

# Jun. Prof. Dr. Nina Merkert (née Gunkelmann)

## Publications

1. D. Thürmer, O. R. Deluigi, H. M. Urbassek, E. M. Bringa, N. Merkert. Atomistic Simulations of the Shock and Spall Behavior of the Refractory High-Entropy Alloy HfNbTaTiZr. *High Entropy Alloys & Materials*, DOI: 10.1007/s44210-024-00042-2, 2024.
2. S. Hampel, I. A. Alhafez, T. Schirmer, N. Merkert, S. Wunderlich, A. Schnickmann, H. Li, M. Fischschweiger, U. E. A. Fittschen. Engineering Compounds for the Recovery of Critical Elements from Slags: Melt Characteristics of  $\text{Li}_5\text{AlO}_4$ ,  $\text{LiAlO}_2$ , and  $\text{LiAl}_5\text{O}_8$ . *ACS Omega*, DOI: 10.1021/acsomega.4c00723, 2024.
3. U. E. A. Fittschen, S. Hampel, T. Schirmer, N. Merkert. Multimodal spectroscopy and molecular dynamic simulations to understand redox-chemistry and compound formation in pyrometallurgical slags: example of manganese oxidation state with respect to lithium recycling. *Appl. Spectrosc. Rev.*, DOI: 10.1080/05704928.2024.2350988, 2024.
4. I. A. Alhafez, O. R. Deluigi, D. Tramontina, N. Merkert, H. M. Urbassek, E. M. Bringa. Nanoindentation into a bcc high-entropy HfNbTaTiZr alloy – an atomistic study of the effect of short-range order. *Sci. Rep.* 14:9112, 2024.
5. D. Thürmer, H.-T. Luu, N. Merkert. Molecular dynamics simulation of shock waves in Fe and Fe-C: Influence of system characteristics. *J. Appl. Phys.* 135:155901, 2024.
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8. G.S. Dutta, D. Meiners, N. Merkert. A Study of Free-Form Shape Rationalization Using Biomimicry as Inspiration. *Polymers* 15:2466, 2023.
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10. S. Homann, H.-T. Luu, N. Merkert. Molecular dynamics simulations of the machining of oxidized and deoxidized titanium work pieces. *Results Surf. Interfaces* 9:100085, 2022.
11. H.-T. Luu, S. Raumel, F. Dencker, M. Wurz, N. Merkert. Nanoindentation in alumina coated Al: Molecular dynamics simulations and experiments. *Surf. Coat. Tech.* 437:128342, 2022.
12. D. Thürmer, N. Gunkelmann. Shock-induced spallation in a nanocrystalline high-entropy alloy: An atomistic study. *J. Appl. Phys.* 131:065902, 2022.

13. D. Thürmer, S. Zhao, O. R. Deluigi, C. Stan, I. A. Alhafez, H. M. Urbassek, M. A. Meyers, E. M. Bringa, N. Gunkelmann. Exceptionally high spallation strength for a high-entropy alloy demonstrated by experiments and simulations. *J. Alloys Compd.* 895:162567, 2022.
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16. H.-T. Luu, S.-L. Dang, T.-V. Hoang, N. Gunkelmann. Molecular dynamics simulation of nanoindentation in Al and Fe: On the influence of system characteristics. *Appl. Surf. Science* 551:149221, 2021.
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23. H.-T. Luu, R. G. A. Veiga, 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, **Journal issue cover image, Volume 9, Issue 10.**
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