ΑΛΕΞΑΝΔΡΟΣ ΧΡΟΝΑΙΟΣ

M.Sc., Ph.D

ΥΠΟΜΝΗΜΑ και ΒΙΟΓΡΑΦΙΚΟ ΣΗΜΕΙΩΜΑ

Σπουδές – Τίτλοι
Διδακτική και Επιστημονική Δραστηριότητα

ΑΘΗΝΑ, 2018

ΒΙΟΓΡΑΦΙΚΟ ΣΗΜΕΙΩΜΑ

Ονοματεπώνυμο: **Χρονάιος Αλέξανδρος**
Ιδιότητα: Καθηγητής
Τόπος-Ημερ/νία Γέννησης: Αθήνα, 20-1-1976
Οικογενειακή κατάσταση: Έγγαμος

Διεύθυνση εργασίας: Faculty of Engineering, Environment & Computing,
Coventry University,
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Εργασιακή Εμπειρία

1/2016-σήμερα	Καθηγητής της Φυσικής των Υλικών (Professor in Materials Physics), τμήμα Μηχανικής, Coventry University, Αγγλία.
9/2014-12/2015	Αναπληρωτής Καθηγητής της Φυσικής των Υλικών (Reader in Materials Physics), τμήμα Μηχανικής, Coventry University, Αγγλία.
10/2012-8/2014	Επίκουρος Καθηγητής, τμήμα Μηχανικής, The Open University, Αγγλία.
6/2013	Επισκέπτης Καθηγητής, Massachusetts Institute of Technology, ΗΠΑ.
9/2015-σήμερα	Αναπληρωτής Καθηγητής (Visiting Reader), τμήμα Υλικών, Imperial College London.
9/2011- 8/2015	Επίκουρος Καθηγητής (Visiting Lecturer), τμήμα Υλικών, Imperial College London.
5/2011-10/2012	Marie Curie Intra-European Fellow, ΕΚΕΦΕ Δημόκριτος.

10/2010-4/2011	Μεταδιδακτορικός ερευνητής, τμήμα Υλικών, Cambridge University, Αγγλία.
3/2010	Επισκέπτης Ερευνητής, Massachusetts Institute of Technology, ΗΠΑ.
03/2010-8/2010	Μεταδιδακτορικός ερευνητής, τμήμα Υλικών, Imperial College London, Αγγλία.
08/2008-10/2009	Μεταδιδακτορικός ερευνητής, τμήμα Υλικών, Imperial College London, Αγγλία.
02/2008-07/2008	Μεταδιδακτορικός ερευνητής, τμήμα Φυσικής, Πανεπιστήμιο του Münster, Γερμανία.
03/2003-05/2004	Στρατιωτική Θητεία.

Σπουδές Τίτλοι

11/2004-02/2008	Διδακτορικό στην Φυσική των Υλικών, τμήμα Υλικών, Imperial College London, Αγγλία.
10/99-06/2002	B.Eng (Hons), Πολιτική Μηχανική, τμήμα Πολιτικών Μηχανικών, Πανεπιστήμιο του Εδιμβούργου , Σκωτία.
10/1998-09/1999	M.Sc, Θεωρητική Χημεία, τμήμα Χημείας, Πανεπιστήμιο της Οξφόρδης, Αγγλία.
10/1995-06/1998	B.Eng (Hons), Επιστήμη των Υλικών και Φυσική, τμήμα Υλικών, Imperial College London, Αγγλία.

Ξένες Γλώσσες:

Αγγλική: Άριστα (O'Level Certificate, grade A)

Γνώσεις Η/Υ:
Λογισμικό: Matlab, Mathematica, Autocad, Abaqus, Gulp, Cascade, Castep (*ab initio*), Microsoft Excel, Microcal Origin.

Λειτουργικά: Unix, Linux and Windows.

Γλώσσα Προγραματισμού: Fortran, Python.

Microsoft Windows, Microsoft Word, Microsoft Access, Microsoft PowerPoint, Origin.

