Curriculum Vitae of

Priv.-Doz. Mgr. David Holec, PhD

Department of Materials Science
Montanuniversität Leoben
Franz-Josef-Straße 18
A-8700 Leoben, Austria

tel: +43 (0)3842 402 4211
e-mail: david.holec@unileoben.ac.at
website: materials.unileoben.ac.at, cms.unileoben.ac.at
orcid: 0000-0002-3516-1061

Education and academic qualifications

2016	Habilitation in the field of "Computational Materials Science" (Priv.-Doz.), Montanuniversität Leoben, AT Thesis: *First principles modelling of alloying trends*
2005–2008	PhD in Material Science, University of Cambridge, Cambridge, UK Dissertation: *"Multi-scale modelling of III-nitrides: from dislocations to the electronic structure"*
2003–2005	Mgr. (equiv. to MSc) in Physics of Condensed Matter, Masaryk University, Brno, CZ Diploma work: *"On the precipitation in NiTi based shape memory alloys"*
1999–2004	Bc. (equiv. to BSc) in Physics, Masaryk University, Brno, CZ Bachelor's project: *"On the motion of low-angle dislocation boundaries in precipitation hardened systems"*
1999–2002	Bc. (equiv. to BSc) in Mathematics, Masaryk University, Brno, CZ Bachelor's project: *"Differential geometry of curves related to a physical practice"*

Career development

2025–	Senior Scientist and Group leader "Materials Modelling Group", Dept. of Materials Science, Montanuniversität Leoben, Leoben, AT
2019–2025	Senior Lecturer and Group leader "Materials Modelling Group", Dept. of Materials Science, Montanuniversität Leoben, Leoben, AT
09–12/2018	Guest Professor, Inst. of Materials Science and Technology TU Wien, Vienna, AT
2018–2019	Visiting scientist at RWTH Aachen, DE (5 weeks)
2017–2018	Senior Lecturer and Group leader "Materials Modelling Group", Dept. of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, AT
2015–2018	Visiting scientist at the Central South University, Chagsha, CN (8 weeks)
2015–	Guest lecturer, Inst. of Materials Science and Technology, TU Wien, Vienna, AT
2013–2015	Guest researcher, Inst. of Materials Science and Technology, TU Wien, Vienna, AT
2010–2017	University assistant, Dept. of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, AT
2008–2010	Postdoctoral research fellow, Dept. of Physical Metallurgy and Materials Testing, Montanuniversität, Leoben, AT
2005–2008	Marie Curie early stage researcher, University of Cambridge, Cambridge, UK
2003–2005	Research fellow, Inst. of Physics of Materials, Academy of Sciences, Brno, CZ

2001–2003 Tutor of mathematical seminars, Faculty of Informatics, Masaryk Univ., Brno, CZ

Research activities and interests

- *ab initio* calculations of structural properties (phase stability, mechanical and thermodynamic properties), electronic structure, phase transformations
- atomistic modelling (molecular dynamics, Monte Carlo) of size effects in nanostructures;
- a multimethod/multiscale approach (from quantum to classical mechanics) to material science problems (polycrystalline and hierarchical structures); *ab initio*-powered Calphad modelling
- defect engineering, e.g. stabilisation by point defects, alloying impact on stacking faults, mobility of dislocations
- hydrogen storage
- material systems: functional coatings (nitrides, oxides, borides); steels; TiAl and related intermetallic alloys; shape memory alloys; C and Au nanostructures

Dissemination of the results (Scopus, January 2026)

peer-reviewed publication:	210
h-index:	45
citations:	6817
list of all publications:	cms.unileoben.ac.at/download/CV-David_Holec.pdf
invited conference presentations:	23

Selected projects

2026–2029 "ReCAllTubes" [FFG], project partner

2024–2027 "TOP-RHEA" (3rd party funding, Plansee SE), project leader

2023–2024 "T3Design" [FFG TakeOff], main project partner

2022–2029 "Knowledge-based Design of Advanced Steels (KnowDAS)" [CDG], area leader

2021–2024 "Additive Manufacturing of Non-Weldable Nickel-Base Superalloys: Process, Microstrucutre and Mechanical Properties" [FFG Bridge], project partner

2021–2022 "Impact of hydrogen on structural and functional properties of NiTi shape memory alloys" [OeAD-WTZ], bi-lateral mobility project with CZ, Austrian co-PI

2020–2023 "Cross-Sectional Microstructure and Stress Design of Tough Diamond Coatings" [FFG Bridge], project partner

2019–2022 "Diffusion control reducing friction of nanocomposite materials" [FWF/GAČR], international joint project with CZ, Austrian co-PI

2018–2022 "Computational-assisted Process Development and Materials Design of Novel CVD Hard Coatings (NovelCVD) " [FFG Comet], key researcher

2017–2021 "Atomistic Principles of Martensitic and Ordering Transformations in Intermetallic Alloys at Finite Temperatures (MOTIF)" [FWF], PI

2017–2020 "Impact of interfaces on mechanical properties of hard coating materials" [FWF], co-PI

2017–2020 "Erosion behaviour of composite AlCr arc cathodes" [FFG Bridge], project partner

Teaching and mentoring experience

- currently supervising 5 PhD students, 3 Master and 1 Bachelor students, all working in the field of atomistic and electronic structure calculations.

	Postdoc	*PhD*	*Master*	*Bachelor*
Finished	4 (+1 co-advised)	4 (+12 co-advised)	15	8
Ongoing	0	5 (+3 co-advised)	3	1

- teaching courses on "Dislocations and Elasticity", "Atomistic Modelling", "Solid State Physics" and "Physical Metallurgy" (Montanuniversität Leoben)
- teaching courses on "Dislocations and Elasticity", "Atomistic Materials Modelling" (TU Wien)

Professional affiliations

- Deutsche Physikalische Gesellschaft (DPG)

Most important scientific achievements

1. ASMET-Forschungspreis 2016 (Feb 2017, 300k€)
2. Theodor Körner Preis, "Understanding the response of filled carbon nanotubes to an applied external stimulus" (Apr 2011, 3k€)
3. PI and co-PI of 3 FWF projects, co-investigator of 4 FFG and 1 FWF project, principle researcher of 2 FFG-Comet projects, area leader of 1 CDL, PI and co-PI of 5 OeAD-WTZ projects
4. editor for Elsevier journal Results in Surfaces and Interfaces
5. reviewer for Phys. Rev. B, Phys. Rev. Lett, Acta Mat., Sci. Rep., Vacuum, Comp. Mat. Sci., Surf. Coat. Technol., Thin Films, J. Phys. D: Appl. Phys, J. Appl. Phys, J. Phys: Cond. Matter, Appl. Lett., Mat. Sci. Eng., Phil. Mag. and other journals
6. session/symposium organiser at ICMCTF (International Conference on Metallurgical Coatings and Thin Films), CA, USA (2012–2014, 2018, 2020–2022, 2024–2025); MSE Congress (Materials Science and Engineering), Darmstadt, DE (2022); Euromat, Graz, AT (2021), ECCOMAS (European Congress on Computational Methods in Applied Sciences and Engineering), Vienna (2012); Austrian-German Workshop on Computational Materials Design, Kirchdorf, AT (2012, 2015, 2018, 2024), International Conference on Multiscale Materials Modeling (2024)
7. member of International Advisory Board of conference on Materials Structure & Micromechanics Of Fracture, Brno, CZ (2019, 2022); 4th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina, Sarajevo, BH (2022)
8. PhD reviewer/examiner at Montanuniversität Leoben, TU Wien (AT), University of Vienna (AT), University of Graz (AT), Brno University of Technology (CZ), University of Cambridge (UK), Université Paris 13 (FR)
9. proposal reviewer for ANR (FR), DFG (DE), OeAD (AT), DoE (US), NCN (PL)

5 selected most relevant recent publications

1. D. Gehringer, M. Friák, and D. Holec. Models of configurationally-complex alloys made simple. *Comput. Phys. Commun.*, 286:108664, 2023. doi: 10.1016/j.cpc.2023.108664
2. N. Abdoshahi, M. Dehghani, A. V. Ruban, M. Friák, M. Šob, J. Spitaler, and D. Holec. On the energetics of the cubic-to-hexagonal transformations in TiAl+Mo alloys. *Acta Mater.*, 240: 118268, 2022. doi: 10.1016/j.actamat.2022.118268

3. M. Dehghani, A. V. Ruban, N. Abdoshahi, D. Holec, and J. Spitaler. Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. *Comput. Mater. Sci.*, 205:111163, 2022. doi: 10.1016/j.commatsci.2021.111163

4. N. Abdoshahi, M. Dehghani, L. Hatzenbichler, P. Spoerk-Erdely, A. V. Ruban, M. Musi, S. Mayer, J. Spitaler, and D. Holec. Structural stability and mechanical properties of TiAl+Mo alloys: A comprehensive ab initio study. *Acta Mater.*, 221:117427, 2021. doi: 10.1016/j.actamat.2021.117427

5. O. Schneeweiss, M. Friák, M. Dudová, D. Holec, M. Šob, D. Kriegner, V. Holý, P. Beran, E. P. George, J. Neugebauer, and A. Dlouhý. Magnetic properties of the CrMnFeCoNi high-entropy alloy. *Phys. Rev. B Condens. Matter*, 96(1):014437, 2017. doi: 10.1103/PhysRevB.96.014437

Publications

Peer-reviewed publications

1. Y. W. Sun, T. Leiner, D. Gehringer, C. J. Humphreys, D. J. Dunstan, and D. Holec. Atmospheric water and graphite lubrication: Insights into surface intercalation and nanoscale confined spaces. *Phys. Rev. Mater.*, 10(3):034002, 2026. doi: 10.1103/5z9j-qrhh
2. B. Han, J. Wang, M. Matas, D. Zhang, Y. Jia, Y. Du, and D. Holec. First-principles study of ti-decorated graphene-based single-atom catalyst for MgH_2 dehydrogenation. *Int. J. Hydrogen Energy*, 207(153379):153379, 2026. doi: 10.1016/j.ijhydene.2026.153379
3. J. L. Neves, T. Wojcik, D. Obersteiner, J. Grillitsch, D. Holec, D. Kiener, and T. Klein. Wire-arc directed energy deposition of metastable-β alloy ti-15 V-3Cr-3Sn-3Al using thick wire feedstock: Microstructure and mechanical response. *Mater. Des.*, 259(114757):114757, 2025. doi: 10.1016/j.matdes.2025.114757
4. P. Ondračka, P. Kümmerl, M. Hans, S. Mráz, D. Primetzhofer, D. Holec, P. Vašina, and J. M. Schneider. Prediction and identification of point defect fingerprints in X-ray photoelectron spectra of TiN with $1.18 \leq x \leq 1.37$. *Mater. Des.*, 259(114752):114752, 2025. doi: 10.1016/j.matdes.2025.114752
5. S. Lin, D. Holec, D. G. Sangiovanni, T. Leiner, L. Hultman, P. H. Mayrhofer, and N. Koutná. Shear-activated phase transformations of diborides via machine-learning potential molecular dynamics. *Acta Mater.*, 301(121606):121606, 2025. doi: 10.1016/j.actamat.2025.121606
6. A. Reiners-Sakic, A. Reichmann, C. Dösinger, L. Romaner, and D. Holec. Interstitials as a key ingredient for P segregation to grain boundaries in polycrystalline α-fe. *Scr. Mater.*, 268 (116864):116864, 2025. doi: 10.1016/j.scriptamat.2025.116864
7. T. Klein, J. L. Neves, D. Obersteiner, J. Grillitsch, and D. Holec. Microstructure and deformation behavior of the wire-arc directed energy deposited high-performance near-β ti-10V-2Fe-3Al alloy. *Mater. Sci. Eng. A Struct. Mater.*, 943(148825):148825, 2025. doi: 10.1016/j.msea.2025.148825
8. M. Seyffertitz, C. J. Balhatchet, M. V. Rauscher, S. Stock, G. Fritz-Popovski, T. Leiner, D. Holec, H. Amenitsch, A. C. Forse, and O. Paris. Selective anion anchoring in MOF-based supercapacitors revealed with operando small-angle X-ray scattering. *Nat. Commun.*, 16(1):8649, 2025. doi: 10.1038/s41467-025-63772-w
9. V. Kundrat, L. Houben, J. Zalesak, D. Holec, I. Pinkas, and R. Tenne. Core–shell WS_2@WTe_2/$MoTe_2$ nanotubes. *Small Struct.*, (2500258):2500258, 2025. doi: 10.1002/sstr.202500258
10. D. Holec, J. Grillitsch, J. L. Neves, D. Obersteiner, and T. Klein. Ab initio modeling of TWIP and TRIP effects in β-ti alloys. *J. Mater. Res.*, 2025. doi: 10.1557/s43578-025-01657-w
11. T. Pogrielz, P. Kunnas, T. Hönigmann, M. Eichinger, J. Todt, A. Weiser, A. Dlouhy, D. Brandl, G. Ressel, G. Mori, D. Holec, J. Keckes, and A. Hohenwarter. Impact of microstructural variations on hydrogen permeation into duplex steel. *Materialia*, 42(102475):102475, 2025. doi: 10.1016/j.mtla.2025.102475
12. T. Leiner and D. Holec. Revealing trends in catalytic activity of adatoms for hydrogen adsorption on carbon: A case study of graphene and carbon nanotube. *Carbon Trends*, 20(100535):100535, 2025. doi: 10.1016/j.cartre.2025.100535
13. F. F. Klimashin, M. Učík, M. Matas, D. Holec, M. Beutner, M. Hackert-Oschätzchen, A. Xomalis, J. J. Schwiedrzik, J. Klusoň, M. Jílek, A. Lümkemann, J. Michler, and T. E. J. Edwards. Su-

perstoichiometric (al,cr)N: Nitrogen's whereabouts and role in structure-property relationships. *Acta Mater.*, 294(121158):121158, 2025. doi: 10.1016/j.actamat.2025.121158

