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Vacancies in MONTAN – a mechanism for tuning hardness–toughness relationshipFedor Klimashin¹, Nikola Koutná¹, David Holec², Paul H. Mayrhofer¹¹TU Wien, Vienna, Austria ²Montanuniversität Leoben, Leoben, Austria

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The cubic-structured nitrides of Mo and Ta exhibit excellent tribo-mechanical and electrical properties and are often used as alloying components to improve, for instance, materials resistance against wear and oxidation. The outstanding properties both materials owe to their inherent driving force to form vacancies. Fusing Mo–N^{1,2} with Ta–N² – experimentally and theoretically – we investigate a novel material system and present here the evolution of structure and mechanical properties of »MoNTaN« coatings triggered by varying the chemical potentials. The insights into the origin of the observed phenomena allow us to tune the hardness–toughness relationship and hence to design materials for applications requiring tailor-made properties.

References:

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MONTAN

Magnetron sputtering

Vacancies

Mechanical properties

Ab initio