

Pierre Hirel - List of scientific communications

International peer-reviewed journals

15. P. Hirel, P. Carrez, P. Cordier, *Scripta Mater.* **120** (2016) 67-70
From glissile to sessile : effect of temperature on $\langle 110 \rangle$ dislocations in perovskite materials
doi:10.1016/j.scriptamat.2016.04.001
14. B. Kozinsky, S.A. Akhade, P. Hirel, A. Hashibon, C. Elsässer, P. Mehta, A. Logéat, U. Eisele, *Phys. Rev. Lett.* **116** (2016) 055901
Effects of sublattice symmetry and frustration on ionic transport in garnet solid electrolytes
doi:10.1103/PhysRevLett.116.055901
13. P. Hirel, P. Carrez, E. Clouet, P. Cordier, *Acta Mater.* **106** (2016) 313-321
The electric charge and climb of edge dislocations in perovskite oxides : the case of high-pressure $MgSiO_3$ bridgmanite
doi:10.1016/j.actamat.2016.01.019
12. A. Kraych, P. Carrez, P. Hirel, E. Clouet, P. Cordier, *Phys. Rev. B* **93** (2016) 014103
Peierls potential and kink-pair mechanism in high-pressure $MgSiO_3$ perovskite : an atomic scale study
doi:10.1103/PhysRevB.93.014103
11. P. Hirel, A.F. Mark, M. Castillo-Rodriguez, W. Sigle, M. Mrovec, C. Elsässer, *Phys. Rev. B* **92** (2015) 214101
Theoretical and experimental study of the core structure and mobility of dislocations and their influence on the ferroelectric polarization in perovskite $KNbO_3$
doi:10.1103/PhysRevB.92.214101
10. P. Hirel, *Comput. Phys. Comm.* **197** (2015) 212-219
Atomsk : a tool for converting and manipulating atomic data files
doi:10.1016/j.cpc.2015.07.012
9. P. Cuvillier, H. Leroux, D. Jacob, P. Hirel, *Meteor. Planet. Sciences* **50** (2015) 1529-1545
Fe-Mg interdiffusion profiles in rimed forsterite grains in the Allende matrix : time-temperature constraints for the parent body metamorphism
doi:10.1111/maps.12493
8. P. Hirel, A. Kraych, P. Carrez, P. Cordier, *Acta Mater.* **79** (2014) 117-125
Atomic core structure and mobility of $[100](010)$ and $[010](100)$ dislocations in $MgSiO_3$ perovskite
doi:10.1016/j.actamat.2014.07.001
7. P. Hirel, M. Mrovec, C. Elsässer, *Acta Mater.* **60** (2012) 329
Atomistic simulation study of $\langle 110 \rangle$ dislocations in strontium titanate
doi:10.1016/j.actamat.2011.09.049
6. P. Hirel, P. Marton, M. Mrovec, C. Elsässer, *Acta Mater.* **58** (2010) 6072
Theoretical investigation of $\{110\}$ generalized stacking faults and their relation to dislocation behavior in perovskite oxides
doi:10.1016/j.actamat.2010.07.025
5. S. Brochard, P. Hirel, L. Pizzagalli, J. Godet, *Acta Mater.* **58** (2010) 4182
Elastic limit for surface step dislocation nucleation in face-centered cubic metals : temperature and step height dependence
doi:10.1016/j.actamat.2010.04.009
4. J. Godet, P. Hirel, S. Brochard, L. Pizzagalli, *Phys. Status Solidi A* **206** (2009) 1885
Dislocation nucleation from surface step in silicon : The glide set versus the shuffle set
doi:10.1002/pssa.200881460
3. J. Godet, P. Hirel, S. Brochard, L. Pizzagalli, *J. Appl. Phys.* **105** (2009) 026104
Evidence of two plastic regimes controlled by dislocation nucleation in silicon nanostructures
doi:10.1063/1.3072707
2. P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp, *Phys. Rev. B* **78** (2008) 064109
Determination of activation parameters for dislocation formation from a surface in fcc metals by atomistic simulations
doi:10.1103/PhysRevB.78.064109
1. P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp, *Scripta Mater.* **47** (2007) 1141
Influence of temperature and surface step on the incipient plasticity in strained aluminium by atomistic simulations
doi:10.1016/j.scriptamat.2007.08.016

