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A stochastic solver based on the residence time algorithm for crystal plasticity models.

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Summary: The deformation of crystalline materials by dislocation motion takes place in discrete amounts determined by the Burgers vector. Dislocations may move individually or in bundles, potentially giving rise to intermittent slip. This confers plastic deformation with a certain degree of variability that can be interpreted as being caused by stochastic fluctuations in dislocation behavior. However, crystal plasticity (CP) models are almost always formulated in a continuum sense, assuming that fluctuations average out over large material volumes and/or cancel out due to multi-slip contributions. Nevertheless, plastic fluctuations are known to be important in confined volumes at or below the micron scale, at high temperatures, and under low strain rate/stress deformation conditions. Here, we develop a stochastic solver for CP models based on the residence-time algorithm that naturally captures plastic fluctuations by sampling among the set of active slip systems in the crystal. The method solves the evolution equations of explicit CP formulations, which are recast as stochastic ordinary differential equations and integrated discretely in time. The stochastic CP model is numerically stable by design and naturally breaks the symmetry of plastic slip by sampling among the active plastic shear rates with the correct probability. This can lead to phenomena such as intermittent slip or plastic localization without adding external symmetry-breaking operations to the model. The method is applied to body-centered cubic tungsten single crystals under a variety of temperatures, loading orientations, and imposed strain rates.

MSC:

74S60 Stochastic and other probabilistic methods applied to problems in solid mechanics

74C20 Large-strain, rate-dependent theories of plasticity

74E15 Crystalline structure

Keywords:

stochastic crystal plasticity; residence time algorithm; rate-dependent plasticity; kinetic Monte Carlo method; body-centered cubic crystal; plastic burst

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References:

- [1] Asaro, RJ, Crystal Plasticity, *J Appl Mech*, 50, 4, 921 (1983) · [Zbl 0557.73033](#) · [doi:10.1115/1.3167205](#)
- [2] Dawson, PR, Computational crystal plasticity, *Int J Solids Struct*, 37, 1-2, 115 (2000) · [Zbl 1075.74021](#) · [doi:10.1016/S0020-7683\(99\)00083-9](#)
- [3] Gurtin, ME; Anand, L.; Lele, SP, Gradient single-crystal plasticity with free energy dependent on dislocation densities, *J Mech Phys Solids*, 55, 9, 1853 (2007) · [Zbl 1170.74013](#) · [doi:10.1016/j.jmps.2007.02.006](#)
- [4] Schmidt-Baldassari, M., Numerical concepts for rate-independent single crystal plasticity, *Comput Methods Appl Mech Eng*, 192, 11-12, 1261 (2003) · [Zbl 1031.74019](#) · [doi:10.1016/S0045-7825\(02\)00563-7](#)
- [5] Gurtin, ME, A finite-deformation, gradient theory of single-crystal plasticity with free energy dependent on densities of geometrically necessary dislocations, *Int J Plast*, 24, 4, 702 (2008) · [Zbl 1131.74006](#) · [doi:10.1016/j.ijplas.2007.07.014](#)
- [6] Aravas, N.; Aifantis, E., On the geometry of slip and spin in finite plastic deformation, *Int J Plast*, 7, 3, 141 (1991) · [Zbl 0735.73034](#) · [doi:10.1016/0749-6419\(91\)90028-W](#)
- [7] Anand, L.; Kothari, M., A computational procedure for rate-independent crystal plasticity, *J Mech Phys Solids*, 44, 4, 525 (1996) · [Zbl 1054.74549](#) · [doi:10.1016/0022-5096\(96\)00001-4](#)
- [8] Harewood, F.; McHugh, P., Comparison of the implicit and explicit finite element methods using crystal plasticity, *Comput Mater Sci*, 39, 2, 481 (2007) · [doi:10.1016/j.commatsci.2006.08.002](#)
- [9] Zhang, K.; Hopperstad, O.; Holmedal, B.; Dumoulin, S., A robust and efficient substepping scheme for the explicit numerical integration of a rate-dependent crystal plasticity model, *Int J Numer Meth Eng*, 99, 4, 239 (2014) · [Zbl 1352.74062](#) · [doi:10.1002/nme.4671](#)
- [10] Zhang M, Nguyen K, Segurado J, Montáns FJ (2021) A multiplicative finite strain crystal plasticity formulation based on

additive elastic corrector rates: theory and numerical implementation. *Int J Plastic* 137:102899

