Curriculum Vitae

Univ.-Prof. Dr. rer. nat.

Karsten Albe

Dipl.-Phys.

Date and place of birth:
03.11.1967, Hildesheim, Germany

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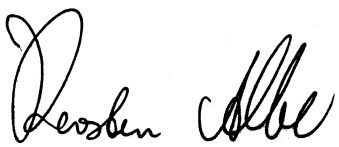

Seeheim-Jugenheim, 2.6.2022

Curriculum Vitae

Professional Employment Record

08/2007 – present	**Professor (W2)**, Materials Modeling Division, Institute of Materials Science, TU Darmstadt • *Modeling of defects in materials for energy conversion and storage, substitution materials and novel nanostructured metals and glasses* • *Particle-based simulation methods and their combination* • *Development of data analysis tools*
04/2020 – 03/2022	**Dean**, Department of Materials- and Geosciences, TU Darmstadt
10/2008 – 03/2009	**Visiting Professor**, VirginiaTech, Blacksburg, USA
11/2002 – 07/2007	**Junior Professor (W1)**, Materials Modeling Division, Institute of Materials Science, TU Darmstadt
07/2000 – 10/2002	**Research Associate**, Thin Films Division (with Prof. Dr. Horst Hahn), Institute of Materials Science, TU Darmstadt
08/1998 – 06/2000	**Postdoctoral Research Associate**, Materials Research Laboratory (Prof. Dr. Robert Averback) and Center for Simulation of Advanced Rockets, University of Illinois, Urbana-Champaign, USA
10/1994 – 07/1998	**Research Assistant**, Research Center Rossendorf-Dresden, Institute of Ion Beam Physics and Materials Research (with Prof. Dr. Wolfhard Möller)
05/1994 – 09/1994	**Research Assistant**, Department of Experimental Physics (with Prof. Dr. Hans-G. Kilian), University of Ulm

Education

08/2005	Positive Interim-Evaluation of Junior-Professorship (equivalent to Habilitation)
06/07/1998	**Doctorate** (*Dr. rer. nat.*) in Physics, TU Dresden *Doctoral Thesis (summa cum laude): "Computer Simulations on Structure and Growth of Boron Nitride"*
02/05/1994	**Diploma (Dipl.-Phys.)** in Physics, University of Ulm *Diploma Thesis: "Isobaric Phase Diagrams and Structure of Crystallizing Mixtures of Higher 1-Mono-Carboxylic Acids"*
10/1990 – 05/1994	University of Ulm, Study of Physics

10/1988 – 09/1990	University of Hamburg, Study of Physics (Intermediate Diploma)
07/1987 – 09/1988	Compulsory Military Service
05/1987	**University-Entrance Diploma** (Abitur), Gymnasium Andreanum, Hildesheim

Further Academic Activities

11/2021 – present	Member of the Scientific Council of NHR4CES
04/2020 – present	Elected Member of the DFG Review Panel 406 "Materials Science"
08/2018– 08/2021	Coordinator of BMBF-Platform "Festbatt - Theorie und Daten"
10/2015 – 11/2021	Member of the Advisory Board of "Hessischer Hochleistungsrechner Lichtenberg"
04/2012 –03/2016	Elected Member of the DFG-Review Panel "Materials Science"
04/2012 –12/2014	Spokesperson of SFB 595, Collaborative Research Center "Electric Fatigue in Functional Materials''
2010 – 2015	Member of the Scientific Council of the John von Neumann-Institute for Computing (NIC)
2010, 2012, 2014	Topic Organizer "Modeling" MSE Congress, Darmstadt
04/2005 – 12/2008	Deputy Editor of Scripta Materialia
06/2005 – 07/2007	Member of the University Assembly of TU Darmstadt

Awards and Distinctions

05/1997	ϵ-MRS–*Young Scientist Award*
12/1998	*Graduate Student Award*, Research Center Rossendorf-Dresden

Professional Society Memberships

Materials Research Society
Deutsche Physikalische Gesellschaft
Deutsche Gesellschaft für Materialkunde
Gesellschaft für Angewandte
Mathematik und Mechanik
Deutscher Hochschulverband