ΥΠΟΤΡΟΦΙΕΣ

2010	Marie Curie Intra-European Fellowship, European Union
06/1996-09/1996	UROP scholarship, τμήμα Υλικών, Imperial College London, Αγγλία.
06/1997-09/1997	UROP scholarship, τμήμα Υλικών, Imperial College London, Αγγλία

ΔΙΔΑΚΤΙΚΟ ΕΡΓΟ

Α. ΜΑΘΗΜΑΤΑ

Ι. Προπτυχιακά

1) Διδασκαλία στο τμήμα Υλικών του Imperial College London την περίοδο 2008-2009. Συγκεκριμένα, δίδαξα σε πρωτοετείς φοιτητές ατομική θεωρία, χημικούς δεσμούς, κύματα στα στερεά, κβαντική θεωρία και κρυσταλλογραφία (κωδικός μαθήματος MSE 105).

2) Διδασκαλία στο τμήμα Μηχανικής του The Open University, Αγγλία. (κωδικός μαθήματος TXR220 Engineering in Action).

3) Διδασκαλία στο τμήμα Μηχανικής του Coventry University.

ΙΙ. Μεταπτυχιακά

1. Διδασκαλία στο MSc in Nuclear Engineering του Imperial College London την περίοδο 2010- σήμερα. Hydrogen Production using Nuclear Energy.

Β. ΦΡΟΝΤΙΣΤΗΡΙΑ

Εχω διδάξει φροντιστηριακές στην ατομική θεωρία, χημικούς δεσμούς, κύματα στα στερεά, κβαντική θεωρία και κρυσταλλογραφία (Imperial College London, κωδικός μαθήματος MSE 105).

Γ. ΕΡΓΑΣΤΗΡΙΑ

Έχω επιβλέψει στα Εργαστήρια Φυσικής επί σειρά ετών στο τμήμα Υλικών, Imperial College London, Αγγλία.

ΜΕΤΑΔΙΔΑΚΤΟΡΕΣ

1. Dr Michael Rushton (Open University) 2014.

2. Dr Stavros Christopoulos (Coventry University) 2015-2016.

3. Dr Nicolaos Kelaidis (Coventry University) 2017- σήμερα.

ΔΙΔΑΚΤΟΡΙΚΕΣ ΔΙΑΤΡΙΒΕΣ

1. Hassan Tahini (Imperial College London), PhD Modelling of Defects in Advanced Semiconductors (2010-2014).

2. Avishek Dey (The Open University), PhD Graphene Based Solar Cell (2014-2017).

3. Olga Thoda (Coventry University/ ΕΚΕΦΕ Δημόκριτος), PhD Development of Ni-based nano- and micro-structured catalysts produced by combustion synthesis and their catalytic activity in liquid phase hydrogenation (9/2015-).

4. Apostolis Kordatos (Coventry University), PhD Disordered ionic conductors: A machine-learning approach (9/2015-).

5. Angeliki Kaiafa (University of Piraeus), PhD Mixed Problems of Boundary Values for Maxwell Equations (12/2016-).

Επίσης, θα πρέπει να αναφερθεί η συνεργασία μου για την επίβλεψη ή/και την ολοκλήρωση των παρακάτω διδακτορικών εργασιών, οι οποίες υλοποιήθηκαν στο τμήμα Φυσικής του Πανεπιστημίου του Münster και στο τμήμα Υλικών του Imperial College London. Σε αγκύλες οι δημοσιεύσεις που προέκυψαν.

1. Rene Kube, τμήμα Φυσικής του Πανεπιστημίου του Münster, [J. Appl. Phys. **106**, 063534 (2009)].

2. Dmitry Rupasov, τμήμα Υλικών του Πανεπιστημίου της Μόσχας/τμήμα Υλικών Imperial College London [Phys. Rev. B **79**, 172102 (2009)].

