

Curriculum Vitae

Dr. Alexandra M. GORYAEVA

Born: June 10, 1989, Kurchatov, USSR
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Research Gate Profile

Research and Education

Scientific Interests

Computational materials science, with particular focus on atomic-scale modeling of solids with complex structure and crystal chemistry. My main scientific interests include:

- Defects in crystalline solids
- Mechanisms of plastic deformation and diffusion
- Phase stability field, thermodynamics and local structure of solid solutions

Research Experience

- **2017 Jan → present:** Post-doc at SRMP, CEA Paris-Saclay, France. The project “LEARN” is aimed to develop machine learning interatomic potentials adapted for modeling irradiation defects and complex energetic landscapes in iron. Advisor: [Dr. M.-C. Marinica](#)
- **2017 Apr → 2017 Sep:** Post-doc at MATEIS, INSA Lyon, France. The 6-month project “Inter-équipes Jeunes Chercheurs MATEIS 2017” dedicated to molecular dynamics modeling of metallic nanoparticles with amorphous shells and their mechanical response upon compression. Advisors: [Dr. J. Amodeo](#), [Dr. C. Fusco](#) and [Dr. M. Bugnet](#)
- **2013 Sep → 2016 Dec:** PhD student at UMET, Université de Lille1, France. The ERC-funded advanced [project RheoMan](#) is aimed to describe plasticity of the essential rock forming minerals of the Earth mantle via multiscale modeling approach. Supervisors: [Prof. P. Cordier](#), [Prof. Ph. Carrez](#)

Education

- **2016 Dec:** PhD degree in computational materials science at Université de Lille1, France. “Modeling defects and plasticity in MgSiO₃ post-perovskite at the atomic scale” ([manuscript in English](#)). Supervisors: [Prof. P. Cordier](#), [Prof. Ph. Carrez](#)
- **2013 Jul:** Master degree with honours in crystallography at Moscow State University, Russia. “Atomistic modeling of mixing properties and the local structure of (Ca, Sr)₁₀[PO₄]₆F₂ solid solutions” ([manuscript in Russian](#)). Supervisors: [Prof. V.S. Urusov](#), [Prof. N.N. Eremin](#)
- **2011 Jul:** Bachelor degree in crystallography at Moscow State University. “Mixing properties of ZrO₂-HfO₂ solid solutions from *ab-initio* simulations and pairwise potential modeling” ([manuscript in Russian](#)). Supervisors: [Prof. V.S. Urusov](#), [Prof. N.N. Eremin](#)

Awards

- **2017: Prize Haüy-Lacroix** from French Society of Mineralogy and Crystallography (SFMC) for outstanding PhD thesis

Teaching

- **2012-2013:** Introduction to Crystallography and Theory of Symmetry: Point Groups, Space Groups, Structural Classification of Minerals (54 hours, in Russian), 1st year students in general geology, Lomonosov Moscow State University, Moscow, Russia

Technical Skills

Operating systems: Linux, MS Windows
Atomic-scale modeling: LAMMPS, GULP, VASP
Programming: MATLAB, bash, notions in Fortran
Data Analysis: Maple, Origin, Gnuplot

Spoken Languages

Russian (native)
English (fluent)
French (intermediate)
German (elementary)

Other Interests

XX Century: fine arts and literature

Publications and Communications

Peer-Reviewed Articles

- (7) Ph. Carrez, **A.M. Goryaeva**, P. Cordier (2017) Prediction of mechanical twinning in magnesium silicate post-perovskite. [Scientific Reports 7: 17640](#)
- (6) **A.M. Goryaeva**, Ph. Carrez, P. Cordier (2017) Modeling defects and plasticity in MgSiO₃ post-perovskite: Part 3 - screw and edge [001] dislocations. [Phys Chem Minerals 44: 521-533](#)
- (5) **A.M. Goryaeva**, Ph. Carrez, P. Cordier (2016). Low viscosity and high attenuation in MgSiO₃ post-perovskite inferred from atomic-scale calculations. [Scientific Reports 6: 34771](#)
- (4) **A.M. Goryaeva**, Ph. Carrez, P. Cordier (2015) Modeling defects and plasticity in MgSiO₃ post-perovskite: Part 2 - screw and edge [100] dislocations. [Phys Chem Minerals 42: 793-803](#)
- (3) **A.M. Goryaeva**, Ph. Carrez, P. Cordier (2015) Modeling defects and plasticity in MgSiO₃ post-perovskite: Part 1 - Generalized stacking faults. [Phys Chem Minerals 42: 781-792](#)
- (2) **A.M. Goryaeva**, V.S. Urusov, N.N. Eremin (2013) Atomistic simulations of mixing properties and the local structure of the (Ca, Sr)₁₀[PO₄]₆F₂ solid solution. [Eur J Miner 25: 947-955](#)

- (1) **A.M. Goryaeva**, V.S. Urusov, N.N. Eremin (2013) Atomistic computer modeling of the local structure and mixing properties of Sr-bearing fluorapatite. *Moscow Univ Geol Bull* 68: 368-379

Oral Presentations

A.M. Goryaeva, Ph. Carrez, P. Cordier. High attenuation in MgSiO₃ post-perovskite resulting from [100] dislocation glide under D'' conditions: an atomic scale study. American Geosciences Union (AGU) General Assembly 2016, San Francisco, USA, December 2016

A.M. Goryaeva, P. Hirel, Ph. Carrez, P. Cordier. Modeling mobility of defects at the atomic scale. Workshop RheoMan-Augury-iGEO-ATUNE. Utrecht, the Netherlands, November 2016

A.M. Goryaeva, Ph. Carrez, P. Cordier. Modeling [100] dislocation glide in MgSiO₃ post-perovskite under D'' conditions. European Mineralogical Conference (EMC²) 2016, Rimini, Italy, September 2016

A.M. Goryaeva, Ph. Carrez, P. Cordier. Atomistic modeling of MgSiO₃ post-perovskite rheology. International School of Earth Sciences (ISES) 2016, Moscow, Russia, May 2016

A.M. Goryaeva, Ph. Carrez, P. Cordier. Anisotropic lattice friction of MgSiO₃ post-perovskite from atomic-scale modeling. European Geosciences Union (EGU) General Assembly 2016, Vienna, Austria, April 2016

P. Cordier, **A.M. Goryaeva**, Ph. Carrez (invited) Modeling dislocations and plasticity in high-pressure polymorphs of MgSiO₃. ppv@10: a meeting for the 10th anniversary of the discovery of post-perovskite, Bristol, United Kingdom, June 2014

A.M. Goryaeva, V.S. Urusov, N.N. Eremin. Theoretical study of thermodynamic mixing properties and the local structure of the (Ca,Sr)₁₀[PO₄]₆F₂ solid solution. Lomonosov 2012, Moscow, Russia, April 2012

A.M. Goryaeva, O.L. Kuskov. Theoretical study of anisotropic acoustic properties of the essential rock forming minerals and its implication for the observed seismic anisotropy in the upper mantle beneath Siberian Craton. VII International School of Earth's Sciences (ISES) 2011, Odessa, Ukraine, September 2011

A.M. Goryaeva, N. Eremin. *Ab initio* modeling of elastic and acoustic properties of low-temperature ZrO₂ and HfO₂ polymorphs. Lomonosov 2011, Moscow, Russia, April 2011