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材料合成及性能

TiN(001)表面上3N1Ti1Si岛构型及其演变的第一性原理研究

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摘要： 为了研究Ti-Si-N薄膜生长过程中界面的形成,采用第一性原理计算了在TiN(001)表面上3N1Ti1Si岛的各构型的总能量和吸附能,并计算了Si-in-3N1Ti构型转向Ti-in-3N1Si构型的两种演变方式所对应的激活能。计算结果表明:在3N1Ti1Si的几种构型中,Ti-in-3N1Si构型是最低能量的稳定结构,这种构型是由SiN相从TiN相中分离出来而形成的;两种演变方式中以Si粒子迁出Ti粒子迁入所需构型演变的激活能较小,更容易实现构型演变;与2Ti2N1Si构型演变相比,3N1Ti-1Si岛演变中SiN与TiN分离比较容易实现,这意味着适当增加氮分量有利于SiN与TiN的分离。

关键词： 界面形成条件 相分离 构型演变 激活能 第一性原理

Configuration and Evolution of 3N1Ti1Si Island on TiN(001) Surface：Ab Initio Study

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Abstract: In order to study the interface formation in the growth process of Ti-Si-N films, a series of calculations have been carried out with the first principle method to investigate the total energies and adsorption energies of some 3N1Ti1Si island configurations on the TiN (001) surface, and also the activation energies of two kinds of transformations from the Si-in-3N1Ti configuration to the Ti-in-3N1Si configuration. The calculations present some interesting results:(1) According to the energies of all 3N1Ti1Si configurations, the Ti-in-3N1Si configuration is a relative stable structure. It implies that silicon atom outside of TiN island could lead to the structure stable. (2) In the island evolution from the Si-in-3N1Ti configuration to the Ti-in-3N1Si configuration, the diffusion of silicon and titanium atoms need less activation energy than the diffusion of nitrogen atoms. (3) Compared with the evolution of 2Ti2N1Si island, the phase separation of SiN and TiN could be easily performed in the evolution of 3N1Ti-1Si island. This means that properly increasing the partial pressure of nitrogen in the deposition is beneficial to the interface formation in Ti-Si-N film growth process.

Keywords: interface formation condition phase separation configuration evolution diffusion energy first-principles

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