Invited seminars

6. **P. Hirel, A. Kraych, P. Carrez, P. Cordier**, "The MgSiO₃ perovskite in Earth's lower mantle : from vacancies to dislocation climb", Fraunhofer-IWM, Freiburg, Germany, 12 July 2013.
5. **P. Hirel, P. Carrez, P. Cordier**, "Étude théorique de dislocations dans des matériaux perovskites : structures de cœur et mobilités", Institut Pprimme, Poitiers, France, Novembre 2012.
4. **P. Hirel, M. Mrovec, C. Elsässer**, "Étude théorique de dislocations dans des matériaux perovskites : structures de cœur et mobilités", UMET, Université Lille 1, France, 19 July 2012.
3. **P. Hirel, S. Brochard, J. Godet, L. Pizzagalli**, "Atomic-scale simulation of the formation of dislocation loops from surface ledges in a stressed metal", Fraunhofer-IWM, Freiburg, Germany, 11 March 2009.
2. **P. Hirel, J. Godet, S. Brochard, L. Pizzagalli**, "Study of the formation of dislocation loops from a free surface in fcc metals by atomistic simulation", Trinity College Dublin, Ireland, 24 October 2008.
1. **P. Hirel, J. Godet, S. Brochard, L. Pizzagalli**, "Simulations à l'échelle atomique de la formation de dislocations depuis une surface libre dans un métal contraint", LEM-ONERA Châtillon, France, 9 October 2008.

