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Influence of Nitrogen Stoichiometry on Properties of Low-Compressibility Advanced Nitrides J. E. LOWTHER, University of the Witwatersrand — The properties of two classes of recently synthesized advanced nitrides are investigated with the aim of considering how nitrogen stoichiometry affects the cohesive properties of this material. One is the class of cubic nitrides with a I43d structure of which Zr- and Hf-nitrides and the other a hexagonal  $P6_3/mmc$  structure and of which MoN and CoN have also recently been synthesized. All materials are considered to have low compressibility and thus speculated to have a high material hardness. Both categories of materials have an underlying nitrogen sub-lattice structure. Using ab-initio techniques the sublattice structure is considered as being a way through which properties of non-stoichiometric forms of these materials can be examined. Consequences of N stoichiometry on the crystal structure and elastic properties of these materials are suggested.

> J. E. Lowther University of the Witwatersrand

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