

List of publications

- 2025 I. Maliyov, **P. Grigorev**, and T. D. Swinburne. “Exploring parameter dependence of atomic minima with implicit differentiation”. In: *npj Computational Materials* 11.1 (Jan. 2025), p. 22.
- 2024 **P. Grigorev** et al. “matsciPy: materials science at the atomic scale with Python”. In: *Journal of Open Source Software* 9.93 (2024), p. 5668.
- S. Starikov, **P. Grigorev**, R. Drautz, and S. V. Divinski. “Large-scale atomistic simulation of diffusion in refractory metals and alloys”. In: *Phys. Rev. Mater.* 8.4 (2024), p. 43603.
- S. Starikov, **P. Grigorev**, and P. A. Olsson. “Angular-dependent interatomic potential for large-scale atomistic simulation of W-Mo-Nb ternary alloys”. In: *Computational Materials Science* 233 (2024), p. 112734.
- 2023 F. J. Domínguez-Gutiérrez, **P. Grigorev**, A. Naghdi, J. Byggmästar, G. Y. Wei, T. D. Swinburne, S. Papanikolaou, and M. J. Alava. “Nanoindentation of tungsten: From interatomic potentials to dislocation plasticity mechanisms”. In: *Physical Review Materials* 7 (4 2023), p. 043603.
- P. Grigorev**, A. M. Goryaeva, M.-C. Marinica, J. R. Kermode, and T. D. Swinburne. “Calculation of dislocation binding to helium-vacancy defects in tungsten using hybrid ab initio-machine learning methods”. In: *Acta Materialia* (2023), p. 118734.
- 2022 V. Grigorev, M. Filianina, Y. Lytvynenko, S. Sobolev, A. R. Pokharel, A. P. Lanz, A. Sapozhnik, A. Kleibert, S. Bodnar, **P. Grigorev**, Y. Skourski, M. Kläui, H.-J. Elmers, M. Jourdan, and J. Demsar. “Optically Triggered Néel Vector Manipulation of a Metallic Antiferromagnet Mn₂Au under Strain”. In: *ACS Nano* 16.12 (2022), pp. 20589–20597.
- 2021 A. M. Goryaeva, J. Dérès, C. Lapointe, **P. Grigorev**, T. D. Swinburne, J. R. Kermode, L. Ventelon, J. Baima, and M.-C. Marinica. “Efficient and transferable machine learning potentials for the simulation of crystal defects in bcc Fe and W”. In: *Phys. Rev. Materials* 5 (10 Oct. 2021), p. 103803.
- 2020 **P. Grigorev**, T. D. Swinburne, and J. R. Kermode. “Hybrid quantum/classical study of hydrogen-decorated screw dislocations in tungsten: Ultrafast pipe diffusion, core reconstruction, and effects on glide mechanism”. In: *Phys. Rev. Materials* 4 (2 Feb. 2020), p. 023601.
- 2018 **P. Grigorev**, A. Zinovev, D. Terentyev, G. Bonny, E. E. Zhurkin, G. V. Oost, and J.-M. Noterdaeme. “Molecular dynamics simulation of hydrogen and helium trapping in tungsten”. In: *Journal of Nuclear Materials* 508 (2018), pp. 451–458.
- 2017 A. Bakaev, **P. Grigorev**, D. Terentyev, A. Bakaeva, E. E. Zhurkin, and Y. A. Mastrikov. “Trapping of hydrogen and helium at dislocations in tungsten: an ab initio study”. In: *Nuclear Fusion* 57.12 (2017), p. 126040.

- A. Bakaev, D. Terentyev, **P. Grigorev**, M. Posselt, and E. E. Zhurkin. "Ab initio study of interaction of helium with edge and screw dislocations in tungsten". In: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 393 (2017), pp. 150–154.
- P. Grigorev**, A. Bakaev, D. Terentyev, G. V. Oost, J.-M. Noterdaeme, and E. E. Zhurkin. "Interaction of hydrogen and helium with nanometric dislocation loops in tungsten assessed by atomistic calculations". In: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 393 (2017), pp. 164–168.
- 2016 A. Bakaeva, D. Terentyev, G. De Temmerman, K. Lambrinou, T. Morgan, A. Dubinko, **P. Grigorev**, K. Verbeken, and J. Noterdaeme. "Dislocation-mediated trapping of deuterium in tungsten under high-flux high-temperature exposures". In: *Journal of Nuclear Materials* 479 (2016), pp. 307–315.
- P. Grigorev**, L. Buzi, A. Bakaeva, D. Terentyev, G. D. Temmerman, G. V. Oost, and J. M. Noterdaeme. "Numerical analysis of TDS spectra under high and low flux plasma exposure conditions". In: *Physica Scripta* 2016.T167 (2016), p. 014039.
- P. Grigorev**, D. A. Terentyev, A. V. Bakaev, and E. E. Zhurkin. "Classical molecular dynamics simulation of the interaction of hydrogen with defects in tungsten". In: *Journal of Surface Investigation* 10.2 (2016), pp. 398–405.
- P. Grigorev**, D. Matveev, A. Bakaeva, D. Terentyev, E. E. Zhurkin, G. Van Oost, and J.-M. Noterdaeme. "Modelling deuterium release from tungsten after high flux high temperature deuterium plasma exposure". In: *Journal of Nuclear Materials* 481 (2016), pp. 181–189.
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- 2014 A. V. Bakaev, D. A. Terentyev, **P. Grigorev**, and E. E. Zhurkin. "Atomistic simulation of the interaction between mobile edge dislocations and radiation-induced defects in Fe-Ni-Cr austenitic alloys". In: *Journal of Surface Investigation* 8.2 (2014), pp. 220–228.

- G. Bonny, D. Terentyev, A. Bakaev, **P. Grigorev**, and D. V. Neck. "Many-body central force potentials for tungsten". In: *Modelling and Simulation in Materials Science and Engineering* 22.5 (2014), p. 053001.
- G. Bonny, **P. Grigorev**, and D. Terentyev. "On the binding of nanometric hydrogen-helium clusters in tungsten". In: *Journal of Physics: Condensed Matter* 26.48 (2014), p. 485001.
- V. I. Dubinko, **P. Grigorev**, A. Bakaev, D. Terentyev, G. van Oost, F. Gao, D. V. Neck, and E. E. Zhurkin. "Dislocation mechanism of deuterium retention in tungsten under plasma implantation". In: *Journal of Physics: Condensed Matter* 26.39 (2014), p. 395001.
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- P. Grigorev** and E. E. Zhurkin. "Simulation of the sputtering of Si nanoclusters with diameters of (2-8) nm under bombardment with monatomic and cluster ions using the method of classical molecular dynamics". In: *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques* 7.2 (2013), pp. 201–210.
- D. Terentyev, G. Monnet, and **P. Grigorev**. "Transfer of molecular dynamics data to dislocation dynamics to assess dislocation-dislocation loop interaction in iron". In: *Scripta Materialia* 69.8 (2013), pp. 578–581.
- E. E. Zhurkin and **P. Grigorev**. "Sputtering of Al nanoclusters by 1-13 keV monatomic or polyatomic ions studied by Molecular Dynamics simulations". In: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 303.0 (2013), pp. 136–141.