Reviewing

Deutsche Forschungsgemeinschaft

Humboldt Foundation
National Science Foundation
European Research Council

Science
Nature, Nature Materials, Nature Communications
Physical Review Letters
Physical Review B
Physical Review Materials
Acta Materialia
Scripta Materialia
Journal of Applied Physics
Applied Physics Letters
Journal of Physics: Cond. Mat.
Material Research Letters
Journal of Alloys & Compounds
Intermetallics
Computational Materials Science
Modeling and Simulation in Materials Science & Engineering
Journal Power Sources
Thin Solid Films
Philosophical Magazine A
Journal of Crystal Growth
Nuclear Instruments and Methods B
Applied Surface Science
Journal of Materials Research

Invited Talks (last 5 years)

MRS Fall Meeting, Boston (2021)
ISMANAM, Chennai (2019)
DPG-Frühjahrstagung Regensburg (2019)
APS Meeting Boston (2019)
Sino-German Symposium, Münster (2019)
CECAM-Workhshop, Bremen (2018)
Mechanics of Multifunctional Materials, Bad Honnef (2018)
Controversial Colloquium on Grain Boundaries, Irvine (2018)
FZ Rossendorf-Dresden, Festvortrag (2017)
RQ 16, Leoben (2017)
Batterieworkshop, Gießen (2017)
Int. Workshop on Hysteresis in magnetocaloric, electrocaloric and elastocaloric refrigeration Dresden (2017)
MSE, Darmstadt (2016)
EMCS, Santiago de Compostella (2016)
DPG Frühjahrstagung, Regensburg (2016)
EMA, Orlando (2016)
DPG Frühjahrstagung, Berlin (2015)

Supervised Theses since 2002

11 Diploma Theses
20 Master Theses
18 (+ 11 ongoing) Doctoral Theses:

1. Utt, Daniel (2021) *Defects in high-entropy alloys studied by atomic scale computer simulations*
2. Koch, Leonie (2021) *First-principles study of the defect chemistry and conductivity in sodium bismuth titanate*
3. Kalcher, Constanze (2019) *Creep of Cu-Zr metallic glasses and metallic glass composites: A molecular dynamics study*
4. Mock, Markus (2019) *Diffusion of point defects in oxide-dispersion strengthened steels*
5. Barragan-Yani, Daniel Antonio (2018) *First-principles study of dislocations in* $\mathrm{Cu(In,Ga)Se_2}$ *solar cell absorbers*
6. Lenchuk, Olena (2017) *Density-functional theory calculations of solutes in molybdenum grain boundaries*
7. Brink, Tobias (2017) *Heterogeneities in Metallic Glasses: Atomistic Computer Simulations on the Structure and Mechanical Properties of Copper–Zirconium Alloys and Composites*
8. Meyer, Kai-Christian (2017) *Phase Transformation Kinetics and Oxygen Transport in the Relaxor Ferroelectric* $\mathrm{Na_{1/2}Bi_{1/2}TiO_3}$ *studied by First-Principles Calculations*
9. Hayn, Silke (2013) *First-principles calculations on the structural and thermodynamic stability of* $\mathrm{Na_{1/2}Bi_{1/2}TiO_3}$ *and* $\mathrm{Pb(Zr,Ti)O_3}$
10. Gröting, Melanie (2013) *Ab-initio Calculations of the Relaxor Ferroelectric* $\mathrm{Na_{1/2}Bi_{1/2}TiO_3}$ *and its Solid Solutions*
11. Pohl, Johan (2013) *Structure and properties of defects in photovoltaics absorber material: Atomic scale computer simulations of Si and* $\mathrm{Cu(In,Ga)Se_2}$
12. Schäfer, Jonathan (2013) *Atomistic simulations of plasticity in nanocrystalline alloys*
13. Ritter, Yvonne (2012) *Molecular Dynamics Simulations of Structure-Property Relationships in Cu-Zr Metallic Glasses*
14. Agoston, Peter (2011) *Point defect and surface properties of* $\mathrm{In_2O_3}$ *and* $\mathrm{SnO_2}$*: A comparative study by first-principles methods*
15. Sopu, Daniel (2011) *Molecular Dynamics Simulations of Metallic Nanoglasses*
16. Stukowski, Alexander (2010) *Atomic-scale modeling of nanostructured metals and alloys*
17. Müller, Michael (2007) *Atomistic Computer Simulations of FePt Nanoparticles*
18. Erhart, Paul (2006) *Intrinsic Point Defects in Zinc Oxide: Modeling of Structural, Electronic, Thermodynamic and Kinetic Properties*

