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THE STRENGTH ANALYSIS OF Cu/α−Al_2O_3 INTERFACES AS A KEY FOR RATIONAL COMPOSITE DESIGN

ANALIZA WYTRZYMAŁOŚCI INTERFAZ Cu/α−Al_2O_3 JAKO KLUCZ DO RACJONALNEGO PROJEKTOWANIA KOMPOZYTÓW

Electron back-scattered diffraction (EBSD) studies carried out for the Cu/α−Al_2O_3 composites manufactured by pulsed laser deposition method and by the powder metal- lurgy enable to uncover a set of orientation relationships characteristic for materials of this type. The identified interfaces are categorized according to the bonding strength. Additionally, their microstructure is reproduced by molecular dynamic (MD) simula- tions. The obtained classification of the phase boundaries constitutes key information for effective composite design.

keywords:

Badania EBSD (Electron Back-Scattered Diffraction) przeprowadzone dla kompozytów Cu/α−Al_2O_3 wytworzonych metodą ablacji laserowej (Pulsed Laser Deposition) oraz metalurgii proszków umożliwiły odkrycie zbioru związków orientacji charakterystycznych dla tego typu materiałów. Zidentyfikowane warstwy przejściowe skategoryzowano zgodnie z wytrzymałością wiązania. Dodatkowo, ich mikrostrukturę odtworzono za pomocą symulacji dynamiki molekularnej (MD). Otrzymana klasyfikacja granic fazowych stanowi kluczową informację do efektywnego projektowania kompozytów.

1. Introduction

Bonding at a phase boundary is one of the important factors determining the toughness of metal/ ceramic composites [1]. The interface bonding strength depends on the relative orientation of crystallites of the both phases [2]. A representative example for junctions of this type constitutes the Cu/α−Al_2O_3 system. The aim of the paper is a theoretical analysis of the Cu/α−Al_2O_3 interface strength for experimentally identified misorientations. EBSD (Electron Back Scattered Diffraction) studies reveal the presence of series of misorientations which are typical for the combined materials regardless of a synthesis method [3, 4]. This is confirmed by the analysis of the results obtained for composites manufactured by powder metallurgy Cu/(5% vol.)α−Al_2O_3 and nanocomposites Cu/α−Al_2O_3 deposited by PLD (Pulsed Laser Deposition) method (Sec.2). Applying the Gautam and Howe method [2] the observed interfaces are categorized according to the bonding strength. Additionally, their atomistic structures are recreated in the form of molecular dynamic (MD) models (Sec.3). In conclusion, it is underlined that the uncovered classification of the interfaces makes a basis for the rational composite design.

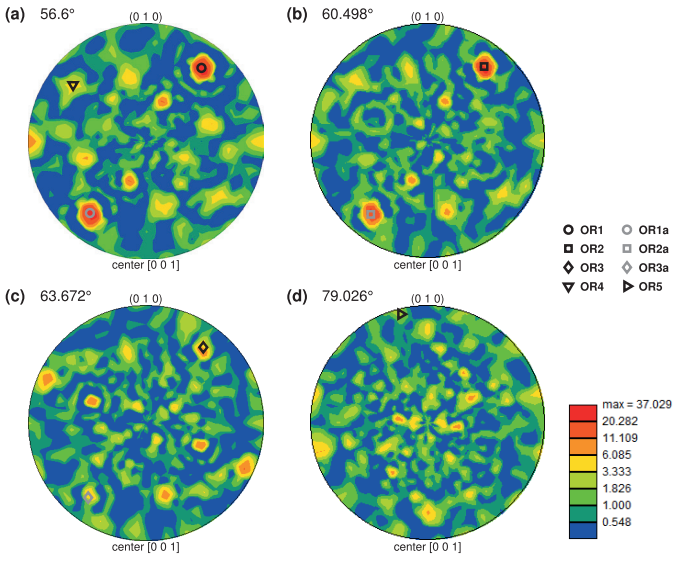

Fig .1. Misorientation Distribution Function for PLD nanocomposites; cross-sections of constant misorientation angle: 56.600°, 60.498°, 63.672° and 79.026°. The representative orientation relationships are denoted by black and gray markers

