ATOMISTIC MODEL OF DECOHESION OF COPPER-CORUNDUM INTERFACE

Marcin Mażdziarz¹, Kinga Nalepka¹, ¹, Zygmunt Szymański¹, Jacek Hoffman¹, Sławomir Kreț², Stanisław Kucharski¹ and Paweł Nalepka³

¹Department of Computational Science, Institute of Fundamental Technological Research Polish Academy of Sciences, Pawiński 5B, 02-106 Warsaw, Poland
²Institute of Physics Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland
³Department of Engineering and Machinery for Food Industry, Agriculture University of Cracow, ul. Balicka 122, 131-149 Cracow, Poland
⁴Department 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-Al₂O₃ 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 misorientation of Cu layer relative to the α-Al₂O₃ 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-Al₂O₃ 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 mm², fluence 2 J/cm²). The sapphire substrate was heated at 800 °C and pressure in the chamber was set to 5×10⁻⁶Pa.

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-Al₂O₃ substrate is (111)|[01T]Cu|[0001]|T00|Al₂O₃, 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
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 microstructure in the interface region is obtained.

The reconstructed Cu layer on the $\alpha$-Al$_2$O$_3$ substrate is used in the molecular static 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

The research was done within the framework of the Project N501 156638 founded by the Polish Ministry of Science and Higher Education.

4. References