Bibliometric Details

ORCID-ID	0000-0003-4669-8056
ResearcherID	F-1139-2011

Publications

Nanostructure Materials and Glasses

Nanoglasses

[1] O. Adjaoud and K. Albe, Mechanical properties of glassy nanopillars: a comparative, computational study of size effects in nanoglasses and homogeneous bulk glasses, FRONTIERS IN MATERIALS **7**, 544660 (2021).

[2] O. Adjaoud and K. Albe, Nanoindentation of nanoglasses tested by molecular dynamics simulations: influence of structural relaxation and chemical segregation on the mechanical response, FRONTIERS IN MATERIALS **8**, 664220 (2021).

[3] C. Kalcher, O. Adjaoud, and K. Albe, Creep deformation of a cu-zr nanoglass and interface reinforced nanoglass-composite studied by molecular dynamics simulations, FRONTIERS IN MATERIALS, 10.3389/fmats.2020.00223 (2020).

[4] C. Kalcher, O. Adjaoud, and K. Albe, Creep deformation of a Cu-Zr nanoglass and interface reinforced nanoglass-composite studied by molecular dynamics simulations, FRONTIERS IN MATERIALS **7**, 10.3389/fmats.2020.00223 (2020).

[5] S. H. Nandam, O. Adjaoud, R. Schwaiger, Y. Ivanisenko, M. R. Chellali, D. Wang, K. Albe, and H. Hahn, Influence of topological structure and chemical segregation on the thermal and mechanical properties of Pd-Si nanoglasses, ACTA MATERIALIA **193**, 252–260 (2020).

[6] O. Adjaoud and K. Albe, Influence of microstructural features on the plastic deformation behavior of metallic nanoglasses, ACTA MATERIALIA **168**, 393–400 (2019).

[7] Y. Ivanisenko, C. Kübel, S. H. Nandam, C. Wang, X. Mu, O. Adjaoud, K. Albe, and H. Hahn, Structure and properties of nanoglasses, ADVANCED ENGINEERING MATERIALS **20**, 10.1002/adem.201800404 (2018).

[8] O. Adjaoud and K. Albe, Microstructure formation of metallic nanoglasses: insights from molecular dynamics simulations, ACTA MATERIALIA **145**, 322–330 (2018).

[9] C. Kalcher, O. Adjaoud, J. Rohrer, A. Stukowski, and K. Albe, Reinforcement of nanoglasses by interface strengthening, SCRIPTA MATERIALIA **141**, 115–119 (2017).

[10] O. Adjaoud and K. Albe, Interfaces and interphases in nanoglasses: surface segregation effects and their implications on structural properties, ACTA MATERIALIA **113**, 284–292 (2016).

[11] D. Sopu and K. Albe, Influence of grain size and composition, topology and excess free volume on the deformation behavior of Cu-Zr nanoglasses, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **6**, 537–545 (2015).

[12] Y. Ritter and K. Albe, Chemical and topological order in shear bands of $Cu_{64}Zr_{36}$ and $Cu_{36}Zr_{64}$ glasses, JOURNAL OF APPLIED PHYSICS **111**, 10.1063/1.4717748 (2012).

[13] Y. Ritter, D. Sopu, H. Gleiter, and K. Albe, Structure, stability and mechanical properties of internal interfaces in $Cu_{64}Zr_{36}$ nanoglasses studied by MD simulations, ACTA MATERIALIA **59**, 6588–6593 (2011).

[14] Y. Ritter and K. Albe, Thermal annealing of shear bands in deformed metallic glasses: recovery mechanisms in $Cu_{64}Zr_{36}$ studied by molecular dynamics simulations, ACTA MATERIALIA **59**, 7082–7094 (2011).

[15] D. Sopu, J. Kotakoski, and K. Albe, Finite-size effects in the phonon density of states of nanostructured germanium: a comparative study of nanoparticles, nanocrystals, nanoglasses, and bulk phases, PHYSICAL REVIEW B **83**, 10.1103/PhysRevB.83.245416 (2011).