3. Nickolas Ashley, τμήμα Υλικών Imperial College London [J. Appl. Phys. **106**, 083502 (2009)].

4. Ankoor Patel, τμήμα Υλικών Imperial College London, [Nucl. Instr. and Meth. in Phys. Res B (Nucl. Instr. and Meth. Phys. Res B **268**, 3111-3113 (2010)].

5. Samuel Murphy, τμήμα Υλικών Imperial College London, έρευνα στο InGaAs [Phys. Rev. B **82**, 073201 (2010); Phys. Rev. B **84**, 184108 (2011)].

ΔΙΑΤΡΙΒΕΣ MSc/MEng

1. Angeliki Kaiafa (University of Athens) MSc Thesis Mixed Problems of Boundary Values for Maxwell Equations (12/2015)

2. Petros-Panagis Filippatos (National Technical University of Athens) Dipl. Thesis Lithium in 312 MAX Phases (2017-)

ΕΡΕΥΝΗΤΙΚΑ ΕΝΔΙΑΦΕΡΟΝΤΑ

Μελέτη της διάχυσης και της αλληλεπίδρασης των προσμίξεων σε κεραμικά, ημιαγώγιμα και υπεραγώγιμα υλικά με πειραματικές και θεωρητικές μεθόδους. Εστιάζω σε υλικά, τα οποία έχουν εφαρμογές στις μικροηλεκτρονικές διατάξεις, τους αισθητήρες ή στην παραγωγή ενέργειας. Συγκεκριμένα εφάρμοσα διάφορες μεθόδους προσομοίωσης σε συνδιασμο με πειραματικές μελέτες για τη μελέτη προβλημάτων που συνδέονται με:

Α) Υλικά υψηλής τεχνολογίας

1. Μελέτη ατελειών σε 2D υλικά (graphene/silicene/germanene/MXene).
2. Ημιαγωγοί στενού ενεργειακού χάσματος, GaSb.
3. Υλικά για αισθητήρες (functional materials for sensors).
4. Οξείδια για μεμβράνες διαχωρισμού οξυγόνου, $Sr_{0.75}Y_{0.25}CoO_{2.625}$.
5. Υλικά για μικροηλεκτρονικές διατάξεις, Si, Ge, SiGe, SiGeSn, SnGe, HfN.
6. Μελέτη της δομής των υδροξειδίων.

Β) Υλικά για ενέργεια

1. Οξείδια για καθόδους σε κυψέλες καυσίμων, $La_2NiO_{4+\delta}$, $Pr_2NiO_{4+\delta}$.
2. Φωτοβολταϊκά, InGaAs.
3. Νέα πυρηνικά καύσιμα, ThC, ThN.
4. Υπεραγώγιμα υλικά, $ReBa_2Cu_3O_{7-d}$.
5. Μελέτη των νανοκρυστάλλων $LiAlSiO_4$ σε μήτρα άμορφου $LiAlSiO_4$.

Μέθοδοι

1. Μελέτη πλεγματικών ατελειών και διάχυσης σε ιοντικούς κρυστάλλους (Secondary Ion Mass Spectrometry, Density Functional Theory, Molecular Dynamics).
2. Μελέτη πλεγματικών ατελειών σε ημιαγώγιμα υλικά (Density Functional Theory, Secondary Ion Mass Spectrometry).
3. Κλασσική Φυσική (Ηλεκτρομαγνητισμός).
4. Μελέτη υπεραγωγίμων υλικών (Ηλεκτρικές Μετρήσεις).
5. Μελέτη ιδιοτήτων σημειακών ατελειών σε ημιαγωγούς (μέθοδος υπερύθρου φασματοσκοπίας (IR).
6. Μελέτη ατελειών σε 2D υλικά (graphene) (XPS, Density Functional Theory).

ΣΥΜΜΕΤΟΧΗ ΣΕ ΕΡΕΥΝΗΤΙΚΑ ΠΡΟΓΡΑΜΜΑΤΑ

Deutsche Forschungsgemeinschaft, SFG 458, European project IST "FRENDTECH", European project "ORAMA", United States Air Force contract number: F33615-01-D-5802 (co-investigator), United Kingdom Energy Research Centre, 2 KAUST research programs in materials (co-investigator in both).

