eastman and J.R. Weertman, *Elastic and tensile behavior of nanocrystalline copper and palladium*, Acta Mater, 1997, vol. 45, no. 10, pp. 4019-4025.](#)
- [12] [Y. Zhou, S. Van Petegem, D. Segers, U. Erb, K.T. Aust and G. Palumbo, *On Young's modulus and the interfacial free volume in nanostructured Ni-P*, Mat Sci Eng a-Struct, 2009, vol. 512, no. 1-2, pp. 39-44.](#)
- [13] [A.P. Sutton, *Grain-boundary structure*, Int metals reviews, 1984, vol. 29, no. 5, pp. 377-404.](#)
- [14] D.V. Bachurin and A.A. Nazarov, *Effect of a relative shift induced by an applied stress on the structure and energy of the Sigma 5 (210)[001] tilt boundary in nickel*, Phys Met Metallogr, 2004, vol. 98, no. 1, pp. 9-15.
- [15] [G.H. Campbell, J. Belak and J.A. Moriarty, *Atomic structure of the Sigma 5 \(310\)\[001\] symmetric tilt grain boundary in molybdenum*, Acta Mater, 1999, vol. 47, no. 15-16, pp. 3977-3985.](#)
- [16] [C.T. Forwood and L.M. Clarebrough, *Rigid body displacements at a faceted epsilon-3 boundary in alpha-iron*, Phys Status Solidi A, 1988, vol. 195, no. 2, pp. 365-375.](#)
- [17] [D.A. Smith, V. Vitek and R.C. Pond, *Computer-simulation of symmetrical high angle boundaries in aluminum*, Acta Metall Mater, 1977, vol. 25, no. 5, pp. 475-483.](#)
- [18] [V.V. Rybin, A.A. Zisman and N.Y. Zolotarevsky, *Junction disclinations in plastically deformed crystals*, Acta Metall et Mater, 1993, vol. 41, no. 7, pp. 2211-2217.](#)
- [19] V.V. Rybin, N.Y. Zolotarevsky and I.M. Zhukowskij, *Structure evolution and internal stresses on stage of developed plastic deformation of crystalline solids*, Phys Met Metallogr, 1990, vol. 69, no. 1, pp. 5-26.
- [20] V.V. Rybin, A.A. Zisman and N.Y. Zolotarevsky, *Junction disclinations in plastically deformed crystals*, Phys Solid State, 1985, vol. 27, no. 1, pp. 181-186.
- [21] A.E. Romanov and V.I. Vladimirov, *Disclinations in crystalline solids*, In: *Dislocations in Crystals*, ed. by F. R. N. Nabarro (Amsterdam: North Holland, 1992), pp. 191-402.
- [22] [A.E. Romanov, *Screened disclinations in solids*, Mat Sci Eng a-Struct, 1993, vol. 164, no. 1-2, pp. 58-68.](#)
- [23] [A.E. Romanov, *Mechanics and physics of disclinations in solids*, Eur J Mech a-Solid, 2003, vol. 22, no. 5, pp. 727-741.](#)
- [24] [A. Torrents, H. Yang and F.A. Mohamed, *Effect of annealing on hardness and the modulus of elasticity in bulk nanocrystalline nickel*, Metall Mater Trans A, 2010, vol. 41a, no. 3, pp. 621-630.](#)
- [25] [R.Z. Valiev, A.V. Sergueeva and A.K. Mukherjee, *The effect of annealing on tensile deformation behavior of nanostructured SPD titanium*, Scripta Mater, 2003, vol. 449, no. 7, pp. 669-674.](#)
- [26] [G.J. Tucker and D.L. McDowell, *Non-equilibrium grain boundary structure and inelastic deformation using atomistic simulations*, Int J Plasticity, 2011, vol. 27, no. 6, pp. 841-857.](#)

- [27] [A. Hasnaoui, H. Van Swygenhoven and P.M. Derlet, *On non-equilibrium grain boundaries and their effect on thermal and mechanical behaviour: a molecular dynamics computer simulation*, Acta Mater, 2002, vol. 50, no. 15, pp. 3927-3939.](#)
- [28] [T.S. Orlova, A.M. Mavlyutov, A.S. Bondarenko, I.A. Kasatkin, M.Y. Murashkin and R.Z. Valiev, *Influence of grain boundary state on electrical resistivity of ultrafine grained aluminium*, Philos Mag, 2016, vol. 996, no. 3, pp. 2429-2444.](#)
- [29] [A.A. Nazarov and R.T. Murzaev, *Nonequilibrium grain boundaries and their relaxation under oscillating stresses in columnar nickel nanocrystals studied by molecular dynamics*, Comp Mater Sci, 2018, vol. 141, pp. 204-213.](#)
- [30] [A.A. Nazarov and R.T. Murzaev, *Molecular dynamics study of nonequilibrium \[112\] tilt grain boundaries in ni and their relaxation under cyclic deformation*, Journal of Metastable and Nanocrystalline Materials, 2018, vol. 30, pp. 1-10.](#)
- [31] J.P. Hirth and J. Lothe, *Theory of dislocations* (New York, Wiley, 1982).