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2. EBSD investigation of Cu/α−Al_2O_3 interfaces

The analysis of EBSD results reveals that the four following misorientations appear with a high frequency: (-1 1 1)[1 1 0]Cu||(0 0 0 1)[0 1 -1 0] α−Al_2O_3, (1 -1 1)[1 1 0]Cu (0 0 0 1)[0 1 -1 0] α−Al_2O_3 and (-7 7 6)[1 1 0]Cu (0 0 0 1)[0 1 -1 0] α−Al_2O_3, (7 -7 6)[1 1 0]Cu (0 0 0 1)[0 1 -1 0] α−Al_2O_3 (Fig. 1a, b and Fig. 2a, b). In this paper they are referred to as OR1, OR1a and OR2, OR2a orientation relationships. The misorientations are strongly preferred both in composites deposited by the laser beam and in those obtained by means of the powder metallurgy. The orientation relationships OR1a and OR2a can be described in a symmetrically equivalent way: (-1 1 1)[-1 -1 0]Cu||(0 0 0 1)[0 1 -1 0] α−Al_2O_3 and (-7 7 6)[-1 -1 0]Cu||(0 0 0 1)[0 1 -1 0] α−Al_2O_3. The formulation shows that the four identified misorientations form pairs whose components differ in the Cu crystal rotation of 180° about the normal to the (0 0 0 1)α−Al_2O_3 surface. If we compose the two-fold axis with the inversion center of the sapphire crystal, the coupled misorientations can be perceived as such in which the α−Al_2O_3 crystal is reflected by the (0 0 0 1) mirror plane. The orientation relationship OR2 arises from OR1 by the Cu crystal rotation of 4° about the close-packed direction [1 1 0].

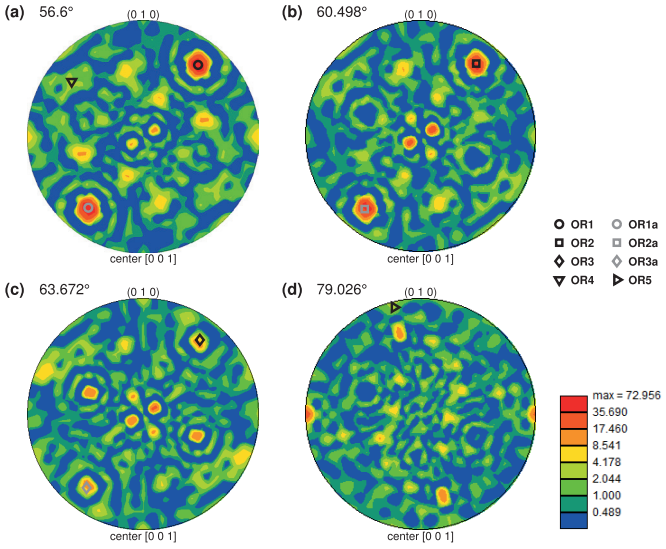

Figure 2: Misorientation Distribution Function for Cu/(5% vol) Al_2O_3 composites; Cross-sections of constant misorientation angle: 56.600°, 60.498°, 63.672° and 79.026°. The representative orientation relationships are denoted by black and gray markers.

The continuation of the process generates other misorientations with lower but significant frequencies. Finally, at the rotation angle of 7.4° we obtain the OR3 orientation relationship (-4 4 3)[1 1 0]Cu||(0 0 0 1)[0 1 -1 0] α−Al_2O_3 in which the strongest bonding at the phase boundary is formed. Like previously, we can distinguish the configuration OR3a that differs from OR3 by the sapphire crystal position (Fig. 1c, Fig. 2c). In order to show dependence of the interface bonding strength on orientation relationships, two other representative mis- orientations are taken into account: OR4 (-1 -1 1)[1 -1 0] Cu||(0 0 0 1)[2 -1 -1 0] α−Al_2O_3 and OR5 (5 -1 -1)[1 1 4]Cu||(0 0 0 1)[0 1 -1 0] α−Al_2O_3 (Fig. 1a,d and Fig. 2a,d).