Oral presentations

26. **P. Hirel, P. Carrez, P. Cordier**, « De glissile vers sessile : la transition ductile-fragile dans les perovskites », Colloque Plasticité 2016, Poitiers, France, 11-13 April 2016.
25. **P. Carrez, A. Kraych, P. Hirel, P. Cordier**, "Peierls Potential and Kink Pair Mechanism in High Pressure MgSiO₃ Perovskite", TMS 2016, Nashville, USA, 14-18 February 2016.
24. **P. Carrez, A. Kraych, P. Hirel, P. Cordier**, "Computational Mechanics of Bridgmanite at High-Pressure, High-temperature and as a Function of Strain-Rate", AGU Fall Meeting 2015, San Francisco, USA, 14-18 December 2015.
23. **P. Hirel, P. Carrez, P. Cordier**, "Can ceramics be ductile? Structure and mobility of dislocations in perovskite materials", EMRS Fall Meeting 2015, Warsaw, Poland, 15-18 September 2015.
22. **P. Hirel, P. Carrez, P. Cordier**, "Les céramiques peuvent-elles être ductiles ? Structure et mobilité des dislocations dans les perovskites", Colloque Plasticité 2015, Autrans, France, 28-30 April 2015.
21. **P. Carrez, P. Hirel, A. Kraych, P. Cordier**, "Plasticité de la perovskite MgSiO₃ sous pression : étude atomique des propriétés de cœur des dislocations [100] et [010]", GDR ModMat Réunion Plénière 2015, Lyon, France, 8-9 January 2015.
20. **P. Cordier, P. Carrez, A. Goryaeva, P. Hirel, A. Kraych, S. Ritterbex**, "How modelling of crystal defects at the atomic scale can provide information on seismic anisotropy", AGU Fall Meeting 2014, San Francisco, USA, 15-19 December 2014.
19. **P. Hirel, P. Carrez, P. Cordier**, "Modeling dislocation climb at the atomic scale in MgSiO₃ perovskite in the conditions of Earth's lower mantle", MMM 2014, Berkeley, USA, 6-10 October 2014.
18. **P. Hirel, A. Kraych, K. Gouriet, P. Carrez, P. Cordier**, "Atomic-Scale Study of Dislocation Climb in MgSiO₃ Perovskite in the Conditions of Earth's Lower Mantle", MRS Fall Meeting 2013, Boston, USA, 1-5 December 2013.
17. **P. Hirel, M. Mrovec, C. Elsässer**, "Étude théorique de dislocations dans les matériaux perovskites", Colloque Plasticité 2012, Metz, France, 11-13 April 2012.
16. **P. Hirel, M. Mrovec, C. Elsässer**, "Atomic-scale study of dislocations in perovskite oxides», DPG Spring Meeting 2012, Berlin, Germany, 25-30 March 2012.
15. **P. Hirel, M. Mrovec, C. Elsässer**, "Atomistic simulations of dislocations in strontium titanate", DPG Spring Meeting 2011, Dresden, Germany, 13-18 March 2011.
14. **S. Brochard, L. Pizzagalli, J. Godet, P. Hirel**, "L'initiation de la plasticité dans les nanostructures : rôle des surfaces", Conférence Invitée, Journées Surface et Interfaces 2011, Poitiers, France, 26-28 January 2011.
13. **P. Hirel, M. Mrovec, C. Elsässer**, "Atomic-scale simulation of extended defects in strontium titanate", Multiscale Materials Modelling 2010, Freiburg, Germany, 4-8 October 2010.
12. **P. Hirel, M. Mrovec, C. Elsässer**, "Planar defects and dislocations in perovskite materials", DPG Spring Meeting 2010, Regensburg, Germany, 22-26 March 2010.
11. **P. Hirel, P. Marton, M. Mrovec, C. Elsässer**, "Modélisation de défauts planaires et linéaires dans le titanate de strontium", Colloque Plasticité 2009, Toulouse, France, 8-10 March 2010.
10. **S. Brochard, P. Hirel, L. Pizzagalli, J. Godet**, "Onset of plasticity in thin aluminum film : determination of activation parameters", Euromat 2009, Glasgow, United Kingdom, 7-10 September 2009.
9. **J. Godet, P. Hirel, S. Brochard, L. Pizzagalli**, "Déformation des objets de taille nanométrique : des défauts de surface aux défauts de volume", colloque Plasticité 2009, Marseille, France, 15-17 April 2009.

8. **S. Brochard, P. Hirel, J. Godet, L. Pizzagalli**, "Détermination des paramètres d'activation de la nucléation des dislocations à partir de marches de surface", Colloque Plasticité 2009, Marseille, France, 15-17 June 2009.
7. **J. Godet, P. Hirel, S. Brochard, L. Pizzagalli**, "Characterization of the mechanical behavior in nanostructures submitted to large stresses : the cases of Al and Si", MRS 2009 Spring Meeting, San Francisco, USA, 13-17 April 2009.
6. **P. Hirel, S. Brochard, J. Godet, L. Pizzagalli**, "Study of dislocation nucleation activation from surface step by atomistic simulation", Multiscale Materials Modelling, Talahassee Floride, États-Unis, 27-31 October 2008.
5. **J. Godet, P. Hirel, S. Brochard, L. Pizzagalli**, "Dislocation nucleation from surface in silicon : the glide set versus the shuffle set", Extended Defects in Semiconductors 2008, Poitiers, France, 15-19 September 2008.
4. **P. Hirel, J. Godet, S. Brochard, L. Pizzagalli**, "Détermination par simulation des paramètres d'activation de la nucléation de dislocations depuis une surface libre", Colloque Plasticité 2008, INPL Nancy, France, 10-12 March 2008.
3. **L. Pizzagalli, S. Brochard, P. Hirel, J. Godet, M.J. Soler, P. Beauchamp**, "Étude théorique de la nucléation de dislocations à partir de surfaces", Journées Surfaces et Interfaces, INSP Paris, France, 29-31 January 2007.
2. **S. Brochard, P. Hirel, J. Godet, L. Pizzagalli, P. Beauchamp**, "Nucléation de dislocations à partir de surfaces : étude par simulation à l'échelle atomique", Colloque Matériaux, Mécanique, Microstructures (3M), INSTN-CEA Saclay, France, 14-15 June 2006.
1. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Atomic-scale simulations of the nucleation of dislocations from a surface step in a FCC metal", Workshop Nanomaterials, Poitiers, France, 12-13 December 2006.