14. D. Gehringer, L. Romaner, and D. Holec. Segregation to grain boundaries in disordered systems: an application to a ni-based multi-component alloy. *Mater. Des.*, 254(114074):114074, 2025. doi: 10.1016/j.matdes.2025.114074

15. M. Friák, P. Čípek, P. Roupcová, O. Schneeweiss, J. Pavlů, D. Fink, Š. Msallamová, D. Holec, and A. Michalcová. Impact of thermal vibrations on the stability of the $FeSn_2$ intermetallics. *Intermetallics*, 182(108755):108755, 2025. doi: 10.1016/j.intermet.2025.108755

16. C. Gutschka, L. Zauner, T. Glechner, D. Holec, and H. Riedl. Metastable AlB_2 structured TM-si-B2±z (TM = ti, zr, hf) solid solutions from first-principles. *Acta Mater.*, 289(120857):120857, 2025. doi: 10.1016/j.actamat.2025.120857

17. L. Hatzenbichler, C. Vincely, P. Haslberger, M. Galler, O. Glushko, D. Holec, H. Clemens, and R. Schnitzer. Effect of tramp elements on the microstructural evolution of a ferritic-pearlitic steel. *Prakt. Metallogr.*, 62(3):148–175, 2025. doi: 10.1515/pm-2025-0010

18. G. K. Nayak, P. Srinivasan, J. Todt, R. Daniel, P. Nicolini, and D. Holec. Accurate prediction of structural and mechanical properties on amorphous materials enabled through machine-learning potentials: A case study of silicon nitride. *Comput. Mater. Sci.*, 249(113629):113629, 2025. doi: 10.1016/j.commatsci.2024.113629

19. Y. Huang, Z. Chen, M. Meindlhumer, R. Hahn, D. Holec, T. Leiner, V. Maier-Kiener, Y. Zheng, Z. Zhang, L. Hatzenbichler, H. Riedl, C. Mitterer, and Z. Zhang. Harvesting superior intrinsic plasticity in nitride ceramics with negative stacking fault energy. *Acta Mater.*, (120774):120774, 2025. doi: 10.1016/j.actamat.2025.120774

20. M. Matas, P. H. Mayrhofer, and D. Holec. Magnetic moments in CrN-based systems are robust: An ab initio study of alloys and superlattices. *Surf. Coat. Technol.*, 496(131540):131540, 2025. doi: 10.1016/j.surfcoat.2024.131540

21. A. Weiser, J. Todt, J. Holcova, T. Zalezak, A. M. Paulik, D. Holec, M. Jary, O. Zobac, J. Mrazek, J. Frenzel, J. Keckes, and A. Dlouhy. Hydrogen penetration into the NiTi superelastic alloy investigated in-situ by synchrotron diffraction experiments. *Acta Mater.*, 277(120217):120217, 2024. doi: 10.1016/j.actamat.2024.120217

22. A. Sakic, R. Schnitzer, and D. Holec. Interplay between alloying and tramp element effects on temper embrittlement in bcc iron: DFT and thermodynamic insights. *Acta Mater.*, 275:120044, 2024. doi: 10.1016/j.actamat.2024.120044

23. N. Schalk, Y. Moritz, G. K. Nayak, D. Holec, C. Hugenschmidt, V. V. Burwitz, L. Mathes, M. Schiester, C. Saringer, C. Czettl, M. Pohler, C. Mitterer, and M. Tkadletz. Nanocomposite versus solid solution formation in the TiSiN system. *Acta Mater.*, 275:120063, 2024. doi: 10.1016/j.actamat.2024.120063

24. P. H. Mayrhofer, L. Zhou, and D. Holec. Influence of Sc, Y, Ti, Zr, Hf, V, Nb, and Ta on structural and mechanical properties of Cr-Al-N coatings. *Berg Huttenmann. Monatsh.*, 169(7):375–380, 2024. doi: 10.1007/s00501-024-01481-5

25. U. Pototschnig, M. Matas, D. Scheiblehner, D. Neuschitzer, R. Obenaus-Emler, H. Antrekowitsch, and D. Holec. Predictive model for catalytic methane pyrolysis. *J. Phys. Chem. C*, 128(22):9034–9040, 2024. doi: 10.1021/acs.jpcc.4c01690

26. D.-L. Zhang, J. Wang, Q. Wu, Y. Du, and D. Holec. Ab initio study of oxygen vacancy filament formation at Ta/HfO_2 interface. *Surfaces and Interfaces*, 49:104418, 2024. doi: 10.1016/j.surfin.2024.104418

27. M. Friák, P. Čípek, J. Pavlů, O. Zobač, P. Roupcová, I. Miháliková, D. Holec, Š. Msallamová, and A. Michalcová. Structure–property relations in Pb-supersaturated metastable Sn-rich Pb-Sn alloys. *Metall. Mater. Trans. A*, 55(6):1867–1877, 2024. doi: 10.1007/s11661-024-07362-3

28. J. Ženíšek, P. Souček, P. Ondračka, Z. Czigány, V. Buršíková, D. Holec, K. Balázsi, and P. Vašina. Effect of nb incorporation in Mo_2BC coatings on structural and mechanical properties — ab initio modelling and experiment. *Acta Mater.*, 268(119741):119741, 2024. doi: 10.1016/j.actamat.2024.119741

29. R. Roy, D. Holec, L. Michal, D. Hemzal, S. Sarkar, G. S. Kumar, D. Nečas, M. Dhankhar, P. Kaushik, J. Gomez, and L. Zajickova. Possible charge ordering and anomalous transport in graphene/graphene quantum dotheterostructure. *J. Phys. Condens. Matter*, 2024. doi: 10.1088/1361-648X/ad31bf

30. I. Spacil, D. Gehringer, D. Holec, M. Albu, and J. Li. Elucidating effects of eu and P on solidification and precipitation of Al-7Si-0.3Mg based alloys refined by ta and TiB_2. *J. Alloys Compd.*, 978:173343, 2024. doi: 10.1016/j.jallcom.2023.173343

31. V. Kundrat, K. Bukvisova, L. Novak, L. Prucha, L. Houben, J. Zalesak, A. Vukusic, D. Holec, R. Tenne, and J. Pinkas. $W_{18}O_{49}$ nanowhiskers decorating SiO_2 nanofibers: Lessons from in situ SEM/TEM growth to large scale synthesis and fundamental structural understanding. *Cryst. Growth Des.*, 2023. doi: 10.1021/acs.cgd.3c01094

32. G. Graf, M. Seyffertitz, P. Spoerk-Erdely, H. Clemens, A. Stark, L. Hatzenbichler, D. Holec, M. Burtscher, D. Kiener, X. Li, and K. Liu. On the stability of $Ti(Mn,Al)_2$ C14 laves phase in an intermetallic Ti–42Al–5Mn alloy. *Intermetallics*, 161(107962):107962, 2023. doi: 10.1016/j.intermet.2023.107962

33. T. Leiner, N. Koutná, J. Janovec, M. Zelený, P. H. Mayrhofer, and D. Holec. On energetics of allotrope transformations in transition-metal diborides via plane-by-plane shearing. *Vacuum*, 215:112329, 2023. doi: 10.1016/j.vacuum.2023.112329

34. G. K. Nayak, A. Kretschmer, P. H. Mayrhofer, and D. Holec. On correlations between local chemistry, distortions and kinetics in high entropy nitrides: An ab initio study. *Acta Mater.*, 255:118951, 2023. doi: 10.1016/j.actamat.2023.118951

35. I. Spacil, D. Holec, M. Albu, and J. Li. Revealing effects of solute ta on solidification and precipitation of Al-7Si-0.3Mg based alloys. *Materialia*, 30:101846, 2023. doi: 10.1016/j.mtla.2023.101846

36. L. Hatzenbichler, S. Zeisl, H. Clemens, and D. Holec. Phase stability of TiAl-based BCC high entropy alloys. *Intermetallics*, 158:107893, 2023. doi: 10.1016/j.intermet.2023.107893

37. D. Gehringer, L. Huber, J. Neugebauer, and D. Holec. Segregation to α_2/γ interfaces in TiAl alloys: A multiscale QM/MM study. *Phys. Rev. Mater.*, 7(6):063604, 2023. doi: 10.1103/PhysRevMaterials.7.063604

38. G. K. Nayak, D. Holec, and M. Zelený. Impact of d-states on transition metal impurity diffusion in TiN. *Sci. Rep.*, 13(1):8244, 2023. doi: 10.1038/s41598-023-34768-7

39. D. Gehringer, M. Friák, and D. Holec. Models of configurationally-complex alloys made simple. *Comput. Phys. Commun.*, 286:108664, 2023. doi: 10.1016/j.cpc.2023.108664

40. I. J. Gómez, M. V. Sulleiro, N. Pizúrová, A. Bednařík, P. Lepcio, D. Holec, J. Preisler, and L. Zajíčková. Spontaneous formation of carbon dots helps to distinguish molecular fluorophores species. *Appl. Surf. Sci.*, 610:155536, 2023. doi: 10.1016/j.apsusc.2022.155536

41. L. Michal, R. Roy, D. Holec, I. J. Gómez, N. Pizúrová, D. Nečas, A. Dolečková, J. Medalová, P. Lepcio, and L. Zajíčková. Long-Range magnetic order in nickel Hydroxide-Functionalized graphene quantum dots. *J. Phys. Chem. Lett.*, 13(49):11536–11542, 2022. doi: 10.1021/acs.jpclett.2c02964

42. M. Musi, S. Kardos, L. Hatzenbichler, D. Holec, A. Stark, M. Allen, V. Güther, H. Clemens, and P. Spoerk-Erdely. The effect of zirconium on the ti-(42-46 at.%)al system. *Acta Mater.*, 241:118414, 2022. doi: 10.1016/j.actamat.2022.118414

43. N. Abdoshahi, M. Dehghani, A. V. Ruban, M. Friák, M. Šob, J. Spitaler, and D. Holec. On the energetics of the cubic-to-hexagonal transformations in TiAl+Mo alloys. *Acta Mater.*, 240:118268, 2022. doi: 10.1016/j.actamat.2022.118268

44. A. Sakic, C. Hofer, R. Schnitzer, and D. Holec. Ab initio study of alloying impact on the stability of cementite in transformation-induced plasticity-assisted advanced steels. *Adv. Eng. Mater.*, page 2200532, 2022. doi: 10.1002/adem.202200532

45. J. Li, X. Zhou, A. Breen, Z. Peng, J. Su, P. Kürnsteiner, M. J. D. Correa, M. L. Chwałek, H. Wang, D. Holec, J. Mayer, and G. Dehm. Elucidation of formation and transformation mechanisms of ca-rich laves phase in Mg-Al-Ca-Mn alloys. *J. Alloys Compd.*, 928:167177, 2022. doi: 10.1016/j.jallcom.2022.167177

46. M. Meindlhumer, T. Ziegelwanger, J. Zalesak, M. Hans, L. Löfler, S. Spor, N. Jäger, A. Stark, H. Hruby, R. Daniel, D. Holec, J. M. Schneider, C. Mitterer, and J. Keckes. Precipitation-based grain boundary design alters inter- to trans-granular fracture in AlCrN thin films. *Acta Mater.*, 237:118156, 2022. doi: 10.1016/j.actamat.2022.118156

47. M. Hans, Z. Czigány, D. Neuß, J. A. Sälker, H. Rueß, J. Krause, G. K. Nayak, D. Holec, and J. M. Schneider. Probing the onset of wurtzite phase formation in (v, al) N thin films by transmission electron microscopy and atom probe tomography. *Surf. Coat. Technol.*, page 128235, 2022

48. R. Roy, D. Holec, M. Kratzer, P. Muenzer, P. Kaushik, L. Michal, G. S. Kumar, L. Zajíčková, and C. Teichert. Probing the charge transfer and electron-hole asymmetry in graphene-graphene quantum dot heterostructure. *Nanotechnology*, 33(32), 2022. doi: 10.1088/1361-6528/ac6c38

49. J. Buchinger, N. Koutná, A. Kirnbauer, D. Holec, and P. H. Mayrhofer. Heavy-element-alloying for toughness enhancement of hard nitrides on the example Ti-W-N. *Acta Mater.*, page 117897, 2022

50. Y. W. Sun, D. Holec, D. Gehringer, L. Li, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Graphene on silicon: Effects of the silicon surface orientation on the work function and carrier density of graphene. *Phys. Rev. B Condens. Matter*, 105(16):165416, 2022. doi: 10.1103/PhysRevB.105.165416

51. P. Ondračka, M. Hans, D. M. Holzapfel, D. Primetzhofer, D. Holec, and J. M. Schneider. Ab initio-guided X-ray photoelectron spectroscopy quantification of Ti vacancies in $Ti_{1-\delta}O_xN_{1-x}$ thin films. *Acta Mater.*, 230(117778):117778, 2022. doi: 10.1016/j.actamat.2022.117778

52. N. Koutná, L. Löfler, D. Holec, Z. Chen, Z. Zhang, L. Hultman, P. H. Mayrhofer, and D. G. Sangiovanni. Atomistic mechanisms underlying plasticity and crack growth in ceramics: a case study of AlN/TiN superlattices. *Acta Mater.*, page 117809, 2022. doi: 10.1016/j.actamat.2022.117809

53. J. Ženíšek, P. Ondračka, J. Čechal, P. Souček, D. Holec, and P. Vašina. W 4f electron binding energies in amorphous W-B-C systems. *Appl. Surf. Sci.*, 586:152824, 2022. doi: 10.1016/j.apsusc.2022.152824

54. F. Schmid, D. Gehringer, T. Kremmer, L. Cattini, P. J. Uggowitzer, D. Holec, and S. Pogatscher. Stabilization of Al_3Zr allotropes in dilute aluminum alloys via the addition of ternary elements. *Materialia*, 21:101321, 2022. doi: 10.1016/j.mtla.2022.101321

55. M. Dehghani, A. V. Ruban, N. Abdoshahi, D. Holec, and J. Spitaler. Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. *Comput. Mater. Sci.*, 205:111163, 2022. doi: 10.1016/j.commatsci.2021.111163

