

## **Hardness characterization parameters of Niobium Carbide and Niobium Nitride: A first principles study**

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### **Abstract**

Niobium carbides and nitrides have been proposed as potential candidates for hardness and related applications, however, comprehensive studies are still needed for better understanding that may pave way for their re-engineering for the ultra-hard industry. Here we present ab initio Density Functional Theory calculations that provide a comprehensive description of various hardness characterization parameters. Our results show that NbC in rocksalt (RS) had a higher shear modulus, Young's modulus, and Voigt-Reuss-Hill shear modulus compared to other phases of NbC and NbN considered in this work. Further, it was noted that NbC in RS had a higher value of Vickers hardness amongst the various phases NbC and NbN studied, thus identified as a potential candidate for hardness and related application. Finally, we showed that compounds with Vickers hardness ( $H_v$ ) > 20 GPa were found to be brittle while those with  $H_v$  < 20 GPa were ductile.

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