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Preface

This volume contains all ICTAM 2016 Papers presented as:
- Plenary Lectures,
- Prize Lectures - Batchelor and Hill
- Sectional Lectures
- Mini-symposia presentations
- Thematic Session presentations, and
- Short Talk with Poster presentations.

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Foreword

The organizers are proud to present the ICTAM2016 papers.

The electronic collection contains all submissions accepted for either oral or poster presentation as of July 8, 2016.

Papers received after this date, as well as those included here, can be accessed using the my*ICTAM2016* congress mobile app.

After the Congress itself all papers will be archived on the permanent IUTAM website.

We would like to thank all the members of the International Program Committee, for generating the content for such an inspiring scientific program. We would also like to acknowledge the tremendous work performed by the National Research Council of Canada and Legend Conference Planning for converting all our ideas into an actual Congress program.

Papers are presented as they were submitted. The organisers take no responsibility for the content language and errors in the texts.

The International Program Committee
ICTAM 2016
Montreal, Canada

ASSESSMENT OF THE STRENGTH OF NANOCOMPOSITES BASED ON INTERFACE BONDING ANALYSIS

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Summary Recent investigations reveal that interface bonding strength is dependent on the relative orientation of crystallites of the both phases [2]. The experimental, theoretical and computational investigations confirm this observation in the case of Cu/α-Al_2O_3 system, [3], [4]. It is shown that the statistical distribution of the values of interface strength for different relative orientations of bonded phases should be included in the phenomenological model of the damage initiation in nanocomposites. The novelty of the presented study is the combination of different experimental techniques: HRTEM, EBSD and molecular dynamics simulations with phenomenological theory of damage development in nanocomposites due to debonding at the interphase boundary [5], [6], [7]. A class of new models with the yield condition determined by one of quadric surfaces, in particular paraboloid or ellipsoid one is considered and the comparison with popular Gurson approach is discussed, [8].

INTRODUCTION

In recent studies on modern materials the information from sophisticated observation techniques and molecular simulations at different levels flows across scales into the decision process of modelling and design, which enables rational tailoring of materials [1]. The concept of workflow integration rather than multiscale integration is applied in the presented paper.

The experimental studies show that the geometry of interphase boundaries and in particular the relative orientation of crystallites of the both phase is one of the crucial factors determining the toughness of metal/ceramic composites [2]. The experimental, theoretical and computational investigations presented in [3], [4] confirm this observation in the case of Cu/α-Al_2O_3 system. Until now there is lack of a model adequately tuned to include the dependence of the strength of the interface bonding on the phase orientation . It is also known observation that the size of the ceramic inclusion embedded in metal matrix decides about the mode of fracture initiation in the composite. If the inclusion is of nanosize diameter the far-field stresses produce the particle/matrix debonding, while in the case of larger particles cracks in ceramic inclusion are developing, [5].

The aim of the paper is identification of the structure, strain, bonding strength and the fracture process at the bimaterial interface. The particular value of the final result consists in using the series of experimental data from complementary investigation methods: EBSD and HRTEM. The first of them provides the information statistically valid and the other one enables detailed local characterization. The experimental data are supplemented by the results of molecular dynamics (MD) computations and a theoretical analysis. The discussed complex characterization of the bimaterial interface is performed on the example of Cu/α-Al_2O_3 boundary. As a result the mechanism of bonding is revealed and a new phenomenological model is proposed that enables introducing the statistical distribution of the bonding strength into the prediction of nanocomposite material toughness.

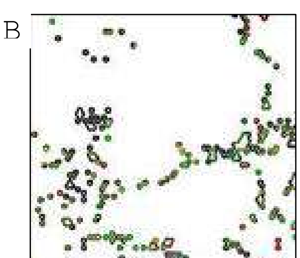
PHYSICAL MOTIVATION

EBSD examination: orientation relationships at interphase boundaries

Corundum nano-particles (red) embedded in a copper matrix (green) were investigated with the use of Electron Back Scattered Diffraction technique (EBSD), [3], [4], Fig. A. Picture B demonstrates an example of EBSD results showing the interphase boundaries: basic orientation relationship (red) and new ones with improved bonding strength (green and yellow).