56. M. Tkadletz, N. Schalk, A. Lechner, L. Hatzenbichler, D. Holec, C. Hofer, M. Deluca, B. Sartory, A. Lyapin, J. Julin, and C. Czettl. Influence of B content on microstructure, phase composition and mechanical properties of CVD Ti(B,N) coatings. *Materialia*, 21:101323, 2022. doi: 10.1016/j.mtla.2022.101323

57. A. Kretschmer, D. Holec, K. Yalamanchili, H. Rudigier, M. Hans, J. M. Schneider, and P. H. Mayrhofer. Strain-stabilized al-containing high-entropy sublattice nitrides. *Acta Mater.*, 224:117483, 2022. doi: 10.1016/j.actamat.2021.117483

58. Y. W. Sun, D. Gehringer, D. Holec, D. G. Papageorgiou, O. Fenwick, S. M. Qureshi, C. J. Humphreys, and D. J. Dunstan. Significant interlayer coupling in bilayer graphene and double-walled carbon nanotubes: A refinement of obtaining strain in low-dimensional materials. *Phys. Rev. B Condens. Matter*, 105(2):024103, 2022. doi: 10.1103/PhysRevB.105.024103

59. N. Abdoshahi, M. Dehghani, L. Hatzenbichler, P. Spoerk-Erdely, A. V. Ruban, M. Musi, S. Mayer, J. Spitaler, and D. Holec. Structural stability and mechanical properties of TiAl+Mo alloys: A comprehensive ab initio study. *Acta Mater.*, 221:117427, 2021. doi: 10.1016/j.actamat.2021.117427

60. D. Holec, N. Abdoshahi, D. Gehringer, L. Hatzenbichler, A. Sakic, and H. Clemens. Electrons meet alloy development: a γ-TiAl-based alloys showcase. *Adv. Eng. Mater.*, 2021. doi: 10.1002/adem.202100977

61. L. Löfler, R. Hahn, P. H. Mayrhofer, M. Bartosik, and D. Holec. Mechanical properties of CrN-based superlattices: Impact of magnetism. *Acta Mater.*, 218:117095, 2021. doi: 10.1016/j.actamat.2021.117095

62. D. M. Holzapfel, Music, Denis, M. Hans, S. Wolff-Goodrich, D. Holec, D. Bogdanovski, M. Arndt, A. O. Eriksson, K. Yalamanchili, D. Primetzhofer, C. H. Liebscher, and J. M. Schneider. Enhanced thermal stability of (Ti,Al)N coatings by oxygen incorporation. *Acta Mater.*, 218:117204, 2021. doi: 10.1016/j.actamat.2021.117204

63. G. K. Nayak, M. N. Popov, and D. Holec. Pressure- and temperature-dependent diffusion from first-principles: A case study of V and ti in a TiN matrix. *Surf. Coat. Technol.*, 422:127491, 2021. doi: 10.1016/j.surfcoat.2021.127491

64. Z. Chen, Y. Zheng, L. Löfler, M. Bartosik, G. K. Nayak, O. Renk, D. Holec, P. H. Mayrhofer, and Z. Zhang. Atomic insights on intermixing of nanoscale nitride multilayer triggered by nanoindentation. *Acta Mater.*, 214:117004, 2021. doi: 10.1016/j.actamat.2021.117004

65. Z. Zhang, A. Ghasemi, N. Koutná, Z. Xu, T. Grünstäudl, K. Song, D. Holec, Y. He, P. H. Mayrhofer, and M. Bartosik. Correlating point defects with mechanical properties in nanocrystalline TiN thin films. *Mater. Des.*, 207:109844, 2021. doi: 10.1016/j.matdes.2021.109844

66. D. Holec, L. Löfler, G. A. Zickler, D. Vollath, and F. D. Fischer. Surface stress of gold nanoparticles revisited. *Int. J. Solids Struct.*, 224:111044, 2021. doi: 10.1016/j.ijsolstr.2021.111044

67. Y. W. Sun, D. Holec, D. Gehringer, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Erratum: Unexpected softness of bilayer graphene and softening of A-A stacked graphene layers [phys. rev. B 101, 125421 (2020)]. *Phys. Rev. B Condens. Matter*, 103(11):119901, 2021. doi: 10.1103/PhysRevB.103.119901

68. A. Wagner, D. Holec, P. H. Mayrhofer, and M. Bartosik. Enhanced fracture toughness in ceramic superlattice thin films: On the role of coherency stresses and misfit dislocations. *Materials and Design*, 202, 2021. doi: 10.1016/j.matdes.2021.109517

69. Z. Chen, Y. Zheng, L. Löfler, M. Bartosik, H. Sheng, C. Gammer, D. Holec, and Z. Zhang. Real-time atomic-resolution observation of coherent twin boundary migration in CrN. *Acta Mater.*, 208:116732, 2021. doi: 10.1016/j.actamat.2021.116732

70. F. F. Klimashin, L. Lobmaier, N. Koutná, D. Holec, and P. H. Mayrhofer. The MoN–TaN system: Role of vacancies in phase stability and mechanical properties. *Mater. Des.*, 202:109568, 2021. doi: 10.1016/j.matdes.2021.109568

71. N. Koutná, A. Brenner, D. Holec, and P. H. Mayrhofer. High-throughput first-principles search for ceramic superlattices with improved ductility and fracture resistance. *Acta Mater.*, 206: 116615, 2021. doi: 10.1016/j.actamat.2020.116615

72. J. Buchinger, A. Wagner, Z. Chen, Z. L. Zhang, D. Holec, P. H. Mayrhofer, and M. Bartosik. Fracture toughness trends of modulus-matched TiN/(Cr,Al)N thin film superlattices. *Acta Mater.*, 202:376–386, 2021. doi: 10.1016/j.actamat.2020.10.068

73. N. Abdoshahi, P. Spoerk-Erdely, M. Friák, S. Mayer, M. Šob, and D. Holec. Ab initio study of chemical disorder as an effective stabilizing mechanism of bcc-based TiAl+Mo. *Phys. Rev. Materials*, 4(10):103604, 2020. doi: 10.1103/PhysRevMaterials.4.103604

74. J. Buchinger, L. Löfler, J. Ast, A. Wagner, Z. Chen, J. Michler, Z. L. Zhang, P. H. Mayrhofer, D. Holec, and M. Bartosik. Fracture properties of thin film TiN at elevated temperatures. *Mater. Des.*, 194:108885, 2020. doi: 10.1016/j.matdes.2020.108885

75. F. Anğay, L. Löfler, F. Tetard, D. Eyidi, P. Djemia, D. Holec, and G. Abadias. Structure, stress, and mechanical properties of Mo-Al-N thin films deposited by dc reactive magnetron cosputtering: Role of point defects. *J. Vac. Sci. Technol. A*, 38(5):053401, 2020. doi: 10.1116/6.0000292

76. R. Hahn, N. Koutná, T. Wójcik, A. Davydok, S. Kolozsvári, C. Krywka, D. Holec, M. Bartosik, and P. H. Mayrhofer. Mechanistic study of superlattice-enabled high toughness and hardness in MoN/TaN coatings. *Communications Materials*, 1(1):62, 2020. doi: 10.1038/s43246-020-00064-4

77. Z. Zhang, Z. Chen, D. Holec, C. H. Liebscher, N. Koutná, M. Bartosik, Y. Zheng, G. Dehm, and P. H. Mayrhofer. Mapping the mechanical properties in nitride coatings at the nanometer scale. *Acta Mater.*, 2020. doi: 10.1016/j.actamat.2020.04.024

78. F. Moitzi, D. Şopu, D. Holec, D. Perera, N. Mousseau, and J. Eckert. Chemical bonding effects on the brittle-to-ductile transition in metallic glasses. *Acta Mater.*, 188:273–281, 2020. doi: 10.1016/j.actamat.2020.02.002

79. P. Ondračka, D. Nečas, M. Carette, S. Elisabeth, D. Holec, A. Granier, A. Goullet, L. Zajíčková, and M. Richard-Plouet. Unravelling local environments in mixed TiO_2–SiO_2 thin films by XPS and ab initio calculations. *Appl. Surf. Sci.*, 510:145056, 2020. doi: 10.1016/j.apsusc.2019.145056

80. J. Svoboda, D. Holec, M. Popov, G. A. Zickler, and F. D. Fischer. Modelling of short-range ordering kinetics in dilute multicomponent substitutional solid solutions. *Philos. Mag.*, pages 1–20, 2020. doi: 10.1080/14786435.2020.1750097

81. M. N. Popov, T. Dengg, D. Gehringer, and D. Holec. Adsorption of H_2 on Penta-Octa-Penta graphene: Grand canonical monte carlo study. *C — Journal of Carbon Research*, 6(2):20, 2020. doi: 10.3390/c6020020

82. D. Gehringer, T. Dengg, M. N. Popov, and D. Holec. Interactions between a H_2 molecule and carbon nanostructures: A DFT study. *C — Journal of Carbon Research*, 6(1):16, 2020. doi: 10.3390/c6010016

83. Y. W. Sun, D. Holec, D. Gehringer, O. Fenwick, D. J. Dunstan, and C. J. Humphreys. Unexpected softness of bilayer graphene and softening of A-A stacked graphene layers. *Phys. Rev. B Condens. Matter*, 101(12):125421, 2020. doi: 10.1103/PhysRevB.101.125421

84. D. Holec, P. Dumitraschkewitz, D. Vollath, and F. D. Fischer. Surface energy of au nanoparticles depending on their size and shape. *Nanomaterials (Basel)*, 10(3):484, 2020. doi: 10.3390/nano10030484

85. S. Mirzaei, M. Alishahi, P. Souček, J. Ženíšek, D. Holec, N. Koutná, V. Buršíková, M. Stupavská, L. Zábranský, F. Burmeister, B. Blug, Z. Czigány, K. Balázsi, R. Mikšová, and P. Vašina. The effect of chemical composition on the structure, chemistry and mechanical properties of magnetron sputtered W-B-C coatings: Modeling and experiments. *Surf. Coat. Technol.*, 383: 125274, 2020. doi: 10.1016/j.surfcoat.2019.125274

86. M. Friák, D. Lago, N. Koutná, D. Holec, T. Rebok, and M. Šob. Multi-phase ELAStic aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. *Comput. Phys. Commun.*, 247:106863, 2020. doi: 10.1016/j.cpc.2019.106863

87. N. Koutná, R. Hahn, J. Zálešák, M. Friák, M. Bartosik, J. Keckes, M. Šob, P. H. Mayrhofer, and D. Holec. Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. *Mater. Des.*, 186:108211, 2020. doi: 10.1016/j.matdes.2019.108211

88. F. Guo, D. Holec, J. Wang, S. Li, and Y. Du. Impact of v, hf and si on oxidation processes in Ti–Al–N: Insights from ab initio molecular dynamics. *Surf. Coat. Technol.*, 381:125125, 2020. doi: 10.1016/j.surfcoat.2019.125125

89. S. Zöhrer, M. Golizadeh, N. Koutná, D. Holec, A. Anders, and R. Franz. Erosion and cathodic arc plasma of Nb–Al cathodes: composite versus intermetallic. *Plasma Sources Sci. Technol.*, 29 (2):025022, 2020. doi: 10.1088/1361-6595/ab5e32

90. M. Friák, M. Golian, D. Holec, N. Koutná, and M. Šob. An ab initio study of magnetism in disordered Fe-Al alloys with thermal antiphase boundaries. *Nanomaterials (Basel)*, 10(1), 2019. doi: 10.3390/nano10010044

91. M. Zelený, M. Heczko, J. Janovec, D. Holec, L. Straka, and O. Heczko. The effect of local arrangement of excess mn on phase stability in Ni–Mn–Ga martensite: An ab initio study. *Shape Memory and Superelasticity*, 2019. doi: 10.1007/s40830-019-00247-0

92. T. Glechner, R. Hahn, T. Wojcik, D. Holec, S. Kolozsvári, H. Zaid, S. Kodambaka, P. H. Mayrhofer, and H. Riedl. Assessment of ductile character in superhard Ta-C-N thin films. *Acta Mater.*, 179:17–25, 2019. doi: 10.1016/j.actamat.2019.08.015

93. M. Friák, V. Buršíková, N. Pizúrová, J. Pavlů, Y. Jirásková, V. Homola, I. Miháliková, A. Slávik, D. Holec, M. Všianská, N. Koutná, J. Fikar, D. Janičkovič, M. Šob, and J. Neugebauer. Elasticity

of phases in Fe-Al-Ti superalloys: Impact of atomic order and Anti-Phase boundaries. *Crystals*, 9(6):299, 2019. doi: 10.3390/cryst9060299

94. I. Miháliková, M. Friák, N. Koutná, D. Holec, and M. Šob. An ab initio study of vacancies in disordered magnetic systems: A case study of Fe-Rich Fe-Al phases. *Materials*, 12(9), 2019. doi: 10.3390/ma12091430

95. J. Buchinger, N. Koutná, Z. Chen, Z. Zhang, P. H. Mayrhofer, D. Holec, and M. Bartosik. Toughness enhancement in TiN/WN superlattice thin films. *Acta Mater.*, 172:18–29, 2019. doi: 10.1016/j.actamat.2019.04.028

96. D. Holec, N. Abdoshahi, S. Mayer, and H. Clemens. Thermal expansion and other thermodynamic properties of α_2-Ti_3Al and γ-TiAl intermetallic phases from first principles methods. *Materials*, 12(8), 2019. doi: 10.3390/ma12081292

97. N. Koutná, P. Erdely, S. Zöhrer, R. Franz, Y. Du, S. Liu, P. H. Mayrhofer, and D. Holec. Experimental chemistry and structural stability of $AlNb_3$ enabled by antisite defects formation. *Materials*, 12(7):1104, 2019. doi: 10.3390/ma12071104

