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Niobium/alumina bicrystal interface fracture: A theoretical interlink between local adhesion capacity and macroscopic fracture energies

A. Siddiq [a,*], S. Schmauder [a], M. Ruehle [b]

[a] Institut für Materialprüfung, Werkstoffkunde und Festigkeitslehre (IMWF), Universität Stuttgart, Pfaffenwaldring 32, 70569 Stuttgart, Germany
[b] Max-Planck Institute for Metal Research, Heisenberg Strasse 3, 70569 Stuttgart, Germany

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Abstract

In the presented work, an effort has been put to clear up the theoretical interlink between local adhesion capacity and macroscopic fracture energies by bridging different length scales, such as nano-, meso-, and macro-scale. Crystal plasticity theory along with a cohesive modelling approach has been used during this work. The influence of different cohesive law parameters (cohesive strength, work of adhesion) on the macroscopic fracture energies for three different orientations of niobium/alumina bicrystal specimens has been presented. It is found that cohesive strength has a stronger effect on macroscopic fracture energies as compared to work of adhesion. In the last part a generalized correlation among macroscopic fracture energy, cohesive strength, work of adhesion and yield stress is derived. The presented results can provide a great help to experimentalists in order to design better metal/ceramic interfaces.

Keywords: Metal/ceramic interface; Crystal plasticity; Cohesive model; Fracture mechanics; Work of adhesion

1. Introduction

Interfaces between metal and ceramic play an important role in many applications, because they combine the properties of metals like ductility, high electrical and thermal conductivity and the properties of ceramics like high hardness, corrosion resistance and capacity of resistance to wear. Some of the applications of metal/ceramic joints include automotive industry, turbine blades, high pressure sodium lamps, squid magnetometers and dental implants. The fracture at or near such interfaces often limits the reliability of these joints. In the past, niobium/alumina interfaces have been studied experimentally [1–5] and numerically [6–8]. Single crystalline alumina/niobium/alumina joints were investigated in [1,2] for different orientations of single crystalline

* Corresponding author. Tel.: +44 114 22 28874; fax: +49 711 685 62365.
E-mail addresses: a.siddiq@shef.ac.uk, amir.siddiq@gmail.com (A. Siddiq).

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niobium. The results showed that the orientations of single crystalline materials have significant effects on the energies of the niobium/alumina interface fracture. It has been observed experimentally [3,4] that the amount of plasticity initiated in the metal during fracture of such interfaces is strongly influenced by both, the interface chemistry and the orientations of slip systems relative to the crack surface due to which the fracture energy of niobium/alumina bicrystal interfaces changes dramatically with relative crystallographic orientation of the two constituents, i.e. metal and ceramic. Isotropic polycrystalline niobium/alumina interfaces were studied experimentally as well as numerically in [5,6]. It was shown that a low yield stress results in high plastic deformation in the metal part and consequently a higher plastic energy is dissipated before the critical stress value for fracture is reached. In order to study crystal orientation effects on crack initiation energies of bicrystalline niobium/alumina interfaces, crystal plasticity theory [7,8] was used in [9,10]. The results showed that by changing the orientation of the single crystalline material, one can change the amount of plasticity induced due to the activation of different slip systems, also, the level of stresses induced at and near the crack tip were found to be different. The reason of the variation in fracture energies for various orientations were explained on the basis of induced stresses and plasticity due to the activation of different slip systems around the crack tip. Interface fracture of a metal/ceramic bicrystalline interface (niobium$(1\,1\,0)[0\,0\,1]$/alumina$(1\,1\,\bar{2}\,0)[0\,0\,0\,1]$) using a cohesive modelling approach and conventional crystal plasticity theory was studied in [11]. The effect of different cohesive law parameters, such as, cohesive strength and work of adhesion on the macroscopic fracture energy was studied. It was found that the effect of cohesive strength on fracture energies is more profound as compared to the work of adhesion. A comparison between experimental and simulation results was presented and a theoretical interlink among cohesive strength, work of adhesion, yield stress and macroscopic fracture energy was presented.

The aim of the present work is to study the interface fracture behaviour of two other orientations (niobium$(1\,0\,0)[0\,0\,1]$/alumina$(1\,1\,\bar{2}\,0)[0\,0\,0\,1]$ and niobium$(1\,1\,1)[\bar{1}\,\bar{1}\,2]$/alumina$(1\,1\,\bar{2}\,0)[0\,0\,0\,1]$) of niobium/alumina bicrystal specimens using crystal plasticity theory [7,8] and a cohesive modelling approach [12]. The effect of different cohesive law parameters, such as cohesive strength and work of adhesion, on the fracture energies of the bicrystal niobium/alumina interfaces is studied for the different orientations. Cohesive model parameters are identified for different combinations of cohesive strength and work of adhesion by applying a scale bridging procedure as shown in Fig. 1. For each value of work of adhesion [20–22], the cohesive

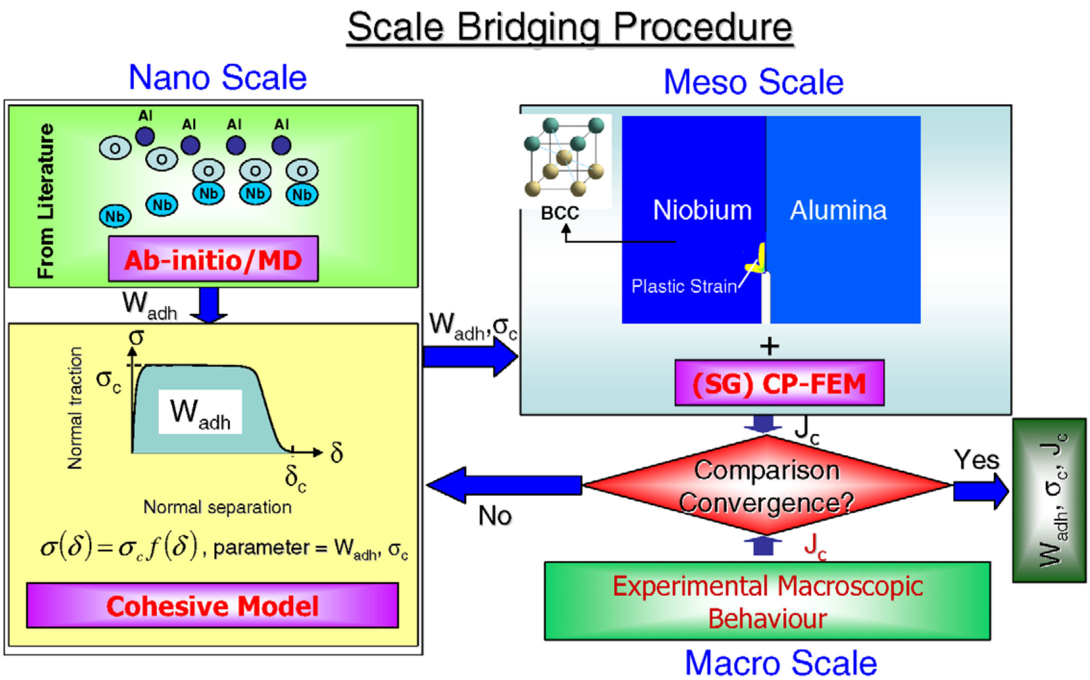

Fig. 1. Scale bridging procedure for metal/ceramic interface fracture.