A

B



HRTEM studies: microstructure observations and modelling

The set of orientation relationships uncovered by EBSD method in composites manufactured by the powder metallurgy is observed also in the Cu/α-Al_2O_3 heterostructures obtained by Pulsed Laser Deposition (PLD). It leads to the conclusion that the revealed misorientations are typical for the copper/ corundum interphase boundary regardless of a synthesis way. The interface with the basic orientation relationship was studied with the use of HRTEM technique. The obtained images are used to three-dimensional reconstruction of the junction microstructure by MD simulations [5]. The results show that strong

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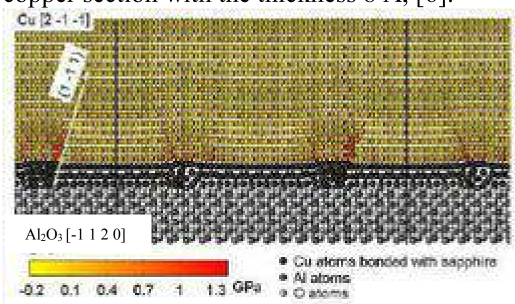
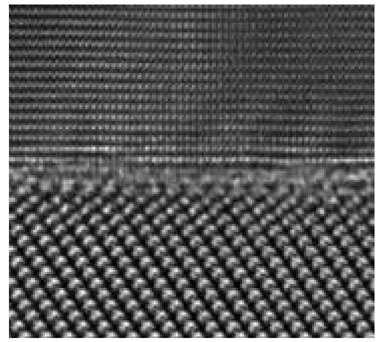
bonding between copper and α-Al_2O_3 induces structural changes in the (111) Cu layer nearest the substrate and leads to formation of the system of partially dissociated dislocations in the next layer. In consequence, the Cu/α-Al_2O_3 interface becomes the semicoherent system. The lattice matching regions of the individual Cu layers are significantly lowered, which results in strong deformations along the closed packed planes (see the pictures below). The interfaces with the improved strength (see images from EBSD investigation) exhibit more intense structural changes which reach much deeper into the metal layer [4].

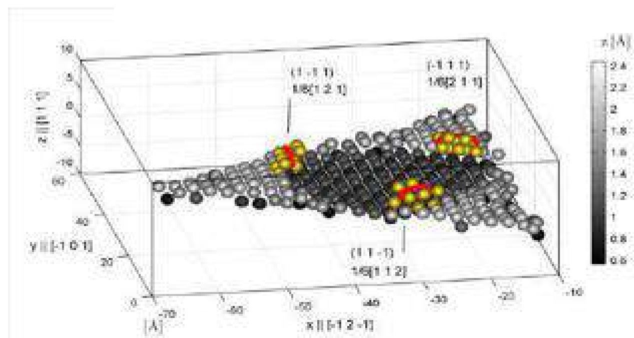
Distribution of elastic strain energy density in the copper section with the thickness 8 Å, [6].





HRTEM image of the Cu/α-Al_2O_3 interface, [6].

An example of the MD simulation of the stacking faults areas. The Cu atoms (yellow) limited by partial dislocations (red) within the planes (1 -1 1), (-1 1 1) and (1 1 -1). The position of atoms belonging to the first Cu layer (grey scale), [7].



MAIN RESULTS AND CONCLUSION

The presented discussion reveals the necessity of accounting for the statistical distribution of the values of interface strength for different relative orientations of bonded phases into the phenomenological model of nanocomposites subjected to damage initiation due to debonding. An energy-based approach resulting in the new model of damaged nanocomposites with the yield condition determined by one of quadric surfaces, in particular paraboloid or ellipsoid one is considered, [8]. Also the comparison with the popular Gurson criterion is discussed. The novelty of the presented multidisciplinary study is the combination of different experimental techniques: HRTEM and EBSD in relation with the results of MD computations with phenomenological theory of damage development in nanocomposites due to ceramic particles debonding.

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