98. N. Koutná, P. Řehák, Z. Chen, M. Bartosik, M. Fallmann, M. Černý, Z. Zhang, M. Friák, M. Šob, P. H. Mayrhofer, and D. Holec. Correlating structural and mechanical properties of AlN/TiN superlattice films. *Scr. Mater.*, 165:159–163, 2019. doi: 10.1016/j.scriptamat.2019.02.021

99. Z. Chen, D. Holec, M. Bartosik, P. H. Mayrhofer, and Z. Zhang. Crystallographic orientation dependent maximum layer thickness of cubic AlN in CrN/AlN multilayers. *Acta Mater.*, 168: 190–202, 2019. doi: 10.1016/j.actamat.2019.02.004

100. F. Guo, J. Wang, Y. Du, D. Holec, P. Ou, H. Zhou, L. Chen, and Y. Kong. Structural evolution of oxygen on the surface of TiAlN: Ab initio molecular dynamics simulations. *Appl. Surf. Sci.*, 470:520–525, 2019. doi: 10.1016/j.apsusc.2018.11.158

101. I. Miháliková, M. Friák, Y. Jirásková, D. Holec, N. Koutná, and M. Šob. Impact of Nano-Scale distribution of atoms on electronic and magnetic properties of phases in Fe-Al nanocomposites: An ab initio study. *Nanomaterials (Basel)*, 8(12), 2018. doi: 10.3390/nano8121059

102. M. Friák, D. Holec, and M. Šob. Quantum-Mechanical study of nanocomposites with low and Ultra-Low interface energies. *Nanomaterials (Basel)*, 8(12), 2018. doi: 10.3390/nano8121057

103. M. Friák, P. Kroupa, D. Holec, and M. Šob. An ab initio study of Pressure-Induced reversal of elastically stiff and soft directions in YN and ScN and its effect in nanocomposites containing these nitrides. *Nanomaterials (Basel)*, 8(12), 2018. doi: 10.3390/nano8121049

104. T. Glechner, P. H. Mayrhofer, D. Holec, S. Fritze, E. Lewin, V. Paneta, D. Primetzhofer, S. Kolozsvári, and H. Riedl. Tuning structure and mechanical properties of Ta-C coatings by N-alloying and vacancy population. *Sci. Rep.*, 8(1):17669, 2018. doi: 10.1038/s41598-018-35870-x

105. M. Friák, M. Zelený, M. Všianská, D. Holec, and M. Šob. An ab initio study of connections between tensorial elastic properties and chemical bonds in $\Sigma5(210)$ grain boundaries in Ni3Si. *Materials*, 11(11):2263, 2018. doi: 10.3390/ma11112263

106. P. Šesták, M. Friák, D. Holec, M. Všianská, and M. Šob. Strength and brittleness of interfaces in Fe-Al superalloy nanocomposites under multiaxial loading: An ab initio and atomistic study. *Nanomaterials*, 8(11), 2018. doi: 10.3390/nano8110873

107. N. Ghafoor, I. Petrov, D. Holec, G. Greczynski, J. Palisaitis, P. O. A. Persson, L. Hultman, and J. Birch. Self-structuring in $Zr_{1-x}Al_xN$ films as a function of composition and growth temperature. *Sci. Rep.*, 8(1):16327, 2018. doi: 10.1038/s41598-018-34279-w

108. R. Schnitzer, C. Hofer, S. Mayer, M. Panzenböck, D. Holec, and H. Clemens. Multi-Scale microstructural characterization. *Pract. Metallogr.*, 55(9):584–602, 2018. doi: 10.3139/147.110531

109. M. Friák, S. Oweisová, J. Pavlů, D. Holec, and M. Šob. An ab initio study of thermodynamic and mechanical stability of Heusler-Based Fe_2AlCo polymorphs. *Materials*, 11(9):1543, 2018. doi: 10.3390/ma11091543

110. D. Vollath, F. D. Fischer, and D. Holec. Surface energy of nanoparticles – influence of particle size and structure. *Beilstein J. Nanotechnol.*, 9:2265–2276, 2018. doi: 10.3762/bjnano.9.211

111. D. Holec, N. Kostoglou, C. Tampaxis, B. Babic, C. Mitterer, and C. Rebholz. Theory-guided metal-decoration of nanoporous carbon for hydrogen storage applications. *Surf. Coat. Technol.*, 351:42–49, 2018. doi: 10.1016/j.surfcoat.2018.07.025

112. V. Moraes, H. Riedl, C. Fuger, P. Polcik, H. Bolvardi, D. Holec, and P. H. Mayrhofer. Ab initio inspired design of ternary boride thin films. *Sci. Rep.*, 8(1):9288, 2018. doi: 10.1038/s41598-018-27426-w

113. Y. W. Sun, D. Holec, Y. Xu, and D. J. Dunstan. Graphite under compression: shift of layer breathing and shear modes frequencies with interlayer spacing. *J. Phys. Commun.*, 2(4):045004, 2018. doi: 10.1088/2399-6528/aab5ea

114. H. Riedl, T. Glechner, T. Wojcik, N. Koutná, S. Kolozsvári, V. Paneta, D. Holec, D. Primetzhofer, and P. H. Mayrhofer. Influence of carbon deficiency on phase formation and thermal stability of super-hard TaC_y thin films. *Scr. Mater.*, 149:150–154, 2018. doi: 10.1016/j.scriptamat.2018.02.030

115. M. Friák, D. Holec, and M. Šob. An ab initio study of mechanical and dynamical stability of $MoSi_2$. *J. Alloys Compd.*, 746:720–728, 2018. doi: 10.1016/j.jallcom.2018.01.241

116. T. Klein, D. Holec, H. Clemens, and S. Mayer. Pathways of phase transformation in β-phase-stabilized σ/γ-TiAl alloys subjected to two-step heat treatments. *Scr. Mater.*, 149:112, 2018. doi: 10.1016/j.scriptamat.2018.02.009

117. N. Koutná, D. Holec, M. Friák, P. H. Mayrhofer, and M. Šob. Stability and elasticity of metastable solid solutions and superlattices in the MoN–TaN system: First-principles calculations. *Mater. Des.*, 144:310–322, 2018. doi: 10.1016/j.matdes.2018.02.033

118. B. Bergk, U. Mühle, I. Povstugar, N. Koutná, D. Holec, H. Clemens, and B. Kieback. Non-equilibrium solid solution of molybdenum and sodium: Atomic scale experimental and first principles studies. *Acta Mater.*, 144(Supplement C):700–706, 2018. doi: 10.1016/j.actamat.2017.11.006

119. P. Dumitraschkewitz, H. Clemens, S. Mayer, and D. Holec. Impact of alloying on stacking fault energies in γ-TiAl. *Appl. Sci.*, 7(11):1193, 2017. doi: 10.3390/app7111193

120. D. Vollath, D. Holec, and F. D. Fischer. Au_{55} , a stable glassy cluster: results of ab initio calculations. *Beilstein J. Nanotechnol.*, 8:2221–2229, 2017. doi: 10.3762/bjnano.8.222

121. K. Leitner (née Babinsky), P. J. Felfer, D. Holec, J. Cairney, W. Knabl, A. Lorich, H. Clemens, and S. Primig. On grain boundary segregation in molybdenum materials. *Mater. Des.*, 135: 204–212, 2017. doi: 10.1016/j.matdes.2017.09.019

122. F. Pacher, P. H. Mayrhofer, and D. Holec. Vacancy-driven extended stability of cubic metastable Ta-Al-N and Nb-Al-N phases. *Surf. Coat. Technol.*, 326:37–44, 2017. doi: 10.1016/j.surfcoat.2017.07.012

123. O. Schneeweiss, M. Friák, M. Dudová, D. Holec, M. Šob, D. Kriegner, V. Holý, P. Beran, E. P. George, J. Neugebauer, and A. Dlouhý. Magnetic properties of the CrMnFeCoNi high-entropy alloy. *Phys. Rev. B Condens. Matter*, 96(1):014437, 2017. doi: 10.1103/PhysRevB.96.014437

124. M. Friák, M. Všianská, D. Holec, and M. Šob. Quantum-mechanical study of tensorial elastic and high-temperature thermodynamic properties of grain boundary states in superalloy-phase Ni3Al. *IOP Conf. Ser.: Mater. Sci. Eng.*, 219(1):012019, 2017. doi: 10.1088/1757-899X/219/1/012019

125. P. Řehák, M. Černý, and D. Holec. Interface-induced electronic structure toughening of nitride superlattices. *Surf. Coat. Technol.*, 325:410–416, 2017. doi: 10.1016/j.surfcoat.2017.06.065

126. Y. X. Xu, H. Riedl, D. Holec, L. Chen, Y. Du, and P. H. Mayrhofer. Thermal stability and oxidation resistance of sputtered TiAlCrN hard coatings. *Surf. Coat. Technol.*, 324:48–56, 2017. doi: 10.1016/j.surfcoat.2017.05.053

127. D. Holec, F. D. Fischer, and D. Vollath. Structure and surface energy of Au_{55} nanoparticles: An ab initio study. *Comput. Mater. Sci.*, 134:137–144, 2017

128. J. Zalesak, D. Holec, I. Matko, M. Petrenec, B. Sartory, N. Koutná, R. Daniel, R. Pitonak, and J. Keckes. Peculiarity of self-assembled cubic nanolamellae in the TiN/AlN system: Epitaxial self-stabilization by element deficiency/excess. *Acta Mater.*, 131:391–399, 2017

129. P. Ondračka, D. Holec, D. Nečas, E. Kedroňová, S. Elisabeth, A. Goullet, and L. Zajíčková. Optical properties of $Ti_xSi_{1-x}O_2$ solid solutions. *Phys. Rev. B Condens. Matter*, 95(19):195163, 2017. doi: 10.1103/PhysRevB.95.195163

130. Z. Zhang, X. Gu, D. Holec, M. Bartosik, P. H. Mayrhofer, and H. P. Duan. Superlattice-induced oscillations of interplanar distances and strain effects in the CrN/AlN system. *Phys. Rev. B Condens. Matter*, 95(15):155305, 2017. doi: 10.1103/PhysRevB.95.155305

131. F. Wang, D. Holec, M. Odén, F. Mücklich, I. A. Abrikosov, and F. Tasnádi. Systematic ab initio investigation of the elastic modulus in quaternary transition metal nitride alloys and their coherent multilayers. *Acta Mater.*, 127:124–132, 2017. doi: 10.1016/j.actamat.2017.01.017

132. D. Holec, L. Zhou, H. Riedl, C. M. Koller, P. H. Mayrhofer, M. Friák, M. Šob, F. Körmann, J. Neugebauer, D. Music, M. A. Hartmann, and F. D. Fischer. Atomistic Modeling-Based design of novel materials. *Adv. Eng. Mater.*, 19(4):1600688, 2017. doi: 10.1002/adem.201600688

133. S. Mayer, P. Erdely, F. D. Fischer, D. Holec, M. Kastenhuber, T. Klein, and H. Clemens. Intermetallic β-Solidifying γ-TiAl based alloys – from fundamental research to application. *Adv. Eng. Mater.*, 19(4):1600735, 2017. doi: 10.1002/adem.201600735

134. H. Lasfargues, T. Glechner, C. M. Koller, V. Paneta, D. Primetzhofer, S. Kolozsvári, D. Holec, H. Riedl, and P. H. Mayrhofer. Non-reactively sputtered ultra-high temperature Hf-C and Ta-C coatings. *Surf. Coat. Technol.*, 309:436–444, 2017. doi: 10.1016/j.surfcoat.2016.11.073

135. M. Bartosik, D. Holec, D. Apel, M. Klaus, C. Genzel, J. Keckes, M. Arndt, P. Polcik, C. M. Koller, and P. H. Mayrhofer. Thermal expansion of Ti-Al-N and Cr-Al-N coatings. *Scr. Mater.*, 127:182–185, 2017. doi: 10.1016/j.scriptamat.2016.09.022

136. T. Klein, M. Schachermayer, D. Holec, B. Rashkova, H. Clemens, and S. Mayer. Impact of Mo on the ω_o phase in β-solidifying TiAl alloys: An experimental and computational approach. *Intermetallics*, 85:26–33, 2017. doi: 10.1016/j.intermet.2017.01.011

137. M. Friák, M. Všianská, D. Holec, M. Zelený, and M. Šob. Tensorial elastic properties and stability of interface states associated with $\Sigma5(210)$ grain boundaries in $Ni_3(Al,Si)$. *Sci. Technol. Adv. Mater.*, 18(1):273–282, 2017. doi: 10.1080/14686996.2017.1312519

138. D. Holec, J. Paulitsch, and P. H. Mayrhofer. First principles study of water-based self-assembled nanobearing effect in CrN/TiN multilayer coatings. *SSP*, 258:373–378, 2016. doi: 10.4028/www.scientific.net/SSP.258.373

139. F. F. Klimashin, N. Koutná, H. Euchner, D. Holec, and P. H. Mayrhofer. The impact of nitrogen content and vacancies on structure and mechanical properties of Mo–N thin films. *J. Appl. Phys.*, 120(18):185301, 2016. doi: 10.1063/1.4966664

140. N. Schalk, J. F. T. Simonet Fotso, D. Holec, G. Jakopic, A. Fian, V. L. Terziyska, R. Daniel, and C. Mitterer. Influence of varying nitrogen partial pressures on microstructure, mechanical and optical properties of sputtered TiAlON coatings. *Acta Mater.*, 119:26–34, 2016. doi: 10.1016/j.actamat.2016.08.007

141. P. Ondračka, D. Holec, D. Nečas, and L. Zajíčková. Accurate prediction of band gaps and optical properties of HfO_2. *J. Phys. D Appl. Phys.*, 49(39):395301, 2016. doi: 10.1088/0022-3727/49/39/395301

142. L. Zhou, F. F. Klimashin, D. Holec, and P. H. Mayrhofer. Structural and mechanical properties of nitrogen-deficient cubic Cr–Mo–N and Cr–W–N systems. *Scr. Mater.*, 123:34–37, 2016. doi: 10.1016/j.scriptamat.2016.05.036