	Τίτλος προγράμματος	**Διάρκεια (months)**	**Έτος**	**Αξία**
USAF	Simulation of Hydroxides	12	2005	12000$
KAUST	Diffusion and Stability of	12	5/2009	62936 UK

	Dopants in Ge and III-V compounds			pounds
KAUST	Controlling Dopant Distribution and Structures in Advanced Semiconductors	36	9/2010	340590$
EU	Rare Earth Oxide Dielectrics for Advanced Ge CMOS Technology	24	2011	154000 Ευρώ
China (Tsingua-Cambridge-MIT Alliance)	Flexible Nuclear Power for Clean Fuels and Peak Electricity Production by Co-Electrolysis of CO_2 and H_2O	24	2011	200000$
EU	MATISSE	36	2013	22000 Ευρώ
EU	STIMULATE	36	2013	96000 Ευρώ
Lloyd's	Joint Research Centre for the Safety of Nuclear Energy	36	2013	500000 UK pounds
Lloyd's	Studying temperature- and ambient-induced band structure changes in tin oxide	36	2018	49400 UK pounds
EU	Energy HarveStorers for Powering the Internet of Things (Horizon 2020)	48	2018	400000 Ευρώ

ΔΙΕΘΝΗΣ ΑΝΑΓΝΩΡΙΣΗ

1. Αναφορές στο δημοσιευμένο έργο

Σύμφωνα με το σύστημα του ISI έχω 4300+ αναφορές και H-index = 41 (google scholar: 5400+ αναφορές και H-index = 48).

2. Αξιολογητής σε διεθνή επιστημονικά περιοδικά

Nature Communications, Physical Review Letters, Accounts of Chemical Research, Energy & Environmental Science, Journal of the American Chemical Society, Chemistry of Materials, ACS Applied Materials & Interfaces, Journal of Physics: Condensed Matter, Journal of Physical Chemistry Letters, Journal of Materials Chemistry A, International Materials Reviews, Journal of Power Sources, International Journal of Hydrogen Energy, Journal of Physical Chemistry, Inorganic Chemistry, Applied Physics Letters, Physical Review B, RSC Advances, Journal of the

Electrochemical Society, Applied Surface Science, Journal of Physics D: Applied Physics, Chemical Physics Letters, Solid State Ionics, Applied Catalysis A, Fuel Cells, Journal of Applied Physics, Journal of Alloys and Compounds, Superconductor Science and Technology, Beilstein Journal of Nanotechnology, Materials Letters, Materials Chemistry and Physics, Solid State Communications, Journal of Solid State Electrochemistry, Computational Materials Science, European Physical Journal B, Journal of Crystal Growth, Energies, Physica Status Solidi (b), Materials Science Engineering B, Thin Solid Films, Journal of Nuclear Materials, Microelectronic Engineering, Journal of Materials Science, Philosophical Magazine, Journal of Physics and Chemistry of Solids, Physics and Chemistry of Minerals, Current Applied Physics, Physica B, IEEE Transactions on Applied Superconductivity, Materials Science and Semiconductor Processing, Materials & Design, Results in Physics, Computational Condensed Matter, Energy Storage Materials, Applied Sciences, Materials, Journal of Computational Methods in Sciences and Engineering, Sustainability, Acta Geophysica, Crystal Research & Technology, Indian Journal of Physics, Advances in Condensed Matter.

3. Αξιολογητής σε Διεθνή προγράμματα

1. Αξιολογητής στο Royal Society.
2. Αξιολογητής στο Κυπριακό πρόγραμμα LinkSCEEM & Cy-Tera.
3. Αξιολογητής στο Netherlands Organisation for Scientific Research.
4. Αξιολογητής στο Georgia National Science Foundation (GNSF).
5. Αξιολογητής στο Austrian Science Fund.
6. Αξιολογητής στο Royal Academy of Engineering.