[16] D. Sopu, Y. Ritter, H. Gleiter, and K. Albe, Deformation behavior of bulk and nanostructured metallic glasses studied via molecular dynamics simulations, PHYSICAL REVIEW B **83**, 10.1103/PhysRevB.83.100202 (2011).

[17] D. Sopu, K. Albe, Y. Ritter, and H. Gleiter, From nanoglasses to bulk massive glasses, APPLIED PHYSICS LETTERS **94**, 10.1063/1.3130209 (2009).

Metallic Glasses and Composites

[18] C. Kalcher, T. Brink, J. Rohrer, A. Stukowski, and K. Albe, Elastostatic loading of metallic glass-crystal nanocomposites: relationship of creep rate and interface energy, PHYSICAL REVIEW MATERIALS **3**, 10.1103/PhysRevMaterials.3.093605 (2019).

[19] D. Sopu, K. Albe, and J. Eckert, Metallic glass nanolaminates with shape memory alloys, ACTA MATERIALIA **159**, 344–351 (2018).

[20] T. Brink and K. Albe, From metallic glasses to nanocrystals: molecular dynamics simulations on the crossover from glass-like to grain-boundary-mediated deformation behaviour, ACTA MATERIALIA **156**, 205–214 (2018).

[21] C. Kalcher, T. Brink, J. Rohrer, A. Stukowski, and K. Albe, Interface-controlled creep in metallic glass composites, ACTA MATERIALIA **141**, 251–260 (2017).

[22] T. Brink, M. Peterlechner, H. Roesner, K. Albe, and G. Wilde, Influence of crystalline nano-precipitates on shear-band propagation in Cu-Zr-based metallic glasses, PHYSICAL REVIEW APPLIED **5**, 10.1103/PhysRevApplied.5.054005 (2016).

[23] T. Brink, D. Sopu, and K. Albe, Solid-state amorphization of Cu nanolayers embedded in a $Cu_{64}Zr_{36}$ glass, PHYSICAL REVIEW B **91**, 10.1103/PhysRevB.91.184103 (2015).

[24] K. A. Avchaciov, Y. Ritter, F. Djurabekova, K. Nordlund, and K. Albe, Effect of ion irradiation on structural properties of $Cu_{64}Zr_{36}$ metallic glass, NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **341**, 22–26 (2014).

[25] J. Bünz, T. Brink, K. Tsuchiya, F. Meng, G. Wilde, and K. Albe, Low temperature heat capacity of a severely deformed metallic glass, PHYSICAL REVIEW LETTERS **112**, 10.1103/PhysRevLett.112.135501 (2014).

[26] K. Albe, Y. Ritter, and D. Sopu, Enhancing the plasticity of metallic glasses: shear band formation, nanocomposites and nanoglasses investigated by molecular dynamics simulations, MECHANICS OF MATERIALS **67**, 94–103 (2013).

[27] K. A. Avchaciov, Y. Ritter, F. Djurabekova, K. Nordlund, and K. Albe, Controlled softening of $Cu_{64}Zr_{36}$ metallic glass by ion irradiation, APPLIED PHYSICS LETTERS **102**, 10.1063/1.4804630 (2013).

[28] S. Mayr, Y Ashkenazy, K Albe, and R. Averback, Mechanisms of radiation-induced viscous flow: role of point defects, PHYSICAL REVIEW LETTERS **90**, 10.1103/PhysRevLett.90.055505 (2003).

Nanocrystalline Materials

[29] J. Schäfer, A. Stukowski, and K. Albe, On the hierarchy of deformation processes in nanocrystalline alloys: grain boundary mediated plasticity vs. dislocation slip, JOURNAL OF APPLIED PHYSICS **114**, 10.1063/1.4821763 (2013).

[30] A. Kobler, J. Lohmiller, J. Schäfer, M. Kerber, A. Castrup, A. Kashiwar, P. A. Gruber, K. Albe, H. Hahn, and C. Kübel, Deformation-induced grain growth and twinning in nanocrystalline palladium thin films, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 554–566 (2013).