143. Q. Long, J. Wang, Y. Du, D. Holec, X. Nie, and Z. Jin. Predicting an alloying strategy for improving fracture toughness of C15 $NbCr_2$ laves phase: A first-principles study. *Comput. Mater. Sci.*, 123:59–64, 2016. doi: 10.1016/j.commatsci.2016.06.009

144. N. Koutná, D. Holec, O. Svoboda, F. F. Klimashin, and P. H. Mayrhofer. Point defects stabilise cubic Mo-N and Ta-N. *J. Phys. D Appl. Phys.*, 49(37):375303, 2016. doi: 10.1088/0022-3727/49/37/375303

145. D. Holec, R. K. Reddy, T. Klein, and H. Clemens. Preferential site occupancy of alloying elements in TiAl-based phases. *J. Appl. Phys.*, 119(20):205104, 2016. doi: 10.1063/1.4951009

146. T. Klein, B. Rashkova, D. Holec, H. Clemens, and S. Mayer. Silicon distribution and silicide precipitation during annealing in an advanced multi-phase γ-TiAl based alloy. *Acta Mater.*, 110:236–245, 2016. doi: 10.1016/j.actamat.2016.03.050

147. R. Hollerweger, L. Zhou, D. Holec, C. M. Koller, R. Rachbauer, P. Polcik, and P. H. Mayrhofer. Controlling microstructure, preferred orientation, and mechanical properties of Cr-Al-N by bombardment and alloying with ta. *J. Appl. Phys.*, 119(6):065304, 2016. doi: 10.1063/1.4941533

148. C. M. Koller, N. Koutná, J. Ramm, S. Kolozsvári, J. Paulitsch, D. Holec, and P. H. Mayrhofer. First principles studies on the impact of point defects on the phase stability of $(Al_xCr_{1-x})_2O_3$ solid solutions. *AIP Adv.*, 6(2):025002, 2016. doi: 10.1063/1.4941573

149. N. Schalk, J. F. T. Simonet Fotso, D. Holec, A. Fian, G. Jakopic, V. L. Terziyska, R. Daniel, and C. Mitterer. Microstructure, mechanical and optical properties of TiAlON coatings sputter-deposited with varying oxygen partial pressures. *J. Phys. D Appl. Phys.*, 49(2):025307, 2016. doi: 10.1088/0022-3727/49/2/025307

150. D. Lang, C. Pöhl, D. Holec, J. Schatte, E. Povoden-Karadeniz, W. Knabl, H. Clemens, and S. Primig. On the chemistry of the carbides in a molybdenum base Mo-Hf-C alloy produced by powder metallurgy. *J. Alloys Compd.*, 654:445–454, 2016. doi: 10.1016/j.jallcom.2015.09.126

151. P. Wan, Z. Zhang, D. Holec, R. Daniel, C. Mitterer, and H. Duan. Nitrogen atom shift and the structural change in chromium nitride. *Acta Mater.*, 98:119–127, 2015. doi: 10.1016/j.actamat.2015.07.019

152. H. Riedl, J. Zálešák, M. Arndt, P. Polcik, D. Holec, and P. H. Mayrhofer. Ab initio studies on the adsorption and implantation of al and fe to nitride materials. *J. Appl. Phys.*, 118(12): 125306, 2015. doi: 10.1063/1.4931665

153. Y. W. Sun, D. Holec, and D. J. Dunstan. Graphite under uniaxial compression along the *c* axis: A parameter to relate out-of-plane strain to in-plane phonon frequency. *Phys. Rev. B Condens. Matter*, 92(9):094108, 2015. doi: 10.1103/PhysRevB.92.094108

154. M. Friák, D. Tytko, D. Holec, P.-P. Choi, P. Eisenlohr, D. Raabe, and J. Neugebauer. Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases. *New J. Phys.*, 17(9):093004, 2015. doi: 10.1088/1367-2630/17/9/093004

155. M. Bartosik, M. Todt, D. Holec, J. Todt, L. Zhou, H. Riedl, H. J. Böhm, F. G. Rammerstorfer, and P. H. Mayrhofer. Thermal expansion of rock-salt cubic AlN. *Appl. Phys. Lett.*, 107(7): 071602, 2015. doi: 10.1063/1.4928911

156. A. Herz, M. Friák, D. Rossberg, M. Hentschel, F. Theska, D. Wang, D. Holec, M. Šob, O. Schneeweiss, and P. Schaaf. Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration. *Appl. Phys. Lett.*, 107(7):073109, 2015. doi: 10.1063/1.4928627

157. D. Holec, D. Legut, L. Isaeva, P. Souvatzis, H. Clemens, and S. Mayer. Interplay between effect of Mo and chemical disorder on the stability of β/β_o-TiAl phase. *Intermetallics*, 61:85–90, 2015. doi: 10.1016/j.intermet.2015.03.001

158. R. Hollerweger, D. Holec, J. Paulitsch, M. Bartosik, R. Daniel, R. Rachbauer, P. Polcik, J. Keckes, C. Krywka, H. Euchner, and P. H. Mayrhofer. Complementary ab initio and x-ray nanodiffraction studies of Ta_2O_5. *Acta Mater.*, 83(0):276–284, 2015. doi: 10.1016/j.actamat.2014.10.006

159. O. Jantschner, S. K. Field, D. Holec, A. Fian, D. Music, J. M. Schneider, K. Zorn, and C. Mitterer. Origin of temperature-induced low friction of sputtered Si-containing amorphous carbon coatings. *Acta Mater.*, 82:437–446, 2015. doi: 10.1016/j.actamat.2014.09.030

160. R. A. Coppeta, D. Holec, H. Ceric, and T. Grasser. Evaluation of dislocation energy in thin films. *Philos. Mag.*, 95(2):186–209, 2015. doi: 10.1080/14786435.2014.994573

161. M. Todt, F. Toth, M. A. Hartmann, D. Holec, M. J. Cordill, F. D. Fischer, and F. G. Rammerstorfer. Computational simulation of lnstability phenomena in nanoparticles and nanofilms. *Comp. Tech. Rev.*, 10:89–119, 2014. doi: 10.4203/ctr.10.4

162. L. Zhou, F. Körmann, D. Holec, M. Bartosik, B. Grabowski, J. Neugebauer, and P. H. Mayrhofer. Structural stability and thermodynamics of CrN magnetic phases from *ab initio* calculations and experiment. *Phys. Rev. B Condens. Matter*, 90(18):184102, 2014. doi: 10.1103/PhysRevB.90.184102

163. D. Holec, F. Tasnádi, P. Wagner, M. Friák, J. Neugebauer, P. H. Mayrhofer, and J. Keckes. Macroscopic elastic properties of textured ZrN–AlN polycrystalline aggregates: From *ab initio* calculations to grain-scale interactions. *Phys. Rev. B Condens. Matter*, 90(18):184106, 2014. doi: 10.1103/PhysRevB.90.184106

164. A. Riedl, R. Daniel, J. Todt, M. Stefenelli, D. Holec, B. Sartory, C. Krywka, M. Müller, C. Mitterer, and J. Keckes. A combinatorial x-ray sub-micron diffraction study of microstructure, residual stress and phase stability in TiAlN coatings. *Surf. Coat. Technol.*, 257(0):108–113, 2014. doi: 10.1016/j.surfcoat.2014.03.045

165. A. O. Monteiro, P. M. F. J. Costa, P. B. Cachim, and D. Holec. Buckling of ZnS-filled single-walled carbon nanotubes – the influence of aspect ratio. *Carbon*, 79(0):529–537, 2014. doi: 10.1016/j.carbon.2014.08.011

166. V. Chawla, D. Holec, and P. H. Mayrhofer. The effect of interlayer composition and thickness on the stabilization of cubic AlN in AlN/Ti–Al–N superlattices. *Thin Solid Films*, 565(0):94–100, 2014. doi: 10.1016/j.tsf.2014.06.051

167. P. H. Mayrhofer, D. Sonnleitner, M. Bartosik, and D. Holec. Structural and mechanical evolution of reactively and non-reactively sputtered Zr–Al–N thin films during annealing. *Surf. Coat. Technol.*, 244:52–56, 2014. doi: 10.1016/j.surfcoat.2014.01.049

168. D. Holec, M. Friák, A. Dlouhý, and J. Neugebauer. Ab initio study of point defects in NiTi-based alloys. *Phys. Rev. B Condens. Matter*, 89:014110, 2014. doi: 10.1103/PhysRevB.89.014110

169. G. Ressel, D. Holec, A. Fian, F. Mendez-Martin, and H. Leitner. Atomistic insights into milling mechanisms in an Fe–Y_2O_3 model alloy. *Appl. Phys. A: Mater. Sci. Process.*, 115(3):851–858, 2014. doi: 10.1007/s00339-013-7877-y

170. H. Riedl, D. Holec, R. Rachbauer, P. Polcik, R. Hollerweger, J. Paulitsch, and P. H. Mayrhofer. Phase stability, mechanical properties and thermal stability of Y alloyed Ti-Al-N coatings. *Surf. Coat. Technol.*, 235:174–180, 2013. doi: 10.1016/j.surfcoat.2013.07.030

171. S. Zhang, W. Y. Fu, D. Holec, C. J. Humphreys, and M. A. Moram. Elastic constants and critical thicknesses of ScGaN and ScAlN. *J. Appl. Phys.*, 114(24):243516, 2013. doi: 10.1063/1.4848036

172. S. Zhang, D. Holec, W. Y. Fu, C. J. Humphreys, and M. A. Moram. Tunable optoelectronic and ferroelectric properties in sc-based III-nitrides. *J. Appl. Phys.*, 114(13):133510, 2013. doi: 10.1063/1.4824179

173. V. Chawla, D. Holec, and P. H. Mayrhofer. Stabilization criteria for cubic AlN in TiN/AlN and CrN/AlN bi-layer systems. *J. Phys. D Appl. Phys.*, 46(4):045305, 2013. doi: 10.1088/0022-3727/46/4/045305

174. R. Hollerweger, D. Holec, J. Paulitsch, R. Rachbauer, P. Polcik, and P. H. Mayrhofer. Magnetic field strength influence on the reactive magnetron sputter deposition of Ta_2O_5. *J. Phys. D Appl. Phys.*, 46(33):335203, 2013. doi: 10.1088/0022-3727/46/33/335203

175. L. Zhou, D. Holec, and P. H. Mayrhofer. First-principles study of elastic properties of cubic $Cr_{1-x}Al_xN$ alloys. *J. Appl. Phys.*, 113:043511, 2013. doi: 10.1063/1.4789378

176. D. Holec, L. Zhou, R. Rachbauer, and P. H. Mayrhofer. Alloying-related trends from first principles: An application to the Ti–Al–X–N system. *J. Appl. Phys.*, 113(11):113510, 2013. doi: 10.1063/1.4795590

177. L. Zhou, D. Holec, and P. H. Mayrhofer. Ab initio study of the alloying effect of transition metals on structure, stability and ductility of CrN. *J. Phys. D Appl. Phys.*, 46(36):365301, 2013. doi: 10.1088/0022-3727/46/36/365301

178. D. Holec, M. Friák, J. Neugebauer, and P. H. Mayrhofer. Trends in the elastic response of binary early transition metal nitrides. *Phys. Rev. B Condens. Matter*, 85(6):064101, 2012. doi: 10.1103/PhysRevB.85.064101

179. M. Friák, W. A. Counts, D. Ma, B. Sander, D. Holec, D. Raabe, and J. Neugebauer. Theory-Guided materials design of Multi-Phase Ti-Nb alloys with Bone-Matching elastic properties. *Materials*, 5(12):1853–1872, 2012. doi: 10.3390/ma5101853

180. D. Holec and P. H. Mayrhofer. Surface energies of AlN allotropes from first principles. *Scr. Mater.*, 67:760–762, 2012. doi: 10.1016/j.scriptamat.2012.07.027

181. V. Chawla, D. Holec, and P. H. Mayrhofer. Interfacial coherency stress distribution in TiN/AlN bilayer and multilayer films studied by FEM analysis. *Comput. Mater. Sci.*, 55:211–216, 2012. doi: 10.1016/j.commatsci.2011.11.024

182. R. Rachbauer, D. Holec, and P. H. Mayrhofer. Increased thermal stability of Ti–Al–N thin films by ta alloying. *Surf. Coat. Technol.*, 211:98–103, 2012. doi: 10.1016/j.surfcoat.2011.07.009

183. A. Dick, B. Grabowski, T. Hickel, F. Liot, D. Holec, A. Schlieter, U. Ku, J. Eckert, Z. Ebrahimi, H. Emmerich, J. Neugebauer, L.-F. Zhu, M. Friák, and U. Kühn. First-principles study of the thermodynamic and elastic properties of eutectic Fe–Ti alloys. *Acta Mater.*, 60(4):1594–1602, 2012. doi: 10.1016/j.actamat.2011.11.046

184. R. Rachbauer, A. Blutmager, D. Holec, and P. H. Mayrhofer. Effect of Hf on structure and age hardening of Ti–Al–N thin film. *Surf. Coat. Technol.*, 206(10):2667–2672, 2012. doi: 10.1016/j.surfcoat.2011.11.020

185. D. Holec, R. Rachbauer, D. Kiener, P. D. Cherns, P. M. F. J. Costa, C. McAleese, P. H. Mayrhofer, and C. J. Humphreys. Towards predictive modeling of near-edge structures in electron energy-loss spectra of AlN-based ternary alloys. *Phys. Rev. B Condens. Matter*, 83(16): 165122, 2011. doi: 10.1103/PhysRevB.83.165122

186. M. Petrov, D. Holec, L. Lymperakis, J. Neugebauer, and C. J. Humphreys. Strain-induced effects on the electronic structure and N k-edge ELNES of wurtzite AlN and $Al_xGa_{1-x}N$. *J. Phys. Conf. Ser.*, 326(1):012016, 2011. doi: 10.1088/1742-6596/326/1/012016