- [11] Arsenlis, A.; Parks, DM, Modeling the evolution of crystallographic dislocation density in crystal plasticity, *J Mech Phys Solids*, 50, 9, 1979 (2002) · [Zbl 1023.74011](#) · [doi:10.1016/S0022-5096\(01\)00134-X](#)
- [12] Forest, S., Modeling slip, kink and shear banding in classical and generalized single crystal plasticity, *Acta Mater*, 46, 9, 3265 (1998) · [doi:10.1016/S1359-6454\(98\)00012-3](#)
- [13] Arsenlis, A.; Parks, D., Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density, *Acta Mater*, 47, 5, 1597 (1999) · [doi:10.1016/S1359-6454\(99\)00020-8](#)
- [14] Kocks, U., Independent slip systems in crystals, *Phil Mag*, 10, 104, 187 (1964) · [doi:10.1080/14786436408225657](#)
- [15] Cuitino, AM; Ortiz, M., Computational modelling of single crystals, *Modell Simul Mater Sci Eng*, 1, 3, 225 (1993) · [doi:10.1088/0965-0393/1/3/001](#)
- [16] Fohrmeister, V.; Díaz, G.; Mosler, J., Classic crystal plasticity theory vs crystal plasticity theory based on strong discontinuities-theoretical and algorithmic aspects, *Int J Numer Meth Eng*, 117, 13, 1283 (2019)
- [17] Barton, NR; Arsenlis, A.; Marian, J., A polycrystal plasticity model of strain localization in irradiated iron, *J Mech Phys Solids*, 61, 2, 341 (2013) · [doi:10.1016/j.jmps.2012.10.009](#)
- [18] Zhang, J.; Jiang, Y., A Study of Inhomogeneous Plastic Deformation of 1045 Steel, *J Eng Mater Technol*, 126, 2, 164 (2004) · [doi:10.1115/1.1647125](#)
- [19] Kang, J.; Wilkinson, D.; Jain, M.; Embury, J.; Beaudoin, A.; Kim, S.; Mishra, R.; Sachdev, A., On the sequence of inhomogeneous deformation processes occurring during tensile deformation of strip cast AA5754, *Acta Mater*, 54, 1, 209 (2006) · [doi:10.1016/j.actamat.2005.08.045](#)
- [20] McDonald RJ, Efstathiou C, Kurath P (2009) The wavelike plastic deformation of single crystal copper. *J Eng Mater Technol* 131(3)
- [21] Feltham, P., A stochastic model of crystal plasticity, *J Phys D Appl Phys*, 6, 17, 2048 (1973) · [doi:10.1088/0022-3727/6/17/311](#)
- [22] Zhang, L.; Dingreville, R.; Bartel, T.; Lusk, MT, A stochastic approach to capture crystal plasticity, *Int J Plast*, 27, 9, 1432 (2011) · [Zbl 1284.74149](#) · [doi:10.1016/j.ijplas.2011.04.002](#)
- [23] Weiss, J.; Rhouma, WB; Richeton, T.; Dechanel, S.; Louchet, F.; Truskinovsky, L., From mild to wild fluctuations in crystal plasticity, *Phys Rev Lett*, 114, 10, 105504 (2015) · [doi:10.1103/PhysRevLett.114.105504](#)
- [24] Askari, H.; Maughan, MR; Abdolrahim, N.; Sagapuram, D.; Bahr, DF; Zbib, HM, A stochastic crystal plasticity framework for deformation of micro-scale polycrystalline materials, *Int J Plast*, 68, 21 (2015) · [doi:10.1016/j.ijplas.2014.11.001](#)
- [25] Zaiser, M.; Moretti, P.; Chu, H., Stochastic crystal plasticity models with internal variables: application to slip channel formation in irradiated metals, *Adv Eng Mater*, 22, 9, 1901208 (2020) · [doi:10.1002/adem.201901208](#)