4. Κριτής σε διεθνή συνέδρια

1. Κριτής **(**International Advisory Board) στο Diffusion in Materials (DIMAT 2014) Münster, Γερμανία.
2. Steering Committee, Workshop on Smart Energy and Power Systems (WINDASPES), Ελλάδα 2014.

5. Editorial Board του περιοδικού

1. Scientific Reports (Nature Publishing Group).
2. Bulletin Kharkov National University (serial Physics, Nuclear, particles, fields).

6. Σημαντικότερες Διεθνείς Συνεργασίες (2008-)

1. Centre of Nuclear Engineering, Imperial College London, Prof. William E. Lee (Διευθυντής του Κέντρου).
2. Τμήμα Υλικών, Imperial College London, Prof. John A. Kilner, BCH Steele Έδρα των Ενεργειακών Υλικών.
3. Τμήμα Υλικών, Imperial College London, Prof. Robin W. Grimes.
4. Massachusetts Institute of Technology, Prof. Bilge Yildiz.
5. Τμήμα Υλικών, Imperial College London, Prof. Stephen Skinner.

6. Τμήμα Υλικών, Imperial College London, Dr David McPhail.
7. Τμήμα Υλικών, Cambridge University, Dr Paul Bristowe.
8. Purdue University, Prof. Lefteri Tsoukalas
9. CEA Grenoble, Dr. Pascal Pochet
10. Los Alamos National Laboratory, Dr Chris Stanek.
11. Los Alamos National Laboratory, Dr Blas Uberuaga.
12. Τμήμα Φυσικής, Πανεπιστήμιο του Münster, Prof. Dr Hartmut Bracht.
13. Πανεπιστήμιο του Χαρκόβου, Prof. Ruslan V. Vovk.
14. KAUST/ Imperial College London, Prof. Udo Schwingenschlögl.
15. IREC Barcelona, Dr Albert Tarancon.
16. Idaho National Laboratory, Dr Chao Jiang

7. Προσκεκλημένες Παρουσιάσεις

1. A. Chroneos, (keynote speaker), *"Defect Engineering Strategies in Energy and Electronic Materials,"* 5th Hellenic Forum for Science Technology and Innovation, Athens, Greece, 5-7/7/2017.
2. A. Chroneos, *"Diffusion in Energy Materials: Insights from Atomistic Modelling,"* 21st International Conference on Solid State Ionics, Padova, Italy, 18-23/6/2017.
3. A. Chroneos, (keynote speaker), "*Solid State Physics Revisited,"* Smart Energy Workshop, Volos, Greece, 15-16/10/2015.
4. A. Chroneos, (keynote speaker), "*Challenges in Energy Materials,"* 5th International Conference on Information, Intelligence, Systems and Applications (IISA), Workshop on Smart Energy and Power Systems (WINDASPES), Chania, Greece, 7-9/7/2014.
5. A. Chroneos, "*Diffusion in Germanium*," Dept. of Physics, National Technical University of Athens, Greece 9/5/2014.
6. A. Chroneos, "*Studies of Ionic Diffusion in Oxides for Energy Applications*," Dept. of Nuclear Engineering, MIT, USA 18/6/2013.
7. A. Chroneos, "*Engineering Defects in Germanium"* Multiscale Materials Modeling (Symposium A: Microstructure Evolution Across Multiple Length Scales: Defects to Materials Properties), Singapore, 15-19/10/2012 (declined).
8. J. A. Kilner, A. Chroneos, D. Parfitt, I. Seymour, R. W. Grimes, and A. Tarancon, "*Intrinsic Disorder and Diffusion in $LnBaCo_2O_{5.5}$ Double Perovskites"* 18th International Conference on Solid State Ionics, Warsaw, Poland, 3-8/7/2011.
9. A. Chroneos, "*Diffusion in Materials for Microelectronic and Energy Applications*," Dept. of Physics, National Technical University of Athens, Greece 6/5/2011.
10. A. Chroneos, "*Diffusion in Materials for Microelectronic and Energy Applications*," Dept. of Chemical Engineering, University of Patras, Greece 8/4/2011.
11. A. Chroneos, "*Engineering Defects in Energy Materials*," Ecole Centrale Paris, France 7/3/2011.
12. A. Chroneos, "*Advanced Materials for Energy Applications*," Dept. of Chemical Engineering, National Technical University of Athens, Greece 31/1/2011.
13. A. Chroneos, "*Molecular Dynamics Studies of Oxygen Diffusion in Oxides for SOFC Applications*," Dept. of Mechanical Engineering, MIT, USA 19/3/2010.