187. R. Daniel, D. Holec, M. Bartosik, J. Keckes, and C. Mitterer. Size effect of thermal expansion and thermal/intrinsic stresses in nanostructured thin films: Experiment and model. *Acta Mater.*, 59(17):6631–6645, 2011. doi: 10.1016/j.actamat.2011.07.018

188. D. Holec, R. Rachbauer, L. Chen, L. Wang, D. Luef, and P. H. Mayrhofer. Phase stability and alloy-related trends in Ti–Al–N, Zr–Al–N and Hf–Al–N systems from first principles. *Surf. Coat. Technol.*, 206(7-5):1698–1704, 2011. doi: 10.1016/j.surfcoat.2011.09.019

189. M. Friák, T. Hickel, B. Grabowski, L. Lymperakis, A. Udyansky, A. Dick, D. Ma, F. Roters, L. F. Zhu, A. Schlieter, U. Kühn, Z. Ebrahimi, R. A. Lebensohn, D. Holec, J. Eckert, H. Emmerich, D. Raabe, and J. Neugebauer. Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. *Eur. Phys. J. Plus*, 126(10):101, 2011. doi: 10.1140/epjp/i2011-11101-2

190. L. Chen, D. Holec, Y. Du, and P. H. Mayrhofer. Influence of zr on structure, mechanical and thermal properties of Ti–Al–N. *Thin Solid Films*, 519(16):5503–5510, 2011. doi: 10.1016/j.tsf.2011.03.139

191. R. Rachbauer, D. Holec, M. Lattemann, L. Hultman, and P. H. Mayrhofer. Electronic origin of structure and mechanical properties in Y and nb alloyed Ti-Al-N thin films. *Int. J. Mater. Res.*, 102(06):735–742, 2011. doi: 10.3139/146.110520

192. R. Rachbauer, S. Massl, E. Stergar, D. Holec, D. Kiener, J. Keckes, J. Patscheider, M. Stiefel, H. Leitner, and P. H. Mayrhofer. Decomposition pathways in age hardening of Ti–Al–N films. *J. Appl. Phys.*, 110(2):23515, 2011. doi: 10.1063/1.3610451

193. M. Todt, F. G. Rammerstorfer, F. D. Fischer, P. H. Mayrhofer, D. Holec, and M. A. Hartmann. Continuum modeling of van der Waals interactions between carbon onion layers. *Carbon*, 49(5): 1620–1627, 2011. doi: 10.1016/j.carbon.2010.12.045

194. D. Holec, M. Friák, A. Dlouhý, and J. Neugebauer. Ab initio study of pressure stabilized NiTi allotropes: Pressure-induced transformations and hysteresis loops. *Phys. Rev. B Condens. Matter*, 84(22):224119, 2011. doi: 10.1103/PhysRevB.84.224119

195. D. Holec, R. Franz, P. H. Mayrhofer, and C. Mitterer. Structure and stability of phases within the NbN–AlN system. *J. Phys. D Appl. Phys.*, 43(14):145403, 2010

196. D. Holec, F. Rovere, P. H. Mayrhofer, and P. B. Barna. Pressure-dependent stability of cubic and wurtzite phases within the TiN–AlN and CrN–AlN systems. *Scr. Mater.*, 62(6):349–352, 2010. doi: 10.1016/j.scriptamat.2009.10.040

197. R. Rachbauer, D. Holec, and P. H. Mayrhofer. Phase stability and decomposition products of Ti–Al–Ta–N thin films. *Appl. Phys. Lett.*, 97(15):151901, 2010. doi: 10.1063/1.3495783

198. P. H. Mayrhofer, R. Rachbauer, and D. Holec. Influence of Nb on the phase stability of Ti–Al–N. *Scr. Mater.*, 63(8):807–810, 2010. doi: 10.1016/j.scriptamat.2010.06.020

199. S. E. Bennett, D. Holec, M. J. Kappers, C. J. Humphreys, and R. A. Oliver. Imaging dislocations in gallium nitride across broad areas using atomic force microscopy. *Rev. Sci. Instrum.*, 81(6): 063701, 2010. doi: 10.1063/1.3430539

200. D. Holec, M. A. Hartmann, F. D. Fischer, F. G. Rammerstorfer, P. H. Mayrhofer, and O. Paris. Curvature-induced excess surface energy of fullerenes: Density Functional Theory and Monte Carlo simulations. *Phys. Rev. B: Condens. Matter Mater. Phys.*, 81(23):235403, 2010. doi: 10.1103/PhysRevB.81.235403

201. B. Jiang, J. M. Zuo, D. Holec, C. J. Humphreys, M. Spackman, and J. C. H. Spence. Combined structure-factor phase measurement and theoretical calculations for mapping of chemical bonds in GaN. *Acta Crystallogr. A*, 66(Pt 4):446–450, 2010. doi: 10.1107/S0108767310008664

202. D. Holec, D. Sridhara Rao, and C. Humphreys. HANSIS software tool for the automated analysis of HOLZ lines. *Ultramicroscopy*, 109(7):837–844, 2009. doi: 10.1016/j.ultramic.2009.03.026

203. M. A. Moram, Y. Zhang, T. B. Joyce, D. Holec, P. R. Chalker, P. H. Mayrhofer, M. J. Kappers, and C. J. Humphreys. Structural properties of wurtzitelike ScGaN films grown by NH_3-molecular beam epitaxy. *J. Appl. Phys.*, 106(11):113533, 2009. doi: 10.1063/1.3268466

204. D. Holec, O. Bojda, and A. Dlouhý. Ni_4Ti_3 precipitate structures in ni-rich NiTi shape memory alloys. *Materials Science and Engineering: A*, 481–482(0):462–465, 2008. doi: 10.1016/j.msea.2006.11.182

205. D. Holec and C. J. Humphreys. Calculations of equilibrium critical thickness for non-polar wurtzite InGaN/GaN systems. *Mater. Sci. Forum*, 2008

206. D. Holec, Y. Zhang, D. V. Sridhara Rao, M. J. Kappers, C. McAleese, and C. J. Humphreys. Equilibrium critical thickness for misfit dislocations in III-nitrides. *J. Appl. Phys.*, 104(12): 123514, 2008. doi: 10.1063/1.3033553

207. D. Holec, P. M. F. J. Costa, P. D. Cherns, and C. J. Humphreys. Electron energy loss near edge structure (ELNES) spectra of AlN and AlGaN: a theoretical study using the Wien2k and Telnes programs. *Micron*, 39(6):690–697, 2008. doi: 10.1016/j.micron.2007.10.013

208. D. Holec, P. M. F. J. Costa, P. D. Cherns, and C. J. Humphreys. A theoretical study of ELNES spectra of using Wien2k and Telnes programs. *Comput. Mater. Sci.*, 44(1):91–96, 2008. doi: 10.1016/j.commatsci.2008.01.029

209. D. Holec, P. Costa, M. Kappers, and C. Humphreys. Critical thickness calculations for InGaN/GaN. *J. Cryst. Growth*, 303(1):314–317, 2007. doi: 10.1016/j.jcrysgro.2006.12.054

210. A. Dlouhý and D. Holec. Stability and motion of low angle dislocation boundaries in precipitation hardened crystals. *Mater. Sci. Forum*, 2005

211. D. Holec and A. Dlouhý. Interactions between particles and low-angle dislocation boundaries during high-temperature deformation. *Z. Metallkd.*, 96(6):558–565, 2005. doi: 10.3139/146.101070

Articles in proceedings

1. I. Spacil, D. Holec, P. Schumacher, and J. Li. Effect of solute ta on grain refinement of Al-7Si-0.3Mg based alloys. In *Semi-Solid of Alloys and Composites XVI*, volume 327, pages 54–64. Trans Tech Publications Ltd, 2022. ISBN 9783035717792. doi: 10.4028/www.scientific.net/SSP.327.54

2. I. Miháliková, A. Slávik, M. Friák, M. Všianská, N. Koutná, D. Holec, and M. Šob. First-principles study of interface energies in Fe-Al-based superalloy nanocomposites. volume 2017-October. TANGER Ltd., 2018. ISBN 9788087294819

3. B. Bergk, U. Mühle, B. Kieback, N. Koutná, D. Holec, and H. Clemens. Nanocrystalline alloys of molybdenum with sodium and yttrium obtained by mechanical alloying. In *Proceedings of Euro PM2017*, Brussels, Belgium, 2017. European Powder Metallurgy Association. ISBN 9781899072491

4. G. Ressel, P. Parz, A. Fian, D. Holec, S. Primig, W. Puff, H. Leitner, and H. Clemens. On the behavior of Yttria/Yttrium during mechanical alloying of a Fe–Y_2O_3 model alloy system. *AMRO*, 922:598–603, 2014. doi: 10.4028/www.scientific.net/AMR.922.598

5. R. A. Coppeta, H. Ceric, D. Holec, and T. Grasser. Critical thickness for GaN thin film on AlN substrate. In *Integrated Reliability Workshop Final Report (IRW), 2013 IEEE International*, pages 133–136, 2013. doi: 10.1109/IIRW.2013.6804177

6. Y. Sun, D. Dunstan, M. Hartmann, and D. Holec. Nanomechanics of carbon nanotubes. *Pammatone*, 13(1):7–10, 2013. doi: 10.1002/pamm.201310003

7. D. Holec, R. Rachbauer, D. Kiener, P. D. Cherns, P. M. F. J. Costa, P. H. Mayrhofer, and C. J. Humphreys. Modelling of electron energy near edge structures of alloys – how well can we do? 2011

8. D. V. S. Rao, K. Muraleedharan, R. Balamuralikrishnan, D. Banerjee, D. Holec, M. J. Kappers, and C. J. Humphreys. Determination of lattice parameters and composition of III-V semiconductor thin films using CBED-HOLZ technique. 2009

9. D. Holec and A. Dlouhý. Stress redistributions and their impact on the precipitation in microstructures. 2005

Book publications

1. P. Cachim, A. O. Monteiro, P. M. F. J. Costa, and D. Holec. Numerical modeling of buckling phenomenon in carbon nanotubes filled with ZnS. In S. Thomas, N. Kalarikkal, C. V. Pious, Z. Ahmad, and J. T. Haponiuk, editors, *Functionalized Engineering Materials and Their Applications*, pages 65–72. Apple Academic Press, 2018. doi: 10.1201/9781315365541-13

2. P. Ondračka, D. Holec, and L. Zajíčková. Predicting optical properties from ab initio calculations. In O. Stenzel and M. Ohlídal, editors, *Optical Characterization of Thin Solid Films*, pages 83–104. Springer International Publishing, Cham, 2018. ISBN 9783319753256. doi: 10.1007/978-3-319-75325-6_4

3. P.H. Mayrhofer, R. Rachbauer, D. Holec, F. Rovere, and J.M Schneider: "Protective Transition Metal Nitride Coatings". In *Comprehensive Materials Processing*, S. Hashmi, G.F. Batalha, C.J.V. Tyne, and B. Yilbas (eds.), Elsevier, Oxford, 2014, pp. 355–388.

4. D. Holec, L. Zhou, R. Rachbauer, and P.H. Mayrhofer: "Alloy-based design of materials from first principles: an application to functional hard coatings". In *Density Functional Theory: Principles, Applications and Analysis*, J. Morin and J.M. Pelletier (eds.), Nova Publishers, New York, 2013.

5. D. Holec: "Multi-scale modelling of III-nitrides: Selected topics from dislocations to the electronic structure". VDM Verlag Dr. Müller, 2010.

6. D. Holec: "Modelling of stresses in polycrystalline materials: The origin and redistribution of stresses in NiTi". LAP Lambert Academic Publishing, 2010.

Conference and workshop contributions
(only those presented by D. Holec; invited presentations are highlighted in bold)

1. G.K. Nayak, D. Holec, J.M. Schneider: "Vacancy-concentration-dependent thermal stability of fcc-(Ti,Al)N_x predicted via chemical-environment-sensitive diffusion activation energies" (oral). *TACT 2025 International Thin Film Conference*, Taipei, Taiwan, October 26–30, 2025.

2. **D. Holec, G.K. Nayak, P. Ondračka: "Multi-method workflow for simulating tensorial properties of amorphous thin films: case studies of a-SiN and a-WBC thin films" (invited oral). *TACT 2025 International Thin Film Conference*, Taipei, Taiwan, October 26–30, 2025.**

3. D. Holec, K. Lechner, J. Zhang, A.S. Jelinek, H. Clemens, W. Knabl, P. Spörk-Erdely, P. Wagatha: "Challenges in predicting trends of structural and mechanical properties of refractory CCAs" (oral). *Intermetallics 2025*, Kloster Banz, Germany, September 29–October 2, 2025.

4. T.Leiner, D. Holec: "Structure of nanoporous carbon for hydrogen storage: an atomistic approach" (oral). *MSMF-11 (Materials Structure & Micromechanics Of Fracture)*, Brno, Czech Republic, June 23–25, 2025.

5. D. Holec, A. Reiners-Sakic, D. Gehringer, C. Dösinger, A. Reichmann, L. Romaner: "Segregation energy spectra as a tool towards modelling real materials" (oral). *MSMF-11 (Materials Structure & Micromechanics Of Fracture)*, Brno, Czech Republic, June 23–25, 2025.

6. A. Reiners-Sakic , C. Dösinger, A. Reichmann, R. Schnitzer, L. Romaner, D. Holec: "Predicting Segregation Behaviour in Polycrystalline Materials: A Case Study of P in Fe" (oral). *ICMCTF 2025 (51th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, May 11–16, 2025.

7. M. Matas, U. Pototschnig, D. Holec: "Finding Optimal Catalysts for Methane Pyrolysis: DFT and AIMD Modelling and Simulation" (poster). *ICMCTF 2025 (51th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, May 11–16, 2025.

8. A. Reiners-Sakic , C. Dösinger, A. Reichmann, L. Romaner, D. Holec: "Segregation of P in polycrystalline Fe: Bringing atomistic predictions towards reality" (oral). *69th Metallkunde-Kolloquium*, Lech am Arlberg, Austria, April 8–10, 2025.