[31] J. Schäfer and K. Albe, Plasticity of nanocrystalline alloys with chemical order: on the strength and ductility of nanocrystalline Ni-Fe, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 542–553 (2013).

[32] J. Schäfer and K. Albe, Competing deformation mechanisms in nanocrystalline metals and alloys: coupled motion versus grain boundary sliding, ACTA MATERIALIA **60**, 6076–6085 (2012).

[33] J. Schäfer, Y. Ashkenazy, K. Albe, and R. S. Averback, Effect of solute segregation on thermal creep in dilute nanocyrstalline Cu alloys, MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING **546**, 307–313 (2012).

[34] J. Schäfer and K. Albe, Influence of solutes on the competition between mesoscopic grain boundary sliding and coupled grain boundary motion, SCRIPTA MATERIALIA **66**, 315–317 (2012).

[35] N. Q. Vo, J. Schäfer, R. S. Averback, K. Albe, Y. Ashkenazy, and P. Bellon, Reaching theoretical strengths in nanocrystalline Cu by grain boundary doping, SCRIPTA MATERIALIA **65**, 660–663 (2011).

[36] J. Schäfer, A. Stukowski, and K. Albe, Plastic deformation of nanocrystalline Pd-Au alloys: on the interplay of grain boundary solute segregation, fault energies and grain size, ACTA MATERIALIA **59**, 2957–2968 (2011).

[37] A. Stukowski, K. Albe, and D. Farkas, Nanotwinned fcc metals: strengthening versus softening mechanisms, PHYSICAL REVIEW B **82**, 10.1103/PhysRevB.82.224103 (2010).

[38] A. Stukowski, J. Markmann, J. Weissmüller, and K. Albe, Atomistic origin of microstrain broadening in diffraction data of nanocrystalline solids, ACTA MATERIALIA **57**, 1648–1654 (2009).

[39] Z.-H. Jin, P. Gumbsch, K. Albe, E. Ma, K. Lu, H. Gleiter, and H. Hahn, Interactions between non-screw lattice dislocations and coherent twin boundaries in face-centered cubic metals, ACTA MATERIALIA **56**, 1126–1135 (2008).

[40] S.-J. Zhao, K. Albe, and H. Hahn, Grain size dependence of the bulk modulus of nanocrystalline nickel, SCRIPTA MATERIALIA **55**, 473–476 (2006).

[41] Z.-H. Jin, P Gumbsch, E Ma, K Albe, K Lu, H Hahn, and H Gleiter, The interaction mechanism of screw dislocations with coherent twin boundaries in different face-centred cubic metals, SCRIPTA MATERIALIA **54**, 1163–1168 (2006).

[42] W Voegeli, K Albe, and H Hahn, Simulation of grain growth in nanocrystalline nickel induced by ion irradiation, NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **202**, 230–235 (2003).

Nanoparticles

[43] A. Tolvanen and K. Albe, Plasticity of Cu nanoparticles: dislocation-dendrite-induced strain hardening and a limit for displacive plasticity, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **4**, 173–179 (2013).

[44] P. M. Diehm, P. Agoston, and K. Albe, Size-dependent lattice expansion in nanoparticles: reality or anomaly?, CHEMPHYSCHEM **13**, 2443–2454 (2012).

[45] J. Pohl, C. Stahl, and K. Albe, Size-dependent phase diagrams of metallic alloys: a Monte Carlo simulation study on order-disorder transitions in Pt-Rh nanoparticles, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **3**, 1–11 (2012).

[46] D. Gross, R. Müller, M. Müller, B.-X. Xu, and K. Albe, On the origin of inhomogeneous stress and strain distributions in single-crystalline metallic nanoparticles, INTERNATIONAL JOURNAL OF MATERIALS RESEARCH **102**, 743–747 (2011).

[47] M. Müller and K. Albe, Kinetic lattice Monte-Carlo simulations on the ordering kinetics of free and supported FePt $L1_0$-nanoparticles, BEILSTEIN JOURNAL OF NANOTECHNOLOGY **2**, 10.3762/bjnano.2.5 (2011).

[48] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Damage production in nanoparticles under light ion irradiation, PHYSICAL REVIEW B **80**, 10.1103/PhysRevB.80.132101 (2009).