14. A. Chroneos, H. Bracht, and R. W. Grimes, "*Diffusion and Defect Reactions of Donor Atoms in Ge and SiGe*," Thermodynamic and Transport Kinetics of Nanostructured Materials, Oranienburg, Germany 17-20/8/2009.
15. A. Chroneos, "*Dopant-Defect Interactions in Inorganic Materials*," Institute of Transuranium Elements, Karlsruhe, Germany 10/7/2009.
16. H. Bracht, S. Schneider, and A. Chroneos, "*Technological and Scientific Aspects of Self- and Dopant Diffusion in Ge,*" European Materials Research Society Spring Meeting (Semiconductor Materials), Strasbourg, France 8-12/6/2009.
17. A. Chroneos, H. Bracht, and S. Brotzmann, "*Diffusion and Defect Reactions of Donors, Carbon, and Vacancies in Germanium*", 7th International Conference on Diffusion in Materials, Lanzarote, Spain 28-31/10/2008.
18. A. Chroneos, "*Atomistic Studies of Impurity-Vacancy Complexes in Germanium*" Institute of Materials Physics, Münster University, Münster, Germany, 4/6/2007.

ΣΥΓΓΡΑΦΙΚΟ ΕΡΕΥΝΗΤΙΚΟ ΕΡΓΟ

220+ Δημοσιεύσεις σε διεθνή περιοδικά με κριτές και ειδικούς τόμους διεθνών συνεδρίων με κριτές. Σε 150 εκ των οποίων είμαι πρώτος ή/και ανταποκριτής συγγραφέας. 80+ παρουσιάσεις σε συνέδρια/Πανεπιστήμια εκ των οποίων 18 Προσκεκλημένες παρουσιάσεις (Invited Presentations). 4200+ αναφορές.

ΕΠΙΣΤΗΜΟΝΙΚΕΣ ΔΗΜΟΣΙΕΥΣΕΙΣ
ΚΑΙ ΑΝΑΚΟΙΝΩΣΕΙΣ

Α) ΔΗΜΟΣΙΕΥΣΕΙΣ ΣΕ ΔΙΕΘΝΗ ΠΕΡΙΟΔΙΚΑ ΜΕ ΚΡΙΤΕΣ

1. R. W. Grimes, G. Busker, M. A. McCoy, A. Chroneos, J. A. Kilner, and S.-P. Chen, "*The Effects of Ion Size on Solution Mechanism and Defect Cluster Geometry*," *Ber. Bunsen. Phys. Chem*. 101 (9), 1204-10 (1997).
2. G. Busker, A. Chroneos, R. W. Grimes and I.-W. Chen, "*Solution Mechanisms for Dopant Oxides in Yttria*," *J. Am. Ceram. Soc.* 82 (6), 1553-59 (1999).
3. A. Chroneos and G. Busker, "*Solution Mechanisms for Li_2O in Sc_2O_3, Y_2O_3 and La_2O_3*," *Acta Chim. Slov.* 52, 417-421 (2005).
4. A. Chroneos, K. Desai, S. E. Redfern, M. O. Zacate and R. W. Grimes, "*New Atomic Scale Simulation Models for Hydroxides and Oxyhydroxides,*" *J. Mater. Sci.* 41, 675-687 (2006).
5. A. Chroneos, R. W. Grimes and C. Tsamis, "*Atomic Scale Simulations of Arsenic-Vacancy Complexes in Germanium and Silicon,*" *Mater. Sci. Semicon. Proc.* 9, 536-540 (2006).
6. A. Chroneos, D. Skarlatos, C. Tsamis, A. Christofi, D.S. McPhail and R. Hung, *"Implantation and Diffusion of Phosphorous in Germanium*," *Mater. Sci. Semicon. Proc.* 9, 640-643 (2006).