3. Analysis of the interface strength

The rational composite design requires precise information about the toughness of interfaces observed experimentally. Appropriately strong bonding at the phase boundary produces deflection and meandering of the crack and in effect enables its closure or bridging. These are ones of the basic mechanisms of composite toughening. The interfacial bonding strength is determined by the interface energy γ. The stronger bonding the lower is the energy γ, thus the cost of its formation [5, 6]. Because of complex interatomic interactions at the metal/ceramic phase boundary, accurate determination of the quantity requires solution of two optimization problems coupled with each other [7]. Therefore in order to categorize interfaces according to bonding strength, we apply a simplified approach proposed by Gautam and Howe [2]. They noted that the interface energy is inversely proportional to the sum of intensities contained in overlapping regions between diffraction spots of two crystals. Thus, the higher total overlapping intensity I the stronger bonding is formed at the phase boundary. The introduced assumption is physically justified because the distribution of the diffraction intensity around a reciprocal lattice point maps the potential distribution in a plane corresponding to that point. In order to calculate the total overlapping intensity, the Cu and α−Al_2O_3 reciprocal lattices are localized in a reference system whose two axes are parallel to edges of the hexagonal sapphire cell. Determining structural factors for the crystals [8], diffraction intensities are ascribed to individual nodes. They are distributed radially according to the Lorentz function within spheres surrounding reciprocal lattice points. We assume that the sapphire crystal is stationary, while the copper crystal rotates to a position determined by an orientation relationship. Performing the analytical integration of intensities contained in overlapping volumes between spheres of two phases, we obtain the quantity I for the distinguished misorientations registered in EBSD studies. The calculated total overlapping intensities enable classification of the interfaces according to the bonding strength (see Tab. 1).

TABLE 1
Total overlapping intensity between diffraction spots of the Cu and α−Al_2O_3 crystals for different orientation relationships

	OR3, 3a	OR4	OR2, 2a	OR1, 1a	OR5
I	3990.1	2614.5	1877.5	1764.1	568.01

The configuration OR1 is well defined in the Literature and therefore it can be treated as a reference orientation relationship. The relatively high value of the total overlapping intensity for OR1 indicates the presence of a certain lattice matching. As a result, bonding formed at the phase boundary is strong enough to enable plastic deformation of the copper under the influence of an externally applied load [9]. The Cu crystal rotation about the [1 1 0] direction leads to a better spatial matching of the lattices. In consequence, we obtain the successive orientation relationships OR2, OR3 which enable the formation of bondings with higher strengths. Another valuable example is the OR4 interface. The symmetrically equivalent description of the orientation relationship (-1 1 1)[-1 -1 0]Cu||(0 0 0 1)[2 -1 -1 0] α−Al_2O_3 shows that OR4 is similar to OR1: the close-packed plane of copper (-1 1 1) is parallel to the analogical one in sapphire

