

List of publications

- 2022 **P. Grigorev**, A. M. Goryaeva, M.-C. Marinica, J. R. Kermode, and T. D. Swinburne. *Synergistic coupling in ab initio-machine learning simulations of dislocations*. Mar. 2022. arXiv: 2111.11262 [under review in Acta Materialia].
- 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.
- P. Grigorev**, D. Terentyev, G. Bonny, E. E. Zhurkin, G. van Oost, and J.-M. Noterdaeme. "Mobility of hydrogen-helium clusters in tungsten studied by molecular dynamics". In: *Journal of Nuclear Materials* 474 (2016), pp. 143–149.
- 2015 **P. Grigorev**, D. A. Terentyev, A. V. Bakaev, and E. E. Zhurkin. "Interaction of hydrogen with dislocations and grain boundaries in Tungsten". In: *Journal of Surface Investigation* 9.6 (2015), pp. 1287–1292.
- P. Grigorev**, D. Terentyev, G. Bonny, E. E. Zhurkin, G. Van Oost, and J.-M. Noterdaeme. "Interaction of hydrogen with dislocations in tungsten: An atomistic study". In: *Journal of Nuclear Materials* 465 (2015), pp. 364–372.
- P. Grigorev**, D. Terentyev, V. Dubinko, G. Bonny, G. Van Oost, J.-M. Noterdaeme, and E. E. Zhurkin. "Nucleation and growth of hydrogen bubbles on dislocations in tungsten under high flux low energy plasma exposure". In: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 352.0 (2015), pp. 96–99.
- 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.
- P. Grigorev**, V. I. Dubinko, D. A. Terentyev, A. V. Bakaev, and E. E. Zhurkin. "Deuterium accumulation in tungsten under low-energy high-flux plasma exposure". In: *Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques* 8.2 (2014), pp. 234–238.

- D. Terentyev, V. Dubinko, A. Bakaev, Y. Zayachuk, W. V. Renterghem, and **P. Grigorev**. "Dislocations mediate hydrogen retention in tungsten". In: *Nuclear Fusion* 54.4 (2014), p. 042004.
- 2013 V. I. Dubinko, E. E. Zhurkin, **P. Grigorev**, D. Terentyev, G. Van Oost, A. Dubinko, and S. V. Dmitriev. "Dislocation mechanism of deuterium trapping and transport in tungsten under sub-threshold plasma implantation". In: *Letters on materials* 3 (2013), p. 5.
- 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.