9. **D. Holec: "Modelling of structural phase transformations in intermetallic and related alloys" (invited oral). *MRS Fall Meeting 2024*, Boston, USA, December 1–6, 2024.**

10. D. Gehringer, L. Romaner, D. Holec: "Solute segregation in compositionally complex alloys: a test case of Σ5(210)[001] grain-boundary Ni-based CCA" (oral). *MMM11 (The 11th International Conference on Multiscale Materials Modeling)*, Prague, Czech Republic, September 24–28, 2024.

11. T. Leiner, D. Holec: "Atomistic Simulations of Hydrogen Storage in Carbon-based Materials" (oral). *ICCCEBH 2024 (5th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina)*, Sarajevo, Bosna and Herzegovina, June 17–30, 2024.

12. D. Holec, M. Matas, P.H. Mayrhofer: "Impact of TM elements on structural and mechanical properties of CrN" (oral). *ICMCTF 2024 (50th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, May 19–24, 2024.

13. D. Holec, J. Grillitsch, J. Neves, T. Klein: "Ab initio insights into compositional dependence of TWIP and TRIP barriers of Ti-alloys" (oral). *DPG Spring meeting 2014*, Berlin, Germany, March 18–22, 2024.

14. D. Holec, A.M. Paulik, A. Weiser, J. Todt, J. Holcová, J. Keckes, A. Dlouhý: "Revealing hydrogen-rich phases in NiTi shape memory alloys" (oral). *DPG Spring meeting 2014*, Berlin, Germany, March 18–22, 2024.

15. **D. Holec, L. Hatzenbichler, S. Zeisl, H. Clemens: "Predicting stability of TiAl-based BCC high entropy alloys" (invited oral). *Intermetallics 2023*, Kloster Banz, Germany, October 2–6, 2023.**

16. D. Gehringer, D. Holec, L. Huber, J. Neugebauer: "Tailoring α_2/γ and γ/γ interfaces in TiAl alloys via segregation: A multi-method study" (poster). *Intermetallics 2023*, Kloster Banz, Germany, October 2–6, 2023.

17. **D. Holec: "Modelling of phase transformations in TiAl-based alloys" (invited oral). *IWTA2023 (International Workshop on Titanium Aluminides 2023)*, Toulouse, France, June 11–16, 2023.**

18. D. Holec, N. Koutná, D. Gehringer, L. Löfler, P.H. Mayrhofer: "Designing strength of interfaces and boundaries" (oral). *MSE-2022 Materials Science & Engineering)*, Darmstadt, Germany, September 27–29, 2022.

19. **D. Holec, L. Hatzenbichler, S. Zeisl: "Ab initio predictions of thermally stable high entropy alloys" (invited oral). *MSMF-10 (Materials Structure & Micromechanics Of Fracture)*, Brno, Czech Republic, September 12–14, 2022.**

20. **D. Holec, D. Gehringer, M.N. Popov, T. Leiner: "Hydrogen adsorption on graphene-based materials" (invited oral). *ICCCEBH 2022 (4th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina)*, Sarajevo, Bosna and Herzegovina, June 30–July 2, 2022.**

21. D. Holec, T. Leiner, N. Koutná, P.H. Mayrhofer: "On the Interplay between Stacking and Stability of Transition-Metal Diborides" (oral). *ICMCTF 2022 (48th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, May 22–27, 2022.

22. D. Holec, D. Vollath, F.D. Fischer, T. Antretter: "Decoupling surface energy and surface stress using a combination of atomistic and continuum mechanics approaches" (oral). *66th Metallkunde-Kolloquium*, Lech am Arlberg, Austria, April 20–22, 2022.

23. **F. Guo, N. Koutná, T. Glechner, Y. Du, H. Riedl, P.H. Mayrhofer, D. Holec: "Insights into oxidation processes of protective coatings from AIMD modelling: a case study of TiAlN and TaC" (keynote oral).** ***SurfCoat Korea 2021, virtual, May 26–28, 2021.***

24. **D. Holec, N. Koutná, L. Löfler, L. Hatzenbichler, M. Bartosik, M. Friák, M. Černý, P.H. Mayrhofer: "Weakest Links in Superlattices: Insights from Ab Initio Modelling" (invited oral).** ***ICMCTF 2021 (47th International Conference on Metallurgical Coatings & Thin Films)*****, virtual, April 26–30, 2021.**

25. **D. Holec, N. Koutná, P. Řehák, Z. Chen, J. Zálešák, R. Hahn, M. Bartosik, M. Friák, M. Černý, J. Keckes, Z. Zhang, M. Šob, P.H. Mayrhofer: "Structure and mechanical properties of nitride superlattices: insights and predictions from modelling corroborated by experiment" (invited oral).** ***APMC 2020 (12th Asia-Pacific Microscopy Conference*****, Hyderabad, India, February 3–7, 2020.**

26. D. Holec, N. Abdoshahi, M. Dehghani, A.V. Ruban, M. Friák, M. Šob, J. Spitaler: "Impact of Mo and disorder on diffusion-less transformations in TiAl intermetallic alloys" (oral). *Intermetallics 2019*, Kloster Banz, Germany, September 30–October 4, 2019.

27. D. Holec, D. Gehringer, F. Schmid, S. Pogatscher: "Alloying impact on phase stability in $ZrAl_3$" (poster). *Intermetallics 2019*, Kloster Banz, Germany, September 30–October 4, 2019.

28. D. Holec, N. Abdoshahi, M. Dehghani, A.V. Ruban, M. Friák, M. Šob, J. Spitaler: "Impact of Mo and disorder on diffusion-less transformations in TiAl intermetallic alloys" (oral). *TCDM 2019 (Theory of Complex Disorder in Materials*, Linköping, Sweden, September 16–18, 2019.

29. L. Hatzenbichler, R. Daniel, J. Zálešák, W. Baumegger, J. Keckes, D. Holec: "Metallic superlattices with naturally sharp interfaces: a case study of immiscible Ti–Ta system" (oral). *MSMF-9 (Materials Structure & Micromechanics Of Fracture)*, Brno, Czech Republic, June 26–28, 2019.

30. N. Koutná, R. Hahn, J. Buchinger, J. Zálešák, M. Friák, J. Keckes, M. Šob, P.H. Mayrhofer, D. Holec: "Vacancies are essential for stabilising metastable nitrides with exceptional properties" (oral). *E-MRS Spring meeting 2019*, Nice, France, May 27–31, 2019.

31. N. Koutná, R. Hahn, J. Zálešák, M. Friák, M. Bartosik, J. Keckes, M. Šob, P.H. Mayrhofer, D. Holec: "Vacancy-controlled design of MoN/TaN superlattices" (oral). *DPG Spring meeting 2019*, Regensburg, Germany, April 1–5, 2019.

32. D. Holec, F.D. Fischer, D. Vollath: "Structure and surface energies of nanoparticles: Insights from atomistic simulations" (oral). *DPG Spring meeting 2019*, Regensburg, Germany, April 1–5, 2019.

33. N. Abdoshahi, M. Friák, M. Šob, D. Holec: "Ab initio study of tetragonal and trigonal bcc-fcc transformations in Ti-Al-Mo system $\beta/\beta_o \rightarrow \gamma$-TiAl phase transformations" (oral). *DPG Spring meeting 2019*, Regensburg, Germany, April 1–5, 2019.

34. **D. Holec, N. Koutná, F. Pacher, M. Friák, M. Šob, P.H. Mayrhofer: "Point-defect engineering of thin film materials: Insights from modelling" (invited oral). *SSC 2018 (Solid State Chemistry*, Pardubice, Czech Republic, September 17–21, 2018.**

35. **D. Holec, N. Abdoshahi, M. Dehghani, S. Mayer, A. Ruban, J. Spitaler: "Stability and ordering in the Ti–Al–Mo system: What happens at the atomic scale?" (invited oral). *Thermec 2018*, Paris, France, July 9–13, 2018.**

36. **D. Holec, N. Koutná, M. Všianská, M. Friák, P.H. Mayrhofer, M. Šob: "Elasticity of interfaces: a multi-method approach" (invited poster). *Thermec 2018*, Paris, France, July 9–13, 2018.**

37. L. Hatzenbichler, D. Holec: "Metallic superlattices: A case study of immiscible Ti–Ta system" (oral). *2nd Workshop on Mechanical Properties of Interfaces*, Leoben, Austria, May 29, 2018.

38. D. Holec, N. Koutná, K. Preininger, S. Zöhrer, R. Franz: "First principles study of the Nb–Al intermetallic systems: Modelling meets experimental reality" (oral). *ICMCTF 2018 (45th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 23–27, 2018.

39. N. Koutná, R. Hahn, J. Zálešák, M. Friák, M. Bartosik, M. Šob, J. Keckes, P.H. Mayrhofer, D. Holec: "MoN/TaN superlattices: from a computer design to a realisation" (poster). *ICMCTF 2018 (45th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 23–27, 2018.

40. **D. Holec, T. Klein, F.F. Klimashin, L. Zhou, S. Mayer, P.H. Mayrhofer, H. Clemens: "Bridging length-scales: From modelling atoms to understanding real microstructures" (invited oral). *64. Metallkundekolloquium*, Lech am Arlberg, Austria, April 9–11, 2018.**

41. D. Holec, T. Klein Ch. Turk, S. Mayer, S. Primig,H. Clemens: "Partitioning of Elements in Multi-Phase Alloys: Modelling vs. Experiment" (oral). *3rd AT-DE Workshop on Complex Landscapes*, Kirchdorf in Tirol, Austria, January 15–19, 2018.

42. D. Holec, T. Klein Ch. Turk, S. Mayer, S. Primig,H. Clemens: "Partitioning of Elements in Multi-Phase Alloys: Modelling vs. Experiment" (oral). *Intermetallics 2017*, Kloster Banz, Germany, October 2–6, 2017.

43. N. Koutná, D. Holec, M. Friák, P.H. Mayrhofer, M. Šob: "Peculiarities of stability and elasticity in the MoN–TaN quasi-binary system" (oral). *EUROMAT 2017*, Thessaloniki, Greece, September 18–22, 2017.

44. D. Holec, F. Pacher, N. Koutná, C.M. Koller, P.H. Mayrhofer: "Role of point defects for predicting phase stability: A case study of Ta-Al-N and Nb-Al-N systems" (highlight oral). *EUROMAT 2017*, Thessaloniki, Greece, September 18–22, 2017.

45. D. Holec, M. Friák, Z. Zhang, M. Bartosik, P.H. Mayrhofer: "Mechanical and structural stability properties of CrN/AlN superlattices" (poster). *ICMCTF 2017 (44th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–28, 2017.

46. D. Holec, N. Koutná, F.F. Klimashin, P.H. Mayrhofer: "Stabilisation of cubic MoN and TaN systems: The role of point defects" (oral). *ICMCTF 2017 (44th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–28, 2017.

47. D. Holec, V. Moraes, M. Arndt, P. Polcik, P.H. Mayrhofer: "On the search for novel borides: High throughput modelling" (oral). *DPG Spring Meeting 2017*, Dresden, Germany, March 20–24, 2017.

48. D. Holec, P. Řehák, M. Černý: "Interface induced electronic structure toughening of nitride bilayers and superlattices" (oral). *MSE-2016 (Materials Science & Engineering)*, Darmstadt, Germany, September 27–29, 2016.

49. D. Holec, M. Friák, M. Všianská, D. Tytko, D. Raabe, M. Šob, J. Neugebauer: "Multiscale approach for predicting mechanical properties of interfaces" (oral). *MSE-2016 (Materials Science & Engineering)*, Darmstadt, Germany, September 27–29, 2016.

50. **D. Holec: "Application of first principles methods in developments of novel intermetallic alloys" (invited oral). *IWTA2016 (5^{th} International Workshop on Titanium Aluminides)*, Tokyo, Japan, August 28– September 2, 2016.**

51. **D. Holec: "Surface adsorption phenomena from first principles" (invited oral). *MSMF-8 (Materials Structure & Micromechanics Of Fracture)*, Brno, Czech Republic, June 27–29, 2016.**

52. D. Holec, P. Dumitraschkewitz, F.D. Fischer, D. Vollath: "Size-dependent surface energies of Au nanoparticles" (oral). *62. Metallkundekolloquium*, Lech am Arlberg, Austria, April 11–13, 2016.

53. **D. Holec: "Phase stability of nitride and oxide solid solutions" (invited oral). *ESTADSM (Electronic Structure Theory for the Accelerated Design of Structural Materials)*, Moscow, Russia, October 26–30, 2015.**

54. P. Dumitraschkewitz, H. Clemens, S. Mayer, and D. Holec: "*Ab initio* study on stacking faults in γ-TiAl" (poster). *Intermetallics*, Kloster Banz, Germany, September 28–October 2, 2015.

55. P. Řehák and D. Holec: "Interface induced electronic structure toughening of nitride bilayers and superlattices" (oral). *ICSMA-17 (17th International Conference on the Strength of Materials)*, Brno, Czech Republic, August 9–14, 2015.

56. **D. Holec: "Surface adsorption phenomena from first principles" (invited oral). *ICMCTF 2015 (42nd International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 20–24, 2015.**

57. D. Holec, P. Ondračka, D. Franta, E. Kedroňová, S. Elisabeth, A. Goullet, and L. Zajíčková: "Compositional variations of electronic and optical properties of Si-doped titanium dioxide" (oral). *MRS Fall Meeting* 2014, Boston, USA, November 30–December 4, 2014.

58. D. Holec, D. Legut, H. Clemens, and S. Mayer: "First principles study on the impact of chemical disorder and Mo alloying on stability of the cubic β/β_o phase in TiAl" (oral). *MRS Fall Meeting* 2014, Boston, USA, November 30–December 4, 2014.

59. D. Holec, J. Keckes, P.H. Mayrhofer: "Impact of a thin film texture on mechanical properties" (oral). *Materials Science and Engineering (MSE)*, Darmstadt, Germany, September 23–25, 2014.

