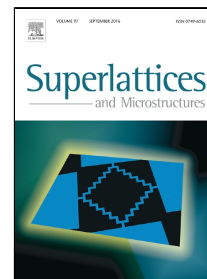


# Accepted Manuscript

Hardness in rare earth diboride systems: Ab initio full-potential study

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PII: S0749-6036(16)30579-1

DOI: [10.1016/j.spmi.2016.10.020](https://doi.org/10.1016/j.spmi.2016.10.020)

Reference: YSPMI 4565

To appear in: *Superlattices and Microstructures*

Received Date: 28 July 2016

Accepted Date: 08 October 2016

Please cite this article as: A. Zaoui, S. Ait Abderrahmane, M. Djermouni, S. Kacimi, F. Zazoua, M. Bejar, E. Dhahri, Hardness in rare earth diboride systems: Ab initio full-potential study, *Superlattices and Microstructures* (2016), doi: 10.1016/j.spmi.2016.10.020

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## Highlights

- > LSDA+*U* calculations were performed on  $\text{Tm}_{1-x}\text{Ti}_x\text{B}_2$  alloys.
- > The mechanical properties and electronic structure has been studied and discussed.
- > B-B bonds play a more important role than the Ti (Tm)-B interaction in these systems.
- > The covalent bond B-B is responsible for the hardness in these systems.

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