

# Veröffentlichungen

- [1] N. Gunkelmann, H. Ledbetter und H. M. Urbassek. Experimental and atomistic study of the elastic properties of  $\alpha'$  Fe-C martensite. *Acta Mater.* 60:4901–4907, 2012.
- [2] N. Gunkelmann, E. M. Bringa, K. Kang, G. J. Ackland und H. M. Urbassek. Polycrystalline iron under compression: Plasticity and phase transitions. *Phys. Rev. B* 86:144111, 2012.
- [3] N. Gunkelmann, D. Serero und T. Pöschel. Temperature of a granular gas with regard to the stochastic nature of particle interactions. *New Journal of Phys.* 15:093030, 2013.
- [4] B. Wang, E. Sak-Saracino, N. Gunkelmann und H. M. Urbassek. Molecular-dynamics study of the  $\alpha \leftrightarrow \gamma$  phase transition in Fe-C. *Comput. Mater. Sci.* 82:399–404, 2014.
- [5] N. Gunkelmann, M. Montaine und T. Pöschel. Stochastic behavior of the coefficient of normal restitution. *Phys. Rev. E* 89:022205, 2014.
- [6] N. Gunkelmann, E. M. Bringa, D. R. Tramontina, C. J. Ruestes, M. J. Suggit, A. Higginbotham, J. S. Wark und H. M. Urbassek. Shock waves in polycrystalline iron: Plasticity and phase transitions. *Phys. Rev. B* 89:140102, 2014.
- [7] N. Gunkelmann, D. R. Tramontina, E. M. Bringa und H. M. Urbassek. Interplay of plasticity and phase transformation in shock wave propagation in nanocrystalline iron. *New J. Phys.* 16:093032, 2014.
- [8] A. Glielmo, N. Gunkelmann und T. Pöschel. Coefficient of restitution of aspherical Particles. *Phys. Rev. E* 90:052204, 2014.
- [9] N. Gunkelmann, D. R. Tramontina, E. M. Bringa und H. M. Urbassek. Morphological changes in polycrystalline Fe after compression and release. *J. Appl. Phys.* 117:085901, 2015.
- [10] C. Ringl, N. Gunkelmann, E. M. Bringa und H. M. Urbassek. Compaction of highly porous granular matter by impacts on a hard wall. *Phys. Rev. E* 91:042205, 2015.
- [11] D. Serero, N. Gunkelmann und T. Pöschel. Hydrodynamics of binary mixtures of granular gases with stochastic coefficient of restitution. *J. Fluid Mech.* 781:595, 2015.

- [12] N. Gunkelmann, E. M. Bringa und H. M. Urbassek. Influence of phase transition on shock-induced spallation in nanocrystalline iron. *J. Appl. Phys.* 118:185902, 2015.
- [13] M. Heckel, A. Glielmo, N. Gunkelmann und T. Pöschel. Can we obtain the coefficient of restitution from the sound of a bouncing ball? *Phys. Rev. E* 93:032901, 2016.
- [14] J. Janßen, N. Gunkelmann und H. M. Urbassek. Influence of C concentration on elastic moduli of  $\alpha'$ -Fe<sub>(1-x)</sub>C<sub>x</sub> alloys. *Phil. Mag.* 96:1448, 2016.
- [15] N. Gunkelmann, C. Ringl und H. M. Urbassek. Instationary compaction wave propagation in highly porous granular media. *Comp. Part. Mech.* 3:429, 2016.
- [16] N. Gunkelmann, Y. Rosandi, C. J. Ruestes, E. M. Bringa und H. M. Urbassek. Compaction and plasticity in nanofoams induced by shock waves: A molecular dynamics study. *Comput. Mater. Sci.* 119:27, 2016.
- [17] N. Gunkelmann, C. Ringl und H. M. Urbassek. Influence of porosity on collisions between dust aggregates. *Astron. Astrophys.* 589:A30, 2016.
- [18] N. Gunkelmann, A. Kataoka, C. P. Dullemond und H. M. Urbassek. Low-velocity collisions of chondrules: How a thin dust cover helps enhance the sticking probability. *Astron. Astrophys.* 599:L4, 2017.
- [19] N. Gunkelmann, I. A. Alhafez, D. Steinberger, H. M. Urbassek und S. Sandfeld. Nanoscratching of iron: A novel approach to characterize dislocation microstructures. *Comput. Mater. Sci.* 135:181, 2017.
- [20] N. Gunkelmann, E. M. Bringa und Y. Rosandi. Molecular Dynamics Simulations of Aluminium Foams under Tension: Influence of Oxidation. *J. Phys. Chem. C* 122:26243, 2018.
- [21] P. Umstätter, N. Gunkelmann, C. P. Dullemond und H. M. Urbassek. Shedding of dust rims in chondrule collisions in the protoplanetary disk. *MNRAS* 483:4398, 2019.
- [22] N. Gunkelmann, D. Serero, A. Glielmo, M. Montaine, M. Heckel und T. Pöschel. Stochastic Nature of Particle Collisions and its Impact on Granular Material Properties. In *Particles in Contact - Micro Mechanics, Micro Process Dynamics and Particle Collective*. Ed: S. Antonyuk, Springer International Publishing, 2019.
- [23] H.-T. Luu und N. Gunkelmann. Pressure-induced phase transformations in Fe-C: Molecular dynamics approach. *Comput. Mater. Sci.* 162:295, 2019.
- [24] F. Lançon, N. Gunkelmann, D. Caliste und J.-L. Rouvière. Incommensurate grain boundary in silicon and the silver-ratio sequence. *Phys. Rev. B.* 100:115307, 2019.

