POLISH ACADEMY OF SCIENCES

INSTITUTE OF FUNDAMENTAL
TECHNOLOGICAL RESEARCH
AND
COMMITTEE ON MECHANICS

40th SOLID MECHANICS CONFERENCE
29.08 - 2.09 2016, WARSAW

URL: http://solmech2016.ippt.pan.pl/table/abstracts.html

Analysis of deformation mechanisms in Cu / α- Al_2O_3 interfaces with the use of HRTEM images

P. Nalepka[1], K. Nalepka[2], R.B. Pęcherski[3]

[1] Department of Engineering and Machinery for Food Industry, Agriculture University in Krakow, Cracow, Poland
[2] Department of Strength and Fatigue of Materials and Structures, AGH University of Science and Technology, Cracow, Poland
[3] Institute of Fundamental Technological Research of the Polish Academy of Sciences, Warsaw, Poland

The composition of metal with ceramics is applied to many devices, structural elements of machines as well as their equipment. Therefore, evaluating the strength of interfaces of this type becomes an important scientific issue of fundamental character. Numerous attempts are made to solve the posed problem, both experimental and theoretical ones. In the first case we receive the results, to a large extent, biased. The strength of the interfacial bonding is defined as the mean value for junctions formed by polycrystalline materials. In addition, testing is associated with the induction of various unwanted processes of energy dissipation. As a matter of fact, the results are neither adequate nor accurate. Theoretical approach enables local, more precise determining the mechanical properties of interfaces. The basis of conducted calculations is the geometry of the interface strongly preferred by the considered system of materials. It is defined by the mutual orientation of crystallites of two phases and the position of the plane boundary. The combination of two advanced research methods: electron back-scatter diffraction (EBSD) and high resolution transmission electron microscopy (HRTEM) enables identification of this crucial characteristics. The second of them additionally reveals a representative microstructure of the interface in the form of a projection. We reconstruct it in three dimensions by means of molecular dynamics (MD) simulations. In this way, we identify deformation mechanisms that enable the formation of the bonding between the metallic phase and ceramic one. The correct mapping the microstructure at the interphase boundary constitutes the direct basis for evaluation of the strength of the junction. The measure of this key mechanical property is a separation work or energy required to separate the heterostructure along the interface plane per unit area.

For calculation, we assume an initial system in the form of a heterostructure consisting of monocrystalline layers of copper and corundum. The α-Al_2O_3 and Cu lattices as well as the interface plane are oriented in accordance with data registered in the HRTEM images. The assumed disorientation belongs to typical ones for the studied system, which is confirmed by the EBSD method [1], [2]. The HRTEM images show also considerable deformations of the metal layer in comparison with these in the ceramic region [3]. Therefore, we assume that the corundum lattice remains undisturbed, while the copper layer matches it by a small uniform compression along the interface plane. In this way, we obtain a computational cell which generates the examined system by the replication in two dimensions. Interatomic interactions in the copper layer are described by means of the embedded atom method (EAM) model which was specified and verified by Nalepka [4], [5]. The interface reconstruction is obtained by applying the canonical ensemble (NVT) at the temperature of 0 K. Due to a strong bonding at the interphase boundary, the semi-coherent system is formed. The neighborhoods of coherency nodes in subsequent Cu planes lying on the corundum surface move toward the interface. As a result, these layers lose the continuity. The coherency regions of the Cu plane nearest the interface undergo structural changes. In this way, they take the symmetry of the Al layer terminating corundum. The separation of the coherency regions of the further Cu layers occurs along the slipping planes (-1 1 1), (1 -1 1), (1 1 -1) (Fig. 1, Fig. 2). As a result, Shockley partial dislocations are formed in these planes.

