ATOMISTIC MODEL OF DECOHESION OF COPPER-CORUNDUM INTERFACE

***Marcin Maździarz*[1], *Kinga Nalepka*[1,4], *Zygmunt Szymański*[1], *Jacek Hoffman*[1], *Sławomir Kret*[2], *Stanisław Kucharski*[1] *and Paweł Nalepka*[3]**

[1]*Department of Computational Science, Institute of Fundamental Technological Research Polish Academy of Sciences, Pawińskiego 5B, 02-106 Warsaw, Poland*

[2]*Institute of Physics Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland*

[3]*Department of Engineering and Machinery for Food Industry, Agriculture University of Cracow, ul. Balicka 122, 131-149 Cracow, Poland*

[4]*Department of Strength and Fatigue of Materials and Structures, Faculty of Mechanical Engineering and Robotics, AGH University of Science and Technology, Al.Mickiewicza 30, 30-059 Cracow, Poland*

1. Aim of the paper

The object of the paper is an atomistic, molecular statics (MS) reconstruction of the Cu- α-Al_2O_3 heterostructure formed by means of a pulsed laser deposition technique (PLD). The molecularly reconstructed copper on sapphire substrate is then used for the examination of decohesion in the region of the interface. For this purpose, a molecular statics nanoindentation simulation is performed.

2. Introduction

The strength of metal-ceramic interfaces is the key properties for the performance of many devices and structural elements: microelectronic devices, thermal barrier coatings used to protect the metallic components and metal-ceramic composites are just a few examples. Therefore, a detailed research of the decohesion in the phase boundary is an important issue.

Applying the PLD technique, an epitaxial Cu layer has been formed on a sapphire substrate. The obtained heterostructure has been examined by means of the High Resolution Transmission Electron Microscopy (HRTEM) (see Figure 1). As a result, the misorientaion of Cu layer relative to the α-Al_2O_3 substrate is determined and subsequently, the system of defects due to the mismatch between the copper and sapphire is identified. Describing the interatomic interaction by the Tight Binding Second Moment Approximation (TB-SMA) potential [2] in the formed proposed in [5], the experimentally observed microstructure in the region of the interface is reconstructed. The obtained, atomistic model of the copper layer is subjected to nanoindentation [1, 3, 4]. During the carried out simulation, the displacement vs. applied force curve is registered, which enable us to identify the decohesion in the interface region [6].

3. Problem description

In this research, copper with purity 99.999% (Kurt J. Lesker Company Ltd.) was deposited on the (0001) α-Al_2O_3 surface (CrysTec GmbH) by PLD. For this purpose, a Nd:YAG laser beam with the wavelength 355 nm, pulse duration 10 ns and the frequency repetition 10 Hz was focused on the copper target (focal spot area 2.5 mm^2, fluence 2 J/cm^2). The sapphire substrate was heated at $800\,^{\circ}\mathrm{C}$ and pressure in the chamber was set to $5\text{x}10^{-6}$Pa.

During the deposition, Cu islands are formed (Volmer-Weber growth mode), (see Figure 1). The reason is that, copper has the higher surface energy then sapphire. The dominant orientation of Cu islands with respect to the α-Al_2O_3 substrate is $(111)\,[01\bar{1}]\mathrm{Cu}\,||\,(0001)[1\bar{1}00]\mathrm{Al_2O_3}$, that is, the closed packed planes and directions of the both crystals are parallel to each other. Additionally, the HRTEM images enable the identification of the Cu lattice deformation resulting from the mismatch between

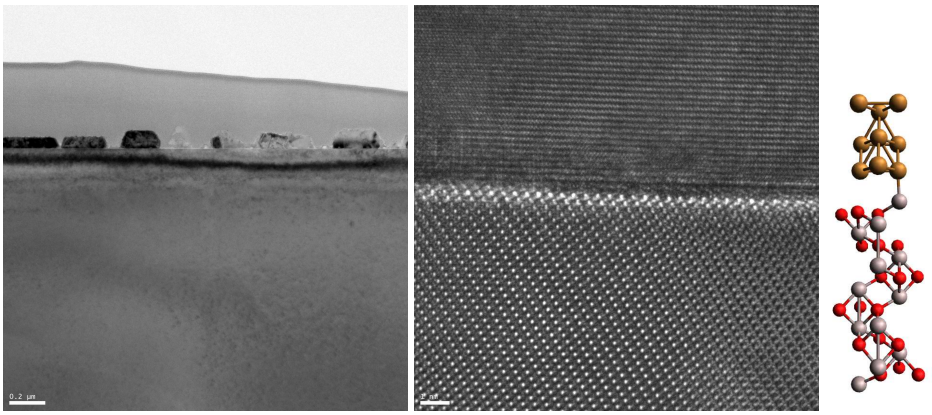

Figure 1. Islands of Cu on Al_2O_3 substrate, HRTEM images of the Cu(*top layer*) Al_2O_3 (*down layer*) interface and periodic cell of Cu-Al_2O_3.

the copper and sapphire. The obtained data are used for the reconstruction of the microstructure in the interface region. For this purpose, the interatomic interaction in the Cu layer are described by the TB-SMA potential [2] in the form determined in [5]. Performing the relaxation of the Cu layer (Molecular Static Simulation), the final microstucture in the interface region is obtained.

The reconstructed Cu layer on the α-Al_2O_3 substrate is used in the molecular statics simulation of nanoindentation in which the behaviour of the defected structure in a nonequilibrium configuration is investigated [4]. Analyzing the obtained displacement vs. applied force curve we try to explain the observed decohesion [6].

Acknowledgments

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4. References

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