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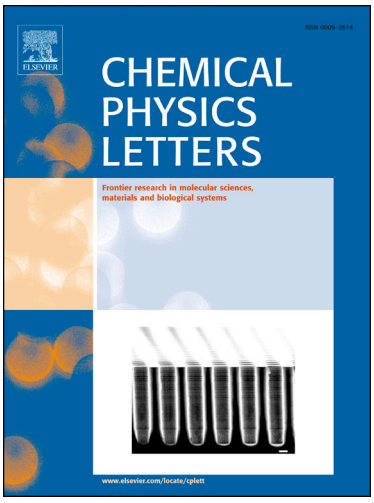

Research paper

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First-principles study of the effect of Cr and Al on the oxidation resistance of WSi_2

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Abstract: By means of first-principles approach, we systematically investigate the effect of Cr and Al on the oxidation resistance of WSi_2. The interstice sites oxygen prefers to occupy are considered. Moreover, Cr and Al tend to occupy the Si sites of WSi_2, and they are thermodynamically stable. The oxygen diffusion in various interstitial sites of undoped and doped WSi_2 are studied, respectively. Importantly, Cr and Al can improve oxidation resistance of WSi_2 obviously, and Cr, Al co-doped system has the best oxidation resistance. The improvement of oxidation resistance is attributed to the formation of Al-O and Cr-O bonds.

Keywords: WSi_2, Oxidation resistance, Alloying, First-principles calculations

1. Introduction

Transition metal disilicides are considered as promising candidate materials for high temperature structural applications due to their outstanding high-temperature performance [1-6]. Among these disilicides, WSi_2 has been regarded as an attractive structural materials due to its high melting point (2160℃), great corrosion resistance and excellent mechanical property at elevated temperature, which makes it have many applications, such as being used as high temperature structural materials and protective coatings for hot components in jet engines [7-9]. Unfortunately, WSi_2 suffers from the so-called "pest oxidation" generating through oxygen diffusion along pores, grain boundaries and internal cracks during low-temperature oxidation, which results in a catastrophic failure of some intermediate range by degradation to powder [10]. Shao et al [11] further reported that tungsten can form a powdered oxide WO_3, which will spall off at higher temperature so that the dense SiO_2 oxide film can no longer protect the alloy. Since the pest oxidation restricts the application of WSi_2 seriously, it is necessary to improve its intrinsic oxidation resistance. Alloying elements such as Cr, Al, Hf and Ti, have been used to improve the oxide's protective ability in transition metal silicides [12-15]. It's worth mentioning that two such elements (Cr and Al) have shown promise due to the nature of their oxidation products. The previous studies have mainly concentrated on improving the mechanical properties