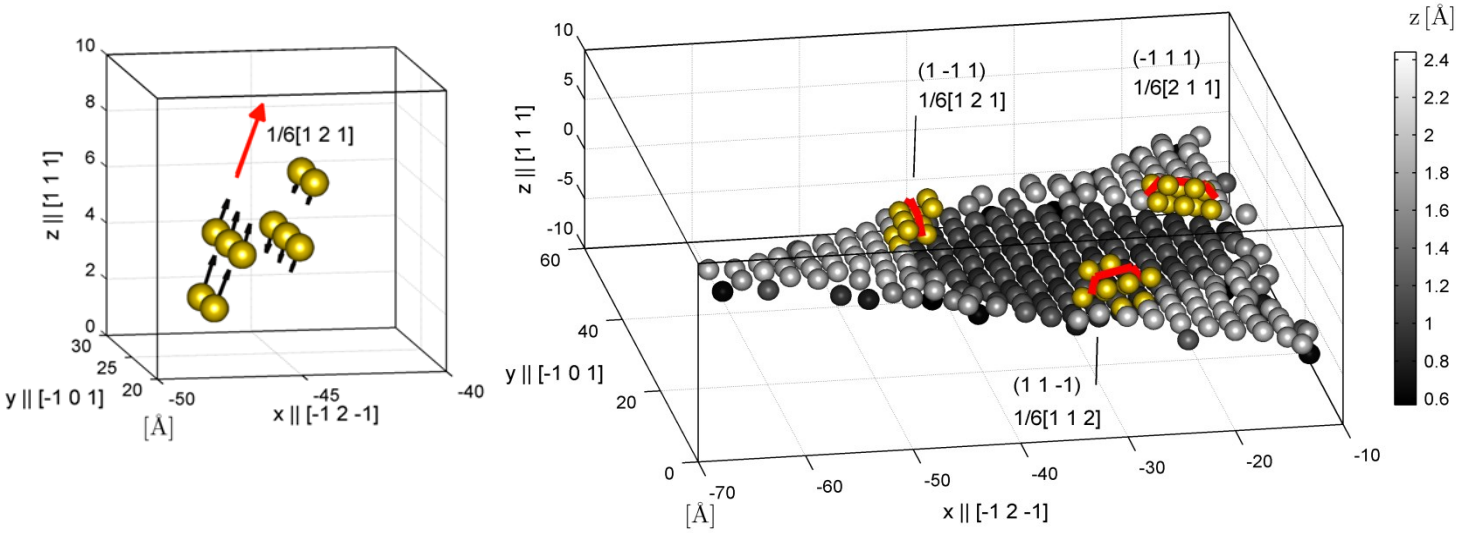

Fig. 1 A slip along (1 -1 1) plane (a), regions of intrinsic stacking faults (marked by yellow color) surrounded by partial dislocation in (1 -1 1), (-1 1 1), (1 1 -1) planes as well as deformation of the Cu layer nearest the interface: the neighborhood of a coherency node (atoms in grey scale) (b).

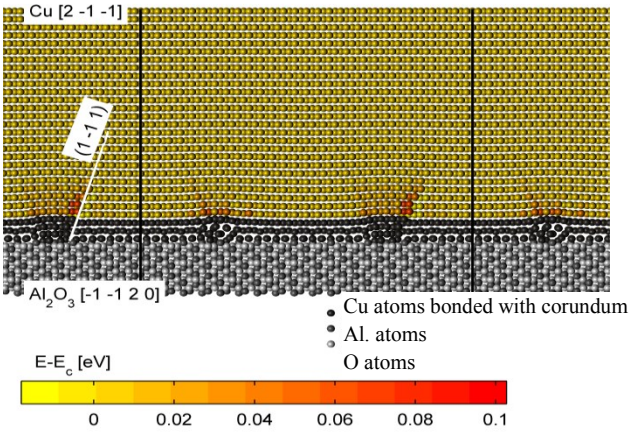

Fig. 2 Distribution of energy changes with respect to the equilibrium state per atom in a section of copper. The chart also illustrates the distribution of an analogical characteristic – density of elastic strain energy.

The obtained reconstruction includes the crucial features of the real microstructure of the copper/ corundum junction. It is confirmed by a good agreement between the HRTEM image generated on the basis of the formulated model and the experimental micrograph. The discussed above changes in the Cu layer are also described by strain fields obtained with the use of the geometrical phase analysis (GPA). The presented results enable in-depth understanding processes registered in HRTEM images as well as identify the mechanisms of deformation and failure in the Cu / α- Al_2O_3 interfaces.

Literature

[1] K. Nalepka, K. Sztwiertnia, P. Nalepka, Acta Materialia 104 (2016) 156-165.
[2] K. Nalepka, K. Sztwiertnia, P. Nalepka, R.B. Pęcherski, Archives of Metallurgy and Materials 60 (2015) 1953-1956
[3] K. Nalepka, J. Hoffman, S. Kret, P. Nalepka, and Z. Szymanski, Applied Physics A 117 (2014) 169-173
[4] K. Nalepka, Computational Materials Science 56 (2012) 100-107.
[5] K. Nalepka, Bulletin of the Polish Academy of Sciences: Technical Sciences 61 (2013) 441 – 450.