金属学报 2009, 45(10) 1185-1189 DOI: ISSN: 0412-1961 CN: 21-1139/TG

论文

第一性原理计算TiN(111)/BN/TiN(111)界面的电子结构、成键特性和结合强度

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摘要：

利用第一性原理计算方法研究了TiN(111)/BN/TiN(111)界面的16个理论界面构型.计算结果表明, 最稳定界面构型为top-top-BN 构型, 此构型中B原子只与周围N原子成键, 为四面体配位. 同时计算了top-top-BN构型的电子结构和成键特性以及界面结合强度, 结果表明, top-top-BN构型界面上的键为较强共价键,
其界面结合强度比TiN(111)板层或TiN块体材料的(111)晶面间的结合强度大, 说明此构型具有强界面特征.

关键词： 纳米复合薄膜 氮化物 界面 第一性原理

FIRST-PRINCIPLES CALCULATION OF ELECTRONIC STRUCTURE, BONDING CHARACTERISTIC AND BONDING STRENGTH OF TiN(111)/BN/TiN(111) INTERFACE

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Abstract:

The nanocomposite nc–TiN/a–BN as a representation of the family of superhard nitride–based nanocomposites, which is a nanocomposite thin film material, exhibits a significant hardness enhancement as compared with the pure constituents. In this paper, first–principles calculations were performed to investigate the role of interfaces in the nanocomposite 'nc–TiN/a–BN', to which less attention has been paid up to now. In order to determine theoretically the stable interface configuration in 'nc–TiN/a–BN', 16 possible theoretical TiN(111)/BN/TiN(111) sandwich interface cnfigurations have been constructed based on the stucture characteristic of 'nc–TiN/a–BN'. It is found in this calculation that the mst favorable interface configuration istop–top–BN, which is closely related to each B atom covalently bonding to its tetahedrally coordinated N atoms in it. ts electronic structure is calculated. The calculated results show that the bnds at the interface in 'top–top–BN'configuration are covalent. Its interface bonding strength is higher than that between two 111 crystalline planes in slab TiN or bulk TiN.

Keywords: nanocomposite film nitride interface first principle

收稿日期 2009-04-08 修回日期 2009-06-29 网络版发布日期 2009-09-15

DOI:

基金项目:

河北省教育厅科研计划资助项目z2008304

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