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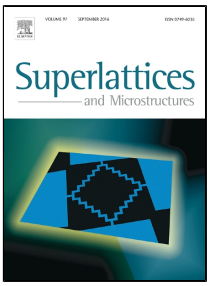

Hardness in rare earth diboride systems: Ab initio full-potential study

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Highlights

> LSDA+*U* calculations were performed on $Tm_{1-x}Ti_xB_2$ 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.