- [32] Y. Ishida, T. Hasegawa and F. Nagata, *Dislocation images on grain boundary and their behavior at elevated temperatures*, T Jpn I Met , 1968, vol. 9, pp. 504-508.
- [33] [R.A. Varin, J.W. Wyrzykowski, W. Lojkowski and M.W. Grabski, *Spreading of extrinsic grain-boundary dislocations in plastically deformed aluminum*, Phys Status Solidi A, 1978, vol. 45, no. 2, pp. 565-569.](#)
- [34] [R.Z. Valiev, V.Y. Gerchman and O.A. Kaibyshev, *On the nature of grain-boundary structure recovery*, Phys Status Solidi A, 1980, vol. 61, no. 2, pp. K95-K99.](#)
- [35] [P.H. Pumphrey and H. Gleiter, *Annealing of dislocations in high-angle grain-boundaries*, Philos Mag, 1974, vol. 30, no. 3, pp. 593-602.](#)
- [36] [W. Lojkowski and M.W. Grabski, *Material purity influence on the spreading temperature of grain-boundary dislocations*, Scripta Metall Mater, 1979, vol. 13, no. 6, pp. 511-514.](#)
- [37] [S. Lartigue and L. Priester, *Stability of extrinsic grain-boundary dislocations in relation with intergranular segregation and precipitation*, Acta Metall Mater, 1983, vol. 31, no. 11, pp. 1809-1819.](#)
- [38] [P.H. Pumphrey and H. Gleiter, *Structure of nonequilibrium high-angle grain-boundaries*, Philos Mag, 1975, vol. 32, no. 4, pp. 881-885.](#)
- [39] [R.A. Varin, *Spreading of extrinsic grain-boundary dislocations in austenitic steel*, Phys Status Solidi A, 1979, vol. 52, no. 1, pp. 347-356.](#)
- [40] [P.R. Howell, A.R. Jones, A. Horsewell and B. Ralph, *Creation and accommodation of extrinsic dislocations at grain-boundaries*, Philos Mag, 1976, vol. 33, no. 1, pp. 21-31.](#)
- [41] [R.C. Pond and D.A. Smith, *Absorption of dislocations by grain-boundaries*, Philos Mag, 1977, vol. 36, no. 2, pp. 353-366.](#)
- [42] [T.P. Darby, R. Schindler and R.W. Balluffi, *Interaction of lattice dislocations with grain-boundaries*, Philos Mag A, 1978, vol. 37, no. 2, pp. 245-256.](#)
- [43] [C.A.P. Horton, J.M. Silcock and G.R. Kegg, *Visibility of extrinsic grain-boundary dislocations in symmetrical \[011\] tilt boundaries in aluminum*, Phys Status Solidi A, 1974, vol. 26, no. 1, pp. 215-224.](#)
- [44] M.W. Grabski, R.Z. Valiev, J.W. Wyrzykowski and W. Lojkowski, *Yield stress dependence on the spreading of the extrinsic grain boundary dislocations and the non-equilibrium of grain boundaries*, Res. Mechanica Lett, 1981, vol. 1, no. 11, pp. 489-496.
- [45] [R.A. Varin and K. Tangri, *The effect of extrinsic grain-boundary dislocations with unrelaxed and relaxed cores on the state of random boundaries in an austenitic steel*, Metall Trans A, 1981, vol. 12, no. 11, pp. 1859-1866.](#)
- [46] [R.Z. Valiev, V.Y. Gertsman and O.A. Kaibyshev, *The migration of grain boundaries having a nonequilibrium structure*, Phys Solid State, 1980, vol. 22, no. 7, pp. 2213-2216.](#)
- [47] [R.Z. Valiev, V.Y. Gertsman and O.A. Kaibyshev, *Study on changes in grain boundary structure during magnesium alloy recrystallization after small deformation*, Phys Met Metallogr, 1984, vol. 55, no. 3, pp. 554-558.](#)
- [48] [R.Z. Valiev, V.Y. Gertsman and O.A. Kaibyshev, *Grain-boundary structure and properties under external influences*, Phys Status Solidi A, 1986, vol. 97, no. 1, pp. 11-56.](#)
- [49] [O.A. Kaibyshev, V.V. Astanin, R.Z. Valiev and V.G. Khairullin, *Grain-boundary slip in zinc bicrystals with a symmetrical inclination boundary*, Phys Met Metallogr, 1981, vol. 51, no. 1, pp. 193-200.](#)

- [50] O.A. Kaibyshev and R.Z. Valiev, *Grain boundaries and properties of metals* (Metallurgiya, Moscow, 1987).
- [51] W. Lojkowski and M.W. Grabski, In: *Deformation of Polycrystals: Mechanisms and Microstructures*, Proceedings of the 2-nd Riso International Symposium on Metallurgy and Materials Science, ed. N. Hansen, A. Horswell, T. Leffers and H. Lilholt, pp. 329-333
- [52] T. Johannesson and A. Thölen, *The role of grain boundaries in creep deformation*, Metal Science Journal, 1972, vol. 6, no. 1, pp. 189-194.
