

Alloying trends from first principles: A case study of ternary and multinary nitrides

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The alloying concept has been long known to allow for fine tuning of material properties, not only in-between the borders set by the boundary systems, but sometimes also reaching beyond the performance limits of the individual constituents. The recent trend in materials science is to effectively combine theoretical modeling with experimental work in order to gain deeper understanding of processes which are e.g., difficult to approach experimentally, but also to guide the experiments. In this paper, we explore the capabilities of standard density functional theory calculations to reliably predict structural, mechanical and electronic properties of alloys. To model the disordered alloys, we employ special quasi-random structures.

As the first example, we will discuss the maximum solubility limit of Al in cubic TiN, an archetype of hard coatings. In agreement with experimental observations, the transition from cubic rock-salt to wurtzite structure (ground state of AlN) is predicted at ~0.7 Al content on the metallic sublattice. Situation gets more complex in isovalent Zr- Al-N and Hf- Al-N systems where a dual-phase region develops between the single phase fields. Single elastic constants are nowadays a standard quantity to calculate. Here, we show the compositional trends for quasi-binary nitride coatings and will demonstrate the strong impact of texture on polycrystalline elastic constants. The latter is especially important for any comparison of theoretical and experimental results. In the final part, we will discuss the predictions of electronic structure and ELNES (electron energy loss near edge structure) for nitride hard coatings and wide band-gap semiconductors.

Biography

David Holec studied mathematics and physics at Masaryk University, Brno, Czech Republic. After completing his Ph.D. in materials science at the age of 28 years from University of Cambridge, UK, he has joined the group of Prof. Paul H. Mayrhofer at Montanuniversität Leoben, Austria. Currently, he is the head of the Materials Modeling Group at the Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Austria. He has published more than 35 papers in peer-review journals.

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