Posters

16. **P. Hirel, P. Carrez, P. Cordier**, "Modeling creep in the lower mantle : insights from the atomic scale", AGU Fall Meeting 2014, San Francisco, USA, 15-19 December 2014.
15. **A. Kraych, P. Hirel, P. Carrez, P. Cordier**, "Temperature-dependent dislocation mobility in MgSiO₃ perovskite", AGU Fall Meeting 2014, San Francisco, USA, 15-19 December 2014.
14. **P. Hirel, P. Carrez, P. Cordier**, "Étude théorique des interactions lacune-dislocation dans la perovskite MgSiO₃", colloque Plasticité 2014, Lyon, France, 28-30 April 2014.
13. **A. Kraych, P. Hirel, P. Carrez, P. Cordier**, "Numerical modeling of MgSiO₃ perovskite plasticity at the atomic scale", American Geophysical Union 2013, San Francisco, USA, 9-13 December 2013.
12. **P. Hirel, M. Mrovec, C. Elsässer**, "Étude des propriétés de dislocations dans la perovskite MgSiO₃ par simulations à l'échelle atomique", Colloque Plasticité 2013, Paris, France, 17-19 April 2013.
11. **P. Hirel, M. Mrovec, C. Elsässer**, "Theoretical Study of Dislocations in Perovskite Oxides", MRS Fall Meeting, Boston, États-Unis, 25-30 November 2012.
10. **P. Hirel, M. Mrovec, C. Elsässer**, "Étude de défauts cristallins dans le titanate de strontium par simulations atomistiques", Colloque Plasticité, Lille, France, 4-6 April 2011.
9. **S. Brochard, P. Hirel**, "Nucléation de dislocations à partir de marches de surface : influence de l'état de surface initial et de la température sur la limite d'élasticité", Colloque Plasticité, Toulouse, France, 8-10 March 2010.
8. **J. Godet, P. Hirel, S. Brochard, L. Pizzagalli**, "Plasticity spreading from surfaces in self-supported nanostructures", Euromat 2009, Glasgow, United Kingdom, 7-10 September 2009.
7. **P. Hirel, J. Godet, S. Brochard, L. Pizzagalli**, "La plasticité naissante dans les matériaux à l'échelle nanométrique : détermination des paramètres d'activation", Congrès Général de la SFP, École Polytechnique de Palaiseau, France, 6-10 July 2009.
6. **P. Hirel, S. Brochard, L. Pizzagalli**, "Onset of plasticity in materials at the nanometer scale : the role of surface defects", MRS Spring Meeting 2009, San Francisco, USA, 13-17 April 2009.
5. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Study of dislocation nucleation activation from surface step by atomistic calculations", Colloque Dislocations 2008, Hong-Kong, China, 13-17 October 2008.
4. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Study of dislocation nucleation activation from surface step by atomistic calculations", Colloque J2NO 2008, Poitiers, France, 15-17 October 2008.
3. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Simulations atomistiques des effets de surface sur la plasticité d'un matériau nanostructuré contraint", Congrès Général de la SFP 2007, Grenoble, France, 9-13 July 2007.
2. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Simulations atomistiques de la nucléation de dislocations à partir d'une marche de surface dans un monocristal CFC", Colloque Plasticité 2007, Poitiers, France, 19-21 March 2007.
1. **P. Hirel, S. Brochard, L. Pizzagalli, P. Beauchamp**, "Simulations atomistiques 3D de la formation de dislocations à partir d'une surface", Colloque Plasticité 2006, Annecy, France, 27-29 March 2006.