60. D. Holec,T. Schmölzer, D. Legut, P. Staron, H. Clemens: "Thermal properties of Ti-Al alloys: A combined theoretical and experimental approach" (poster). *Materials Science and Engineering (MSE)*, Darmstadt, Germany, September 23–25, 2014.

61. D. Holec, L. Zhou, and P.H. Mayrhofer: "Predictive power of electron energy loss spectra modelled by first principles " (oral). *ICMCTF 2014 (41st International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 28–May 2, 2014.

62. S. Zhang, D. Holec, W.Y. Fu, C.J. Humphreys, P.H. Mayrhofer, and M.A. Moram: "Ab initio evaluation of the potential use of Sc-based III-nitrides in optoelectronics" (poster). *ICMCTF 2014 (41st International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 28–May 2, 2014.

63. **D. Holec: "What does a bunch of atoms reveal about behaviour of real materials?" (invited oral). *60. Metallkunde-Jubiläumskolloquium*, Lech am Arlberg, Austria, April 23–25, 2014.**

64. **D. Holec, M. Friák, A. Dlouhý, and J. Neugebauer: "Point defects in NiTi-based alloys" (invited oral). *The Czech-Japanese Workshop on High- Temperature Intermetallics*, Brno, Czech Republic, April 13–16, 2014.**

65. L. Zhou, D. Holec, M. Bartosik, F. Körmann, B. Grabowski, J. Neugebauer, and P.H. Mayrhofer: "Structural stability and thermodynamics of CrN magnetic phases from first principles" (poster). *ViCoM workshop (From Electrons to Phase Transitions)*, Vienna, Austria, February 26–28, 2014.

66. **D. Holec: "Alloying trends from first principles – A case study of ternary and multinary nitrides" (invited oral). *Nanotek 2013*, Las Vegas, USA, December 2–4, 2013.**

67. D. Holec, D. Legut, S. Mayer, and H. Clemens: "Interplay between chemical disorder and Mo content on mechanical stability of cubic body centred TiAl phase" (oral). *Intermetallics 2013*, Kloster Banz, Germany, September 30–October 4, 2013.

68. D. Holec, J. Keckes, P. Wagner, F. Tasnádi, M. Friák, J. Neugebauer, and P.H. Mayrhofer: "Texture dependent elastic constants of polycrystalline Zr–Al–N predicted by *ab initio* calculations" (oral). *ICMCTF 2013 (40th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 29–May 3, 2013.

69. D. Holec, L. Zhou, R. Rachbauer, and P.H. Mayrhofer: "First principles study of alloying trends in Ti–Al–N and Cr–Al–N systems" (poster). *ICMCTF 2013 (40th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 29–May 3, 2013.

70. D. Holec: "Texture influence on elastic constants of nitride alloys – A multiscale approach" (oral). *Max-Planck-Institut für Eisenforschung*, Düsseldorf, Germany, March 27, 2013.

71. **D. Holec, M. Hartmann, O. Paris, and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes; A multi-method density functional theory and monte carlo study" (invited oral). *84th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM)*, Novi Sad, Serbia, March 18–22, 2013.**

72. D. Holec, L. Zhou, R. Rachbauer, and P.H. Mayrhofer: "Alloying trends in Ti–Al–N and Cr–Al–N hard coatings" (oral). *Special Symposium on Simlation Activities at Montanuniversität*, Leoben, Austria, January 15, 2013.

73. **D. Holec: "Alloying Trends from First Principles: How Well Can We Do?" (invited oral). *Materials between Scientific Fields*, Brno, Czech Republic, November 15–16, 2012.**

74. D. Holec, R. Rachbauer, L. Zhou and P.H. Mayrhofer: "Calculational study of alloying effects in Ti–Al–N-based protective hard coatings" (oral). *ECCOMAS 2012 (6th European Congress on Computational Methods in Applied Sciences and Engineering)*, Vienna, Austria, September 10–14, 2012.

75. D. Holec, R. Rachbauer, L. Zhou and P.H. Mayrhofer: "Computer aided understanding and design of protective hard coatings by alloying" (oral). *ECNF 2012 (European Conference on Nanofilms)*, Ancona, Italy, June 17–22, 2012.

76. D. Holec and P.H. Mayrhofer: "Do nitride alloys exhibit Vegard's-like linear behaviour?" (oral). *ICMCTF 2012 (39th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–27, 2012.

77. D. Holec P. Wagner, M. Friák, and P.H. Mayrhofer: "Elasticity in binary and ternary transition metal nitrides" (poster). *ICMCTF 2012 (39th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 24–27, 2012.

78. D. Holec, M. Hartmann, M. Todt, F.D. Fischer, F.G. Rammerstorfer, D. Vollath and P.H. Mayrhofer: "Size-dependent surface properties of nanoparticles: An atomistic study" (oral). *58. Metallkunde-Kolloquium*, Lech am Arlberg, Austria, April 16–18 2012.

79. D. Holec: "Computer-aided modelling ranging from quantum, via atomistic to continuum level is used to support and interpret experimental observations, as well as to explore new basic-research areas" (poster). *WerWasWo*, Leoben, Austria, March 12–23, 2012.

80. D. Holec, M. Friák, A. Dlouhý and J. Neugebauer: "Ab initio study of pressure-induced structural transitions in NiTi: The unexpected appearance of hysteresis" (oral). *1st Austrian-German Workshop on Computational Materials Design*, Kramsach, Austria, January 24–26 2012.

    D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Modelling of electron energy loss near edge structures of alloys" (oral). *Max Planck Institut für Eisenforschung.* Düsseldorf, Germany, November 29, 2011.

81. D. Holec, P. Wagner and P.H. Mayrhofer: "Elasticity in binary and ternary transition metal nitrides" (poster). *Euromat 2011*, Montpellier, France, September 12–16 2011.

82. D. Holec, M. Friák, A. Dlouhý and J. Neugebauer: "Ab initio study of pressure-induced structural transitions in NiTi" (oral). *Euromat 2011*, Montpellier, France, September 12–16 2011.

83. **D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Modelling of electron energy near edge structures of alloys – How well can we do?" (invited oral). *International Conference on Electron Nanoscopy*, Hyderabad, India, July 6–8 2011.**

84. D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Electron energy loss near edge structures of AlN-based ternary thin films" (oral). *E-MRS Spring Meering*, Nice, France, May 9–13, 2011.

85. D. Holec, R. Rachbauer, L. Chen, L. Wang, D. Luef and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *E-MRS Spring Meering*, Nice, France, May 9–13, 2011.

86. D. Holec, R. Rachbauer, and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *SIMNET Symposium*, Graz, Austria,May 2, 2011.

87. D. Holec, M.A. Hartmann, O. Paris and P.H. Mayrhofer: "Structure, surface energy and stability of carbon fullerenes" (poster). *ISSC-18 (Interdisciplinary Surface Science Conference)*, Warwick, United Kingdom, April 1–4, 2011.

88. R. Rachbauer, D. Holec, M. Lattemann, L. Hultman and P.H. Mayrhofer: "Electronic origin of structure and mechanical properties in Y and Nb alloyed Ti–Al–N thin films" (poster). *ISSC-18 (Interdisciplinary Surface Science Conference)*, Warwick, United Kingdom, April 1–4, 2011.

89. D. Holec, R. Rachbauer, D. Kiener, P.D. Cherns, P.M.F.J. Costa, P.H. Mayrhofer and C.J. Humphreys: "Towards reliable modelling of ELNES of $Al_xGa_{1-x}N$ and other AlN based ternary alloys" (poster). *MSM-XVII (Microscopy of Semiconducting Materials)*, Cambridge, United Kingdom, April 1–4, 2011.

90. D. Holec: "Structural and electronic properties of alloys" (oral). *Seminar at the University of Linköping.* Linköping, Sweden, October 27, 2010.

91. D. Holec, M. Hartmann, O. Paris and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *27th Max Born Symposium on Multiscale Modeling of Real Materials*, Wroclaw, Poland, September 18–20, 2010.

92. D. Holec, M. Hartmann, O. Paris and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

93. D. Holec, R. Rachbauer and P.H. Mayrhofer: "Phase stability and electronic structure of Ti-Al-N, Zr-Al-N and Hf-Al-N" (oral). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

94. D. Holec, R. Rachbauer, D. Kiener, P.H. Mayrhofer and C.J. Humphreys: "Towards reliable modelling of electron energy loss near edge structure of ternary alloys" (poster). *MSMF-6 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 28–30, 2010.

95. D. Holec, M. Hartmann, F.G. Rammerstorfer, O. Paris, F.D. Fischer and P.H. Mayrhofer: "Surface energy of carbon fullerenes and nanotubes" (oral). *ICMCTF 2010 (37th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 26–30, 2010.

96. D. Holec, F. Rovere, P.H. Mayrhofer and P. Barna: "Pressure dependent stability of cubic and wurtzite phases within the TiN-AlN and CrN-AlN systems" (poster). *ICMCTF 2010 (37th International Conference on Metallurgical Coatings & Thin Films)*, San Diego, USA, April 26–30, 2010.

97. D. Holec, R. Franz, M.A. Moram and P.H. Mayrhofer: "The Bk phase: a new player on the stage (Phase stability of ternary nitrides)" (oral). *4th Surface Engineering Workshop Leoben–Aaachen*, Aachen, Germany, March 15–16, 2010.

98. D. Holec, R. Franz, P.H. Mayrhofer and C. Mitterer: "Phase stability and electronic structure of the Ti-Al-N and Nb-Al-N pseudo-binary systems" (oral). *CMMP09 (Condensed Matter and Materials Physics 2009)*, Warwick, UK, December 15–17, 2009.

99. D. Holec, P.H. Mayrhofer and C.J. Humphreys: "Ab inito calculations of electron energy loss near edge structure of ternary alloys" (poster). *CMMP09 (Condensed Matter and Materials Physics 2009)*, Warwick, UK, December 15–17, 2009.

100. D. Holec and P.H. Mayrhofer: "First principles studies on Ti-Al-N and Nb-Al-N" (oral). *Euromat 2009*, Glasgow, UK, September 7–10, 2009.

101. D. Holec, M. Petrov, L. Lymperakis, C.J. Humphreys and J. Neugebauer: "Theoretical study of strain effects on ELNES and electronic structure of AlGaN" (poster). *MRS Fall meeting 2008*, Boston, USA, December 1–5, 2008.

102. D. Holec and C.J. Humphreys: "Ab initio calculations of electron energy loss near edge structure of ternary alloys: III-nitrides" (oral). *SP-SSM 2008 (International Symposium on Structure-Property Relationships in Solid State Materials)*, Nantes, France, June 29–July 3, 2008.

103. D. Holec and C.J. Humphreys: "Ab initio calculations of electron energy loss near edge structure of ternary alloys: AlGaN" (poster). *TMCS workshop (Theory, Modelling and Computational Methods for Semiconductor Materials and Nanostructures)*, Manchester, UK, January 31–February 1, 2008.

104. D. Holec and C.J. Humphreys: "Modelling of threading dislocations reduction in GaN" (oral). *UKNC meeting*, Glasgow, UK, January 9–10, 2008.

105. D. Holec and C.J. Humphreys: "A theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes" (poster). *Autumn School on Materials Science and Electron Microscopy 2007*, Berlin, Germany, October 8–11, 2007.

106. D. Holec and C.J. Humphreys: "Modelling of threading dislocations reduction in GaN" (oral). *Euromat 2007*, Nürnberg, Germany, September 10–13, 2007.

107. D. Holec, P.M.F.J. Costa, P.D. Cherns and C.J. Humphreys: "Detailed theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes programs" (poster). *Wien2k workshop*, Singapore, July 6–9, 2007.

108. D. Holec, P.M.F.J. Costa, P.D. Cherns and C.J. Humphreys: "Detailed theoretical study of ELNES spectra of $Al_xGa_{1-x}N$ using Wien2k and Telnes programs" (oral). *ICMAT 2007 (International Conference on Materials for Advanced Technologies)*, Singapore, July 1–6, 2007.

109. D. Holec and C.J. Humphreys: "Critical thickness calculations for non-polar InGaN/GaN systems" (oral). *MSMF-5 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 27–29, 2007.

110. D. Holec and C.J. Humphreys: "On properties of dislocations in wurtzite materials" (oral). *Workshop on Nitride based nanostructures*, Berlin, Germany, February 6–8, 2007.

111. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Critical thickness calculations for $In_xGa_{1-x}N$/GaN" (oral). *EW3NS (European Workshop on III-Nitride Semiconductor Materials and Devices)*, Heraklion, Crete, Greece, September 18–20, 2006.

112. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Critical thickness calculations for $In_xGa_{1-x}N/GaN$" (oral), *5-IWMCG (5th International Workshop on Modelling in Crystal Growth)*, Bamberg, Germany, September 10–13, 2006.

113. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "The effect of the hexagonal symmetry on critical thickness calculations for $In_xGa_{1-x}N/GaN$" (poster), *Junior–Euromat 2006*, Lausanne, Switzerland, September 4–8, 2006.

114. D. Holec, P.M.F.J. Costa, M.J. Kappers and C.J. Humphreys: "Misfit dislocations – theory and experiment" (oral). *UKNC meeting*, Sheffield, UK, July 4, 2006.

115. D. Holec and A. Dlouhý: "Stress redistributions and their impact on the precipitation in microstructures" (oral). *Applied Mechanics 2005*, Hrotovice, Czech Republic, March 29–April 1, 2005.

116. D. Holec and A. Dlouhý: "Properties of low-angle dislocation boundaries in precipitation hardened crystals" (poster). *Junior–Euromat 2004*, Lausanne, Switzerland, September 6–9, 2004.

117. D. Holec and A. Dlouhý: "Stability and motion of low-angle dislocation boundaries in precipitation hardened crystals" (oral). *MSMF-4 (Materials Structure & Micromechanics of Fracture)*, Brno, Czech Republic, June 23–25, 2004.