

Thin film materials design & some thoughts on complexity and sustainability

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- [1] D. Bogdanovski, P.J. Pöllmann, J.M. Schneider, An ab initio investigation of the temperature-dependent energetic barriers towards CrAlB and (Mo,Cr)AlB formation in a metastable synthesis scenario; *Nanoscale* 10(35), 12866-12874 (2022)
[doi.org/10.1039/D2NR01087A]
- [2] P. Ondračka, M. Hans, D. Holzapfel, D. Primetzhofer, D. Holec, J. M. Schneider, Ab initio-guided X-ray photoelectron spectroscopy quantification of Ti vacancies in $Ti_{1-\delta}O_{x}N_{1-x}$ thin films; *Acta materialia* 230, 117778 (2022)
[doi.org/10.1016/j.actamat.2022.117778]
- [3] D. M. Holzapfel, D. Music, M. Hans, S. Woof-Goodrich, D. Holec, D. Bogdanovski, M. Arndt, A. O. Eriksson, K. Yalamanchili, D. Primetzhofer, C. H. Liebscher, J. M. Schneider, Enhanced thermal stability of (Ti,Al)N coatings by oxygen incorporation, *Acta Materialia* 218, 117204 (2021)
[doi.org/10.1016/j.actamat.2021.117204]
- [4] S. Karimi Aghda, D. Music, Y. Unutulmazsoy, H.H. Sua, S. Mráz, M. Hans, D. Primetzhofer, A. Anders, J.M. Schneider, Unravelling the ion-energy-dependent structure evolution and its implications for the elastic properties of (V,Al)N thin films
Acta Materialia 214, 117003 (2021)
[doi.org/10.1016/j.actamat.2021.117003]
- [5] D. Holzapfel, D. Music, S. Mráz, S. Aghda, M. Etter, P. Ondračka, M. Hans, D. Bogdanovski, S. Evertz, L. Patterer, P. Schmidt, A. Schökel, A. O.Eriksson, M. Arndt, D. Primetzhofer, J. Schneider, Influence of ion irradiation-induced defects on phase formation and thermal stability of $Ti_{0.27}Al_{0.21}N_{0.52}$ coatings *Acta Materialia* 237, 118160 (2022)
[doi.org/10.1016/j.actamat.2022.118160]