- [26] Gillespie, DT, A general method for numerically simulating the stochastic time evolution of coupled chemical reactions, *J Comput Phys*, 22, 4, 403 (1976) · [doi:10.1016/0021-9991\(76\)90041-3](#)
- [27] Gardiner, C., *Stochastic methods* (2009), Berlin: Springer, Berlin · [Zbl 1181.60001](#)
- [28] Martínez, E.; Marian, J.; Kalos, MH; Perlado, JM, Synchronous parallel kinetic Monte Carlo for continuum diffusion-reaction systems, *J Comput Phys*, 227, 8, 3804 (2008) · [Zbl 1139.65003](#) · [doi:10.1016/j.jcp.2007.11.045](#)
- [29] Marian, J.; Bulatov, VV, Stochastic cluster dynamics method for simulations of multispecies irradiation damage accumulation, *J Nucl Mater*, 415, 1, 84 (2011) · [doi:10.1016/j.jnucmat.2011.05.045](#)
- [30] Bortz, AB; Kalos, MH; Lebowitz, JL, A new algorithm for Monte Carlo simulation of Ising spin systems, *J Comput Phys*, 17, 1, 10 (1975) · [doi:10.1016/0021-9991\(75\)90060-1](#)
- [31] Kalos, MH; Whitlock, PA, *Monte carlo methods* (2009), New York: Wiley, New York · [Zbl 1170.65302](#)
- [32] Gardiner CW et al (1985) *Handbook of stochastic methods*, vol 3. springer Berlin
- [33] Serebrinsky, SA, Physical time scale in kinetic Monte Carlo simulations of continuous-time Markov chains, *Phys Rev E*, 83, 3, 037701 (2011) · [doi:10.1103/PhysRevE.83.037701](#)
- [34] Martínez E, Caturla M.J, Marian J (2020) DFT-parameterized object kinetic Monte Carlo simulations of radiation damage. *Handbook of materials modeling: applications: current and emerging materials* pp 2457-2488
- [35] Van Siclen C.D (2007) Derivation of the residence time for kinetic Monte Carlo simulations. arXiv preprint arXiv:0712.2464
- [36] Dai H (2019) Bayesian inference on complicated data IntechOpen
- [37] Lee, E.; Liu, D., Finite-strain elastic-plastic theory with application to plane-wave analysis, *J Appl Phys*, 38, 1, 19 (1967) · [doi:10.1063/1.1708953](#)
- [38] Roters, F.; Eisenlohr, P.; Hantcherli, L.; Tjahjanto, DD; Bieler, TR; Raabe, D., Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications, *Acta Mater*, 58, 4, 1152 (2010) · [doi:10.1016/j.actamat.2009.10.058](#)
- [39] Cereceda, D.; Diehl, M.; Roters, F.; Raabe, D.; Perlado, JM; Marian, J., Unraveling the temperature dependence of the yield strength in single-crystal tungsten using atomistically-informed crystal plasticity calculations, *Int J Plast*, 78, 242 (2016) · [doi:10.1016/j.ijplas.2015.09.002](#)
- [40] Stukowski, A.; Cereceda, D.; Swinburne, TD; Marian, J., Thermally-activated non-Schmid glide of screw dislocations in W using atomistically-informed kinetic Monte Carlo simulations, *Int J Plast*, 65, 108 (2015) · [doi:10.1016/j.ijplas.2014.08.015](#)
- [41] Hull, D.; Byron, JF; Noble, FW, Orientation dependence of yield in body-centered cubic metals, *Can J Phys*, 45, 2, 1091 (1967) · [doi:10.1139/p67-080](#)