- [53] [R.Z. Valiev, V.Y. Gertsman and O.A. Kaibyshev, *Non-equilibrium state and recovery of grain-boundary structure. 2. Energetic analysis*, Phys Status Solidi A, 1983, vol. 78, no. 1, pp. 177-186.](#)
- [54] A.A. Nazarov, *On the mechanism and kinetics of the spreading of extrinsic grain-boundary dislocations*, Phys Met Metallogr, 2000, vol. 89, no. 5, pp. 439-444.
- [55] [A.A. Nazarov, *A revision of the models for the accommodation of extrinsic grain boundary dislocations*, Interface Sci, 2000, vol. 8, no. 1, pp. 71-76.](#)
- [56] [A.A. Nazarov, A.E. Romanov and R.Z. Valiev, *Incorporation model for the spreading of extrinsic grain-boundary dislocations*, Scripta Metal et Mater, 1990, vol. 24, no. 10, pp. 1929-1934.](#)
- [57] K.J. Kurzydowski, J.W. Wyrzykowski and G. Garbach, *Analysis of delocalization models for extrinsic grain boundary dislocations*, Phys Met Metallogr, 1988, vol. 65, pp. 385-392.
- [58] [R.A. Varin and E. Romanowska-Haftek, *On the kinetics of the spreading of extrinsic grain-boundary dislocations*, Metall Trans A, 1986, vol. 17, no. 11, pp. 1967-1975.](#)
- [59] W.A.T. Clark and D.A. Smith, *Interaction of lattice dislocations with periodic grain-boundary structures*, J Mater Sci, 1979, vol. 14, no. 4, pp. 776-788.
- [60] [S. Poulat, B. Decamps and L. Priester, *In-situ transmission electron microscopy study of the dislocation accommodation in \[101\] tilt grain boundaries in nickel bicrystals*, Philos Mag A, 1999, vol. 79, no. 11, pp. 2655-2680.](#)
- [61] A.A. Nazarov, *Kinetics of relaxation of disordered grain boundary dislocation arrays in ultrafine grained materials*, Ann Chim-Sci Mat, 1996, vol. 21, no. 6-7, pp. 461-469.
- [62] [A.A. Nazarov, *Kinetics of grain boundary recovery in deformed polycrystals*, Interface Sci, 2000, vol. 8, no. 4, pp. 315-322.](#)
- [63] A.A. Nazarov and D.V. Bachurin, *On the relaxation of quadrupoles of junction disclinations in deformed polycrystals*, Phys Met Metallogr, 2003, vol. 96, no. 5, pp. 446-451.
- [64] [D.V. Bachurin and A.A. Nazarov, *On the annealing of junction disclinations in deformed polycrystals*, Philos Mag, 2003, vol. 83, no. 23, pp. 2653-2667.](#)
- [65] V.N. Perevezentsev, *Modern concepts of the nature of structural superplasticity*, In: *Problems of the theory of defects in crystals*, (Leningrad: Nauka, 1987), pp. 85-100.
- [66] [J.R. Spingarn and W.D. Nix, *Model for creep based on the climb of dislocations at grain-boundaries*, Acta Metall Mater, 1979, vol. 27, no. 2, pp. 171-177.](#)
- [67] [D.V. Bachurin, R.T. Murzaev and A.A. Nazarov, *Discrete dislocation simulation of the ultrasonic relaxation of non-equilibrium grain boundaries in a deformed polycrystal*, Ultrasonics, 2021, vol. 117, art. 106555.](#)
- [68] [D.V. Bachurin, R.T. Murzaev and A.A. Nazarov, *Ultrasonic influence on evolution of disordered dislocation structures*, Model Simul Mater Sc, 2017, vol. 25, art. 085010.](#)
- [69] [R.T. Murzaev, D.V. Bachurin and A.A. Nazarov, *Relaxation of the residual defect structure in deformed polycrystals under ultrasonic action*, Phys Met Metallogr, 2017, vol. 118, no. 7, pp. 621-629.](#)
- [70] [R.T. Murzaev, D.V. Bachurin and A.A. Nazarov, *Simulation of the effect of ultrasound on the dislocation structure of deformed polycrystals*, Phys Met Metallogr, 2018, vol. 119, no. 10, pp. 993-1003.](#)
- [71] [D.V. Bachurin, R.T. Murzaev and A.A. Nazarov, *Relaxation of dislocation structures under ultrasonic influence*, Int J Solids Struct, 2019, vol. 156, pp. 1-13.](#)
- [72] [R.Z. Valiev, A.V. Korznikov and R.R. Mulyukov, *Structure and properties of ultrafine-grained materials produced by severe plastic-deformation*, Mat Sci Eng a-Struct, 1993, vol. 168, no. 2, pp. 141-148.](#)
- [73] I. Kaur, W. Gust and L. Kozma, *Handbook of grain and interface boundary diffusion data* (Stuttgart, Ziegler Press, 1989).

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