7. A. Chroneos, I. L. Goulatis and R. V. Vovk, "*Atomic Scale Models for $RBa_2Cu_3O_{6.5}$ and $R_{1-x}Pr_xBa_2Cu_3O_{6.5}$ Compounds (R= Y and Lanthanides),*" *Acta Chim. Slov.* 54, 179-184 (2007).
8. A. Chroneos and I. L. Goulatis, "*Aluminium-Vacancy Complexes in $Ge_{1-x}C_x$*," *Functional Materials,* 14, 362-364 (2007).
9. R. V. Vovk, M. A. Obolenskii, A. V. Bondarenko, I. L. Goulatis and A. Chroneos, "*2D-3D Crossover of the In-Plane Paraconductivity in Optimal Doped $ReBa_2Cu_3O_{7-\delta}$ (Re=Y, Ho) Single Crystals*" *High Pressure Physics and Technology*, 17, 83-88 (2007).
10. A. I. Chroneos, I. L. Goulatis, R. V. Vovk, A. A. Zavgorodniy, M. A. Obolenskii, A. G. Petrenko, and A. V. Samoilov, "*Atomistic Models for $R_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ (R=Y and Lanthanides) and Related Oxides*" *High Pressure Physics and Technology*, 19, 7-13 (2007).
11. A. Chroneos, N. Ashley, K. Desai, J. F. Maguire and R. W. Grimes, "*Optimized Hydrogen Positions for Aluminium and Iron Hydroxide Minerals*," *J. Mater. Sci.* 42, 2024-2029 (2007).
12. A. Chroneos, "*Isovalent Impurity-Vacancy Complexes in Germanium,*" *Phys. Stat. Sol. B* 244, 3206-3210 (2007).
13. R. V. Vovk, M. A. Obolenskii, A. A. Zavgorodniy, A. V. Bondarenko, I. L. Goulatis and A. Chroneos, "*Excess Conductivity and Pseudo-Gap State in YBCO Single Crystals Slightly Doped with Al and Pr*," *J. Mater. Sci.: Mater. Electron.* 18, 811-815 (2007).
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ΠΕΡΙΛΗΨΗ ΤΗΣ ΔΙΔΑΚΤΟΡΙΚΗΣ ΔΙΑΤΡΙΒΗΣ

Α) ΔΙΔΑΚΤΟΡΙΚΗ ΔΙΑΤΡΙΒΗ

01. Defect Processes in Germanium
Διδακτορική διατριβή, Imperial College London, 2008
Α. Χροναίος

Καθώς η συμβατική τεχνολογία ημιαγωγικών διατάξεων πυριτίου αγγίζει τα φυσικά της όρια, εμφανίζεται η ανάγκη εισαγωγής εναλλακτικών υποστρωμάτων για την κατασκευή τους. Το χαρακτηριστικό των νέων αυτών υποστρωμάτων είναι η υψηλή ευκινησία φορέων που επιτρέπει μία σημαντική απόδοση των διατάξεων, χωρίς να απαιτείται περαιτέρω σμίκρυνση των διαστάσεών τους. Ένα από τα υποστρώματα αυτά είναι το γερμάνιο. Σε αντίθεση με το πυρίτιο, η έρευνα της διάχυσης των προσμίξεων στο γερμάνιο έχει αποκτήσει ενδιαφέρον μόλις τα τελευταία χρόνια. Σκοπός της διδακτορικής μου διατριβής ήταν η μελέτη των τεχνολογικά σημαντικών προσμίξεων στο γερμάνιο με πειραματικές και θεωρητικές μεθόδους.