- [42] Kocks, U.; Mecking, H., Physics and phenomenology of strain hardening: the FCC case, *Prog Mater Sci*, 48, 3, 171 (2003) · doi:10.1016/S0079-6425(02)00003-8
- [43] Roters, F.; Eisenlohr, P.; Hantcherli, L.; Tjahjanto, D.; Bieler, T.; Raabe, D., Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications, *Acta Mater*, 58, 4, 1152 (2010) · doi:10.1016/j.actamat.2009.10.058
- [44] Franciosi, P., The concepts of latent hardening and strain hardening in metallic single crystals, *Acta Metall*, 33, 9, 1601 (1985) · doi:10.1016/0001-6160(85)90154-3
- [45] Franciosi, P.; Le, L.; Monnet, G.; Kahloun, C.; Chavanne, MH, Investigation of slip system activity in iron at room temperature by SEM and AFM in-situ tensile and compression tests of iron single crystals, *Int J Plast*, 65, 226 (2015) · doi:10.1016/j.ijplas.2014.09.008
- [46] Kuchnicki S, Cuitino A (1988) Radovitzky R (2006) Efficient and robust constitutive integrators for single-crystal plasticity modeling. *Int J Plastic* 22(10) · Zbl 1136.74310
- [47] Dumoulin, S.; Hopperstad, O.; Berstad, T., Investigation of integration algorithms for rate-dependent crystal plasticity using explicit finite element codes, *Comput Mater Sci*, 46, 4, 785 (2009) · doi:10.1016/j.commatsci.2009.04.015
- [48] Zhang, K.; Holmedal, B.; Dumoulin, S.; Hopperstad, OS, An explicit integration scheme for hypo-elastic viscoplastic crystal plasticity, *Trans Nonferrous Metals Soc China*, 24, 7, 2401 (2014) · Zbl 1352.74062 · doi:10.1016/S1003-6326(14)63363-X
- [49] van der Giessen, E.; Neale, KW, Analysis of the inverse Swift effect using a rate-sensitive polycrystal model, *Comput Methods Appl Mech Eng*, 103, 1-2, 291 (1993) · doi:10.1016/0045-7825(93)90050-8
- [50] Jennings, AT; Greer, JR, Tensile deformation of electroplated copper nanopillars, *Phil Mag*, 91, 7-9, 1108 (2011) · doi:10.1080/14786435.2010.505180
- [51] Huang, P.; Yu, Q., Dislocation Multiplications in Extremely Small Hexagonal-structured Titanium Nanopillars Without Dislocation Starvation, *Sci Rep*, 7, 1, 15890 (2017) · doi:10.1038/s41598-017-16195-7
- [52] Zaiser, M.; Schwerdtfeger, J.; Schneider, A.; Frick, C.; Clark, B.; Gruber, P.; Arzt, E., Strain bursts in plastically deforming molybdenum micro- and nanopillars, *Phil Mag*, 88, 30-32, 3861 (2008) · doi:10.1080/14786430802132522
- [53] Dutta, A., Compressive deformation of Fe nanopillar at high strain rate: modalities of dislocation dynamics, *Acta Mater*, 125, 219 (2017) · doi:10.1016/j.actamat.2016.11.062
- [54] Martínez, E.; Monasterio, PR; Marian, J., Billion-atom synchronous parallel kinetic Monte Carlo simulations of critical 3D Ising systems, *J Comput Phys*, 230, 4, 1359 (2011) · Zbl 1210.82016 · doi:10.1016/j.jcp.2010.11.006
- [55] Forest, S.; Rubin, M., A rate-independent crystal plasticity model with a smooth elastic-plastic transition and no slip indeterminacy, *Eur J Mech A/Solids*, 55, 278 (2016) · Zbl 1406.74114 · doi:10.1016/j.euromechsol.2015.08.012
- [56] Nguyen, K.; Zhang, M.; Amores, VJ; Sanz, MA; Montáns, FJ, Computational modeling of dislocation slip mechanisms in crystal plasticity: a short review, *Curr Comput-Aided Drug Des*, 11, 1, 42 (2021)
- [57] Valdenaire, PL; Le Bouar, Y.; Appolaire, B.; Finel, A., Density-based crystal plasticity: From the discrete to the continuum, *Phys Rev B*, 93, 21, 214111 (2016) · doi:10.1103/PhysRevB.93.214111
- [58] Forest, S., Strain localization phenomena in generalized single crystal plasticity, *J Mech Behav Mater*, 11, 1-3, 45 (2000) · doi:10.1515/JMBM.2000.11.1-3.45
- [59] Eidel, B., Crystal plasticity finite-element analysis versus experimental results of pyramidal indentation into (0 0 1) fcc single crystal, *Acta Mater*, 59, 4, 1761 (2011) · doi:10.1016/j.actamat.2010.11.042
- [60] Berdichevsky, V., Entropy and temperature of microstructure in crystal plasticity, *Int J Eng Sci*, 128, 24 (2018) · Zbl 1423.74711 · doi:10.1016/j.ijengsci.2018.03.001
- [61] Zhang MH, Shen XH, He L, Zhang KS (2018) Application of differential entropy in characterizing the deformation inhomogeneity and life prediction of low-cycle fatigue of metals. *Materials* 11(10):1917
- [62] Wang EY (2014) Comparison Between Deterministic and Stochastic Biological Simulation. Uppsala University, Department of Mathematics, Tech. rep
- [63] Liberti L, Kucherenko S (2005) Comparison of deterministic and stochastic approaches to global optimization. *Int Trans Oper Res* 12(3):263 · Zbl 1131.90437
- [64] Stoller R, Golubov S, Domain C, Becquart C (2008) Mean field rate theory and object kinetic monte carlo: a comparison of kinetic models. *J Nuclear Mater* 382(2):77. *Microstructural Processes in Irradiated Materials*
- [65] Nabarro, FRN, Dislocations in a simple cubic lattice, *Proc Phys Soc*, 59, 2, 256 (1947) · doi:10.1088/0959-5309/59/2/309

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