- [25] H.-T. Luu, R. G. A. Veiga und N. Gunkelmann. Atomistic Study of the Role of Defects on  $\alpha \rightarrow \epsilon$  Phase Transformations in Iron under Hydrostatic Compression. *Metals* 9(10):1040, 2019.
- [26] N. Gunkelmann und M. Baum (Eds.) Simulation Science, Second International Workshop, SimScience 2019 *Communications in Computer and Information Science (CCIS)* 1199: 153, Springer, Cham, 2020.
- [27] H. Stromberg, N. Gunkelmann und A. Lohrengel. A novel approach to multiscale MD/FE simulations of frictional contacts. In *Simulation Science, Second International Workshop, SimScience 2019: Communications in Computer and Information Science (CCIS)* 1199: 153, Springer, Cham, 2020.
- [28] Y. Rosandi, H.-T. Luu, H. M. Urbassek und N. Gunkelmann. Molecular Dynamics Simulations of the Mechanical Behavior of Alumina Coated Aluminum Nanowires under Tension and Compression. *RSC Advances* 10:1435, 2020.
- [29] N. Gunkelmann und M. Merkert. Improved energy minimization of iron carbon systems: On the influence of positioning interstitial atoms. *MSMSE* 28(4):045005, 2020.
- [30] H.-T. Luu, R. J. Ravelo, M. Rudolph, E. M. Bringa, T. C. Germann, D. Rafaja und N. Gunkelmann. Shock-induced plasticity in nanocrystalline iron: Large-scale molecular dynamics simulations. *Phys. Rev. B* 102:020102(R), 2020.
- [31] K. C. Le, S. L. Dang, H.-T. Luu und N. Gunkelmann. Thermodynamic dislocation theory: Application to bcc-crystals. *MSMSE* 29(1): 015003, 2020.
- [32] H. Song, N. Gunkelmann, G. Po und S. Sandfeld. Data-mining of dislocation microstructures: concepts for coarse-graining of internal energies. *MSMSE* 29:035005, 2021.
- [33] H.-T. Luu, S.-L. Dang, T.-V. Hoang und N. Gunkelmann. Molecular dynamics simulation of nanoindentation in Al and Fe: On the influence of system characteristics. *Appl. Surf. Science* 551:149221, 2021.
- [34] A. Plack, M. Bierwirth, A.P. Weber und N. Gunkelmann. Experimental and atomistic study of high speed collisions of gold nanoparticles with a gold substrate: Validation of interatomic potentials. *J. Aerosol Sci.* 159:105846, 2021.
- [35] D. Thürmer, S. Zhao, O. R. Deluigi, C. Stan, I. A. Alhafez, H. M. Urbassek, M. A. Meyers, E. M. Bringa und N. Gunkelmann. Exceptionally high spallation strength for a high-entropy alloy demonstrated by experiments and simulations. *J. Alloys Compd.* 895:162567, 2022.
- [36] D. Thürmer und N. Gunkelmann. Shock-induced spallation in a nanocrystalline high-entropy alloy: An atomistic study. *J. Appl. Phys.* 131:065902, 2022.

- [37] H.-T. Luu, S. Raumel, F. Dencker, M. Wurz und N. Merkert. Nanoindentation in alumina coated Al: Molecular dynamics simulations and experiments. *Surf. Coat. Tech.* 437:128342, 2022.
- [38] S. Homann, H.-T. Luu und N. Merkert. Molecular dynamics simulations of the machining of oxidized and deoxidized titanium work pieces. *Results Surf. Interfaces* 9:100085, 2022.
- [39] S. Raumel, K. Barenti, H.-T. Luu, N. Merkert, F. Dencker, F. Nürnberg, H.J. Maier und M. C. Wurz. Characterization of the tribologically relevant cover layers formed on copper in oxygen and oxygen-free conditions. *Friction*, DOI: 10.1007/s40544-022-0695-5, 2023.
- [40] G.S. Dutta, D. Meiners und N. Merkert. A Study of Free-Form Shape Rationalization Using Biomimicry as Inspiration. *Polymers* 15:2466, 2023.
- [41] A. Demirci, D. Steinberger, M. Stricker, N. Merkert, D. Weygand und S. Sandfeld. Statistical analysis of discrete dislocation dynamics simulations: initial structures, cross-slip and microstructure evolutions. *MSMSE* 31:075003, 2023.
- [42] L. Hahn, S. A. Blaue, P. Höhn, N. Merkert, P. Klein. Open Educational Resources für den Hochschulbereich. In *PhyDid B, Didaktik der Physik, Beiträge zur virtuellen DPG-Frühjahrstagung*. Ed: H. Grötzebach, S. Heinicke, 2023.