[49] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Low energy cluster deposition of nanoalloys, JOURNAL OF APPLIED PHYSICS **106**, 10.1063/1.3225910 (2009).

[50] J. Pohl and K. Albe, Phase equilibria and ordering in solid Pt-Rh calculated by means of a refined bond-order simulation mixing model, ACTA MATERIALIA **57**, 4140–4147 (2009).

[51] T. T. Järvi, D. Pohl, K. Albe, B. Rellinghaus, L. Schultz, J. Fassbender, A. Kuronen, and K. Nordlund, From multiply twinned to fcc nanoparticles via irradiation-induced transient amorphization, EPL **85**, 10.1209/0295-5075/85/26001 (2009).

[52] T. T. Järvi, A. Kuronen, K. Nordlund, and K. Albe, Structural modification of a multiply twinned nanoparticle by ion irradiation: a molecular dynamics study, JOURNAL OF APPLIED PHYSICS **102**, 10.1063/1.2825045 (2007).

[53] M. Müller and K. Albe, Structural stability of multiply twinned FePt nanoparticles, ACTA MATERIALIA **55**, 6617–6626 (2007).

[54] M. Müller, P. Erhart, and K. Albe, Thermodynamics of l1(0) ordering in FePt nanoparticles studied by Monte Carlo simulations based on an analytic bond-order potential, PHYSICAL REVIEW B **76**, 10.1103/PhysRevB.76.155412 (2007).

[55] M. Müller and K. Albe, Concentration of thermal vacancies in metallic nanoparticles, ACTA MATERIALIA **55**, 3237–3244 (2007).

[56] T. T. Järvi, A. Kuronen, K. Meinander, K. Nordlund, and K. Albe, Contact epitaxy by deposition of Cu, Ag, Au, Pt, and Ni nanoclusters on (100) surfaces: size limits and mechanisms, PHYSICAL REVIEW B **75**, 10.1103/PhysRevB.75.115422 (2007).

[57] P Krasnochtchekov, K Albe, Y Ashkenazy, and R. Averback, Molecular-dynamics study of the density scaling of inert gas condensation, JOURNAL OF CHEMICAL PHYSICS **123**, 10.1063/1.2074247 (2005).

[58] P Erhart and K Albe, Molecular dynamics simulations of gas phase condensation of silicon carbide nanoparticles, ADVANCED ENGINEERING MATERIALS **7**, 937–945 (2005).

[59] M Müller and K Albe, Lattice Monte Carlo simulations of FePt nanoparticles: influence of size, composition, and surface segregation on order-disorder phenomena, PHYSICAL REVIEW B **72**, 10.1103/PhysRevB.72.094203 (2005).

[60] P Erhart and K Albe, The role of thermostats in modeling vapor phase condensation of silicon nanoparticles, APPLIED SURFACE SCIENCE **226**, 12–18 (2004).

[61] P Krasnochtchekov, K Albe, and R. Averback, Simulations of the inert gas condensation processes, ZEITSCHRIFT FUR METALLKUNDE **94**, 1098–1105 (2003).

[62] Y Ashkenazy, R. Averback, and K Albe, Nanocluster rotation on Pt surfaces: twist boundaries, PHYSICAL REVIEW B **64**, 10.1103/PhysRevB.64.205409 (2001).

Nanoporous Metals

[63] N. Beets, D. Farkas, and K. Albe, The mechanical response of nanoporous gold and silver foams with varying composition and surface segregation, ACTA MATERIALIA **203**, 116445 (2021).

[64] A. J. Klomp, A. Stukowski, R. Müller, K. Albe, and F. Diewald, Influence of surface stress on the mechanical response of nanoporous metals studied by an atomistically informed continuum model, ACTA MATERIALIA **221**, 10.1016/j.actamat.2021.117373 (2021).

[65] B.-N. D. Ngo, B. Roschning, K. Albe, J. Weissmüller, and J. Markmann, On the origin of the anomalous compliance of dealloying-derived nanoporous gold, SCRIPTA MATERIALIA **130**, 74–77 (2017).