Το πειραματικό μέρος της διατριβής εστιάστηκε στην εμφύτευση και τη διάχυση του φωσφόρου (P) στο Ge Η ιοντική εμφύτευση είναι συνήθης μέθοδος για την εισαγωγή προσμίξεων στο πυρίτιο και για το λόγο αυτό αναμένεται να είναι σημαντική και στην τεχνολογία γερμανίου. Πραγματοποιήθηκαν πειράματα, όπου σε δισκία γερμανίου εμφυτεύθηκαν ιόντα φωσφόρου με διαφορετικές δόσεις και ενέργειες εμφύτευσης. Τα δισκία γερμανίου καλύφθηκαν με διοξείδιο του πυριτίου (SiO_2), νιτρίδιο του πυριτίου ή παρέμειναν ακάλυπτα. Επακολούθησε ανόπτηση των δειγμάτων σε ατμόσφαιρα αζώτου (N_2) σε διάφορους χρόνους, ενώ η συγκέντρωση των ιόντων φωσφόρου αναλύθηκε με τη μέθοδο SIMS. Στην περίπτωση των ακάλυπτων δειγμάτων παρατηρήθηκε απώλεια της επιφάνειας του γερμανίου και κατά συνέπεια σημαντική μείωση της δόσης του φωσφόρου. Η επικάλυψη με νιτρίδιο του πυριτίου αποδείχθηκε η πιο αποτελεσματική. Η διάχυση του φωσφόρου στο γερμάνιο εξαρτάται από την κατανομή. Στα εμφυτευμένα δείγματα με τη μικρότερη δόση φωσφόρου παρατηρήθηκε αμελητέα διάχυση, σε αντίθεση με τα δείγματα με τη μεγαλύτερη δόση, όπου παρατηρήθηκε σημαντική διάχυση (non-Fickian).

Το θεωρητικό μέρος της διατριβής εστιάστηκε στον υπολογισμό της ενέργειας συμπλεγμάτων ανάμεσα σε σημειακές ατέλειες και σε άτομα προσμίξεων καθώς και στη διάχυση των προσμίξεων. Με την εφαρμογή μεθόδων *ab initio* (density functional theory) μελετήθηκαν συνολικά 11 (B, In, Ga, Al, C, Si, Sn, N, P, As και Sb) τεχνολογικά σημαντικές προσμίξεις στο γερμάνιο και για σύγκριση στο πυρίτιο. Μέσα από τη μελέτη μεγάλου αριθμού προσμίξεων κατέστη δυνατή η αναγνώριση

των ομοιοτήτων και διαφορών των συμπλεγμάτων που σχηματίζονται στο γερμάνιο και το πυρίτιο.

Χρησιμοποιήσα υπολογισμούς *ab initio* για τη μελέτη της σταθερότητας, της συγκέντρωσης και διάχυσης συμπλεγμάτων, τα οποία περιλαμβάνουν πλεγματικές οπές (V) και άτομα φωσφόρου, αρσενικού ή αντιμονίου στο γερμάνιο, το οποίο περιέχει άνθρακα. Η αλληλεπίδραση των ατόμων άνθρακα με τα κινούμενα ζεύγη PV, AsV και SbV μπορεί να οδηγήσει στη δημιουργία συμπλεγμάτων που δεν διαχέονται. Υπολογίσα τις σχετικές συγκεντρώσεις των συμπλεγμάτων αυτών, καθώς και τους παράγοντες που τις επηρεάζουν. Οι θεωρητικές προβλέψεις επιβεβαιώνουν την επιβράδυνση των ζευγών PV, AsV και SbV όταν υπάρχει σημαντική συγκέντρωση άνθρακα στο γερμάνιο και κατά συνέπεια είναι σε συμφωνία με πρόσφατες πειραματικές μελέτες. Επιπλέον, οι υπολογισμοί προσφέρουν πληροφορίες που αφορούν τη δομή, την ενέργεια και την συγκέντρωση των πιο σημαντικών συμπλεγμάτων.