Mixed-mode mechanical strength and failure of Ni/Al_2O_3 interface from first-principles

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INTRODUCTION

Thermal barrier coatings (TBCs) spallation and delamination are well-known problems that have been addressed by a number of experimental and theoretical studies. Premature failure often occur along the interface between bond coat and thermally grown oxide (TGO) by microcrack nucleation, propagation and coalescence, leading eventually to spalling and delaminating of the TBC. To prevent these premature failure in TBCs, it is important to improve the adhesion strength between the bond coat and the TGO. This study focuses on modeling of $Ni/\alpha\text{-}Al_2O_3$ interfaces.

Many researchers have analyzed mechanical response of $Ni/\alpha\text{-}Al_2O_3$ interfaces under tension and shear, in order to give a quantitative evaluation of interfacial adhesion strength [1, 2]. However, little theoretical work has been reported on the $Ni/\alpha\text{-}Al_2O_3$ interfaces under mixed-mode loading so far. Therefore, it is essential to perform such as first-principle calculations on the Ni/Al_2O_3 interfaces to determine their mechanical strengths, as well as the nature of the Ni/Al_2O_3 bondings and failure mechanisms.

In this study, we performed the first-principle mixed-mode simulations for the Al-terminated O-site Ni(111)/α-Al_2O_3(0001) interfaces that displace along 22.5°, 45° and 67.5° orientation with respect to the interface. Firstly, their mechanical strengths are obtained. The evolution of atomic structures of these interface models are observed, and the failure mechanisms are elaborated from the computational results. Furthermore, the implications to failure criterion and fracture toughness of the interface are discussed in detail.

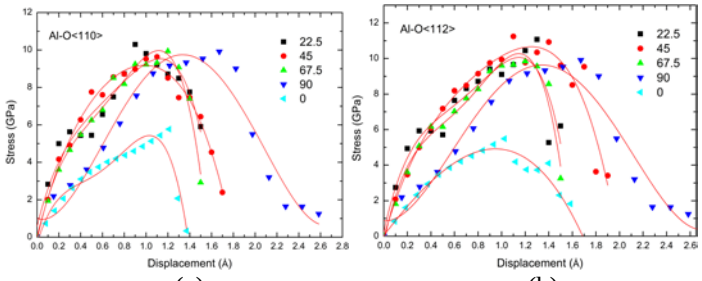
METHODOLOGY

Our first-principle tensile, shear and mixed mode calculations are carried out using the VASP code. The generalized gradient approximation (GGA) of projector augmented wave (PAW) method is adopted for parametrization of the exchange-correlation functional. The *k*-point sampling was attained upon using 5×5×1 points in a regular Monkhorst–Pack (MP) scheme. The plane-wave cutoff energy of 500 eV and an energy convergence criterion of 10^{-5} eV for self-consistency are adopted throughout all the calculations. Relaxation is done until the Hellman-Feynman forces are less than 0.01 eV/Å using a conjugate gradient algorithm. The coherent Ni(111)$(\sqrt{3}\times\sqrt{3})$/α-Al_2O_3(0001)(1×1) interface model was dealt with in present work. Focus was put on the Al-terminated O-site model (in short, Al-O model hereafter).

RESULTS AND DISCUSSION

Stress- displacement curves

The first output of our first principle calculations is the stress-displacement curves for the interface model along <110> and <112> directions of the Ni lattice, as shown in Fig. 1. It is seen that the maximum stresses of the Al-O model at 0° loading case (i.e. shear) are relatively smaller than that at other cases, probably due to the difference of the simulation methods adopted. Secondly, first principle study gives directly the evolution of atomic structures during loadings, and therefore it is rather easy to identify their deformation and failure characteristics. Furthermore, the potential usage of these results that could offer in fabricating thermal barrier coatings and in analyzing their mechanical response are discussed in particular.



(a) (b)

Fig. 1. The stress versus displacement curves: (a) Al-O<110> and (b) Al-O<112>.

References

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