[66] B.-N. D. Ngo, A. Stukowski, N. Mameka, J. Markmann, K. Albe, and J. Weissmüller, Anomalous compliance and early yielding of nanoporous gold, ACTA MATERIALIA **93**, 144–155 (2015).

[67] P Erhart, E. Bringa, M Kumar, and K Albe, Atomistic mechanism of shock-induced void collapse in nanoporous metals, PHYSICAL REVIEW B **72**, 10.1103/PhysRevB.72.052104 (2005).

High Entropy Alloys

[68] T. Keil, D. Utt, E. Bruder, A. Stukowski, K. Albe, and K. Durst, Solid solution hardening in CrMnFeCoNi-based high entropy alloy systems studied by a combinatorial approach, JOURNAL OF MATERIALS RESEARCH **2021**, 1–13 (2021).

[69] J. Kottke, D. Utt, M. Laurent-Brocq, A. Fareed, D. Gärtner, L. Perriere, L. Rogal, A. Stukowski, K. Albe, S. Divinski V, and G. Wilde, Experimental and theoretical study of tracer diffusion in a series of $CoCrFeMn_{(100-x)}Ni_x$ alloys, ACTA MATERIALIA **194**, 236–248 (2020).

[70] F. Thiel, D. Utt, A. Kauffmann, K. Nielsch, K. Albe, M. Heilmaier, and J. Freudenberger, Breakdown of varvenne scaling in $(AuNiPdPt)_{(1-x)}Cu_x$ high-entropy alloys, SCRIPTA MATERIALIA **181**, 15–18 (2020).

[71] D. Utt, A. Stukowski, and K. Albe, Grain boundary structure and mobility in high-entropy alloys: a comparative molecular dynamics study on a Σ 11 symmetrical tilt grain boundary in face-centered cubic CuNiCoFe, ACTA MATERIALIA **186**, 11–19 (2020).

[72] F. Thiel, D. Geissler, K. Nielsch, A. Kauffmann, S. Seils, M. Heilmaier, D. Utt, K. Albe, M. Motylenko, D. Rafaja, and J. Freudenberger, Origins of strength and plasticity in the precious metal based high-entropy alloy AuCuNiPdPt, ACTA MATERIALIA **185**, 400–411 (2020).

[73] E. Levo, F. Granberg, D. Utt, K. Albe, K. Nordlund, and F. Djurabekov, Radiation stability of nanocrystalline single-phase multicomponent alloys, JOURNAL OF MATERIALS RESEARCH **34**, 854–866 (2019).

[74] L. Koch, F. Granberg, T. Brink, D. Utt, K. Albe, F. Djurabekova, and K. Nordlund, Local segregation versus irradiation effects in high-entropy alloys: steady-state conditions in a driven system, JOURNAL OF APPLIED PHYSICS **122**, 10.1063/1.4990950 (2017).

[75] T. Brink, L. Koch, and K. Albe, Structural origins of the boson peak in metals: from high-entropy alloys to metallic glasses, PHYSICAL REVIEW B **94**, 10.1103/PhysRevB.94.224203 (2016).

Energy Materials

Photovoltaic Absorbers and Buffer Materials

[76] O. Cojocaru-Mirédin, E. Ghorbani, M. Raghuwanshi, X. Jin, D. Pandav, J. Keutgen, R. Schneider, D. Gerthsen, K. Albe, and R. Scheer, Intense sulphurization process can lead to superior heterojunction properties in $Cu(In,Ga)(S,Se)_2$ thin-film solar cells, NANO ENERGY, 10.1016/j.nanoen.2021.106375 (2021).

[77] E. Ghorbani, D. Barragan-Yani, and K. Albe, Towards intermediate-band photovoltaic absorbers: theoretical insights on the incorporation of Ti and Nb in In_2S_3, NPJ COMPUTATIONAL MATERIALS **6**, 10.1038/s41524-020-00350-2 (2020).

[78] C. Li, E. S. Sanli, D. Barragan-Yani, H. Stange, M.-D. Heinemann, D. Greiner, W. Sigle, R. Mainz, K. Albe, D. Abou-Ras, and P. A. van Aken, Secondary-phase-assisted grain boundary migration in $CuInSe_2$, PHYSICAL REVIEW LETTERS **124**, 10.1103/PhysRevLett.124.095702 (2020).

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