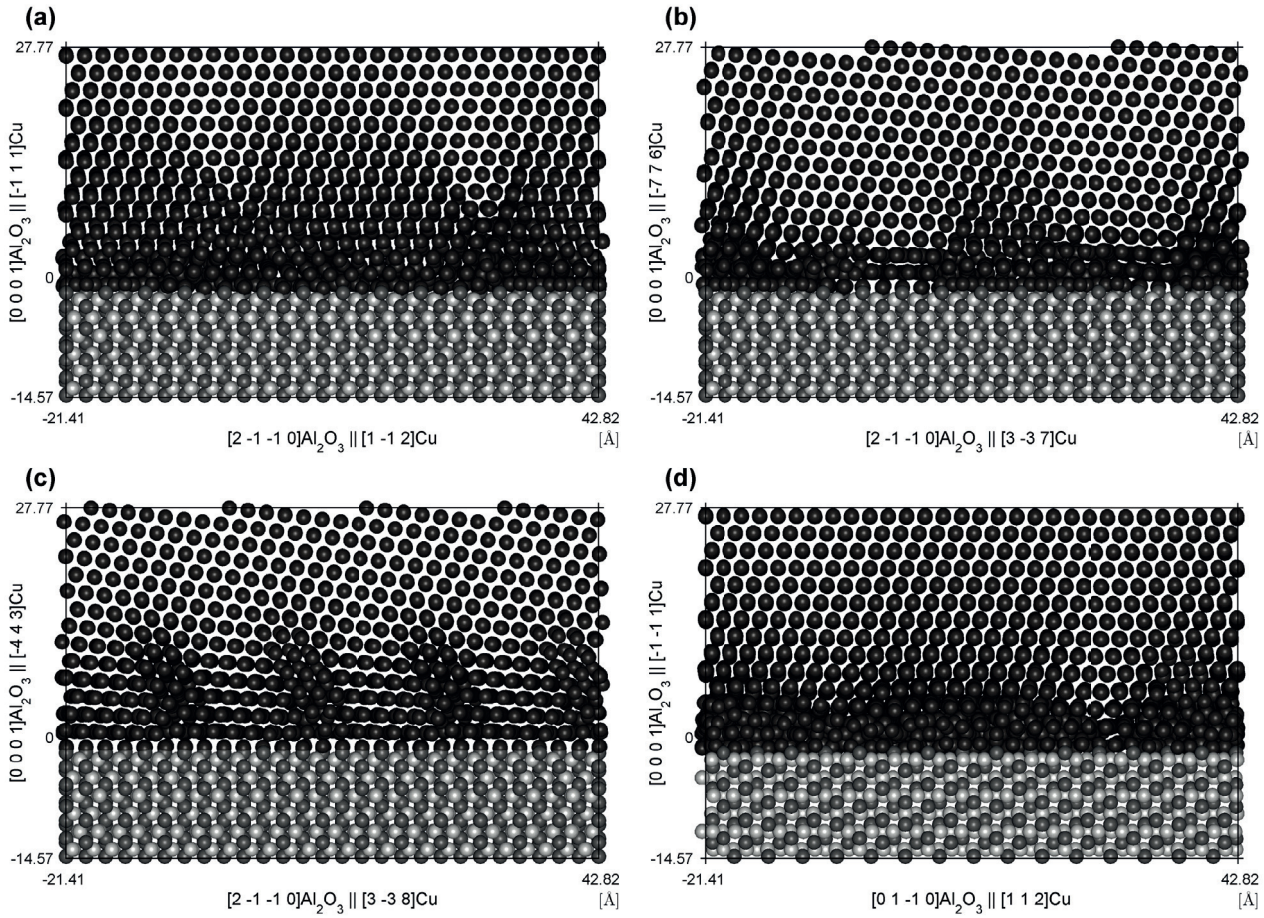

Fig. 3. MD models for microstructures of the representative interfaces: OR1 (a), OR2 (b), OR3 (c), OR4 (d)

(0 0 0 1). The difference constitutes the Cu crystal rotation of 90° about the normal to the (0 0 0 1) surface. The orientation relationship OR4 enables the formation of the interfacial bonding stronger than it is in the case of OR1. Unfortunately, it appears in synthesized composites with a lower frequency. Performed studies [10] show that the orientation relationship OR4 can be assumed as often as OR1 if the manufacture conditions are changed. This example indicates that the appropriate selection of methods of the composite synthesis can promote the formation of interfaces with strong bondings, such as OR3 ones.

Improvement of the composite toughness requires an increase in participation of the phase boundaries with the above mentioned orientation relationships. Additionally, interfaces with a weak bonding should be eliminated. An example can be OR5 misorientation, in which the lattice matching is low. It leads to the amorphization of the interface region, which enables easy crack propagation.

The experimentally identified interfaces with strong bonding are reconstructed by MD simulations. For this purpose, the bonding in the interface is approximated by the Long- Chen potential [11] and the interatomic interactions in the Cu phase are described by the Voter model [12] specified by means of the symmetry-based method [13, 14]. The initial heterostructures are equilibrated with the use of the canonical ensemble (NVT). The recon- struction of the four interfaces discussed above is presented in Fig. 3.

4. Conclusions

The series of misorientations typical for the Cu/α−Al_2O_3 system is identified by EBSD investigations. The registered orientation relationships are categorized according to the strength of bonding formed at the phase boundary. The obtained hierarchy enables manufacture of composites with strong interfaces and thus the rational design of these materials.

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