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PLASTIC FLOW AND FAILURE OF SOLIDS. MODELLING ACROSS SCALES

K. Nalepka[1], R. B. Pęcherski[2]

[1]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 Krakow, Poland, e-mail: knalepka@agh.edu.pl

[2]Department of Mechanics of Materials, Institute of Fundamental Technological Research, Polish Academy of Sciences
A. Pawińskiego 5B, 02-106 Warsaw, Poland, e-mail: rpecher@ippt.pan.pl

1. Introduction

The aim of the presentation is to discuss the classical problems of elastic limit criteria from the perspective of basic quantum mechanical approach [1]. In the case of metallic solids the multiscale mechanisms of plastic deformation and failure are analysed [2]. In particular, the role of shear banding responsible for plastic flow is elucidated [3].

New and original aspects of the presentation are related with our recent studies on metal-ceramic composites. Final functional and mechanical properties of such materials depend largely on interface microstructures [4]. Particularly, it concerns to nanocomposites. Therefore, in cooperation with specialists of leading research centers in Poland, we undertook experimental and theoretical studies on microstructures of metal/ceramic interfaces. As an example, copper/ sapphire nanocomposites were considered. As a result of the carried out research, the interface microstructure of Cu/α-Al_2O_3 nanocomposites obtained by the pulsed laser deposition (PLD) method is reconstructed [5]. The synthesized heterostructures were examined using the aberration corrected high-resolution transmission electron microscopy (Cs-HRTEM) and the electron backscatter diffraction (EBSD). The results reveal that copper deposited by a laser pulse on the (0 0 0 1) α-Al_2O_3 surface

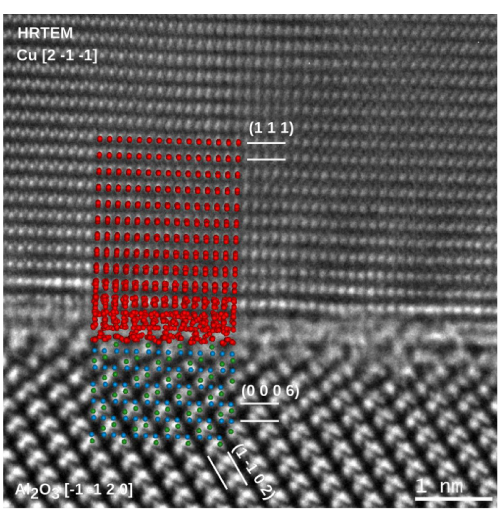

Fig. 1. Atomistic reconstruction (Cu, Al, and O atoms are denoted by red, green and blue spheres, respectively) compared with Cs-HRTEM image.

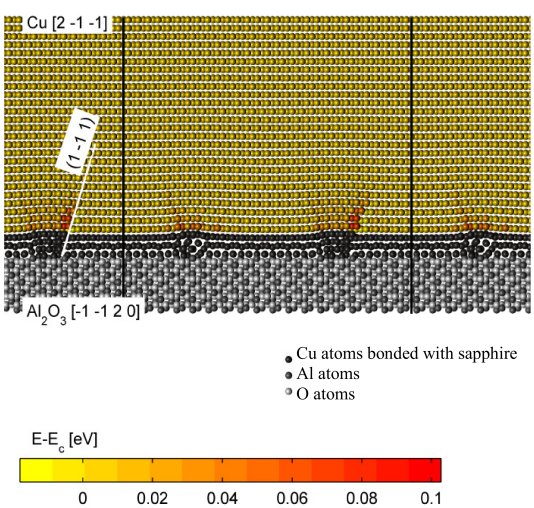

Fig. 2. Distribution of energy changes relative to the equilibrium state per atom in the copper section with the thickness 8 Å.

forms islands (the Volmer-Weber growth type) with one main orientation. In the preferred arrangement, the close packed planes and directions of copper are parallel to their equivalents in sapphire: (1 1 1)[−1 0 1]Cu|| (0 0 0 1)[0 1 −1 0] α-Al_2O_3. This gives an opportunity to form a strong bonding at the phase boundary. EBSD studies showed that the identified disorientation is also characteristic for copper matrix composites reinforced by sapphire particles. The strong bonding between Cu and α-Al_2O_3 induces structural changes in the (1 1 1) Cu layer nearest the substrate and leads to plastic deformations in subsequent layers (Fig. 1, 2). 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 formation of the system of partially dissociated dislocations in the close packed planes {1 -1 1}. The reconstructed interface is used for Cs-HRTEM image simulation. A good accordance with the experimental results indicates that the proposed model correctly maps the microstructure at the phase boundary of the synthesized nanocomposite.

The reconstruction is obtained by Molecular Dynamic and Static (MD and MS) simulations under the assumption that the sapphire substrate is rigid, while the copper undergoes deformations according to the model of interatomic interactions by A.F. Voter [6]. The interatomic potential is specified by a new method which is based on symmetry of considered material (S-B method) [7, 8]. According to the proposed approach, in the equilibrium state, the cohesive energy and eigenvalues of the elasticity tensor $\mathbf{C}$ predicted by the model are consistent with the experimental data. Additionally, the pressure in the crystal should amount to zero. The derived conditions take a simpler form than those proposed in the literature thanks to double application of material symmetry: at the continuum and atomistic level. At the first of them, symmetry determines the spectral decomposition of the elasticity tensor, which enables to formulate the initial form of parameterization relationships. The obtained conditions undergo further simplifications at the atomistic level due to application of orthogonality relations in the point group of the considered crystal. The proposed specification method enables us to asses accuracy with which a model reproduces arbitrary processes of small strains. It is shown that errors in eigenvalues of the tensor $\mathbf{C}$ constitute extreme values of errors with which a model predicts energy densities stored during elastic deformations. Formulated S-B conditions are used to specify the Voter model. The obtained potential more accurately reproduces processes of small strains (Fig. 3) and the key paths of large deformations [7]. At the end perspectives of further research on the strength of the Cu/α-Al_2O_3 interface are discussed.

References

1. K. Nalepka, R.B. Pęcherski, T. Frąś, M. Nowak (2014). Inelastic flow and failure of metallic solids. Material effort: study across scales, in: T. Łodygowski, A. Rusinek (eds.), Constitutive Relations under Impact Loadings. Experiments, Theoretical and Numerical Aspects, CISM International Centre for Mechanical Sciences, vol. 552, Udine, 245–285.
2. R.B. Pęcherski (1983). Relation of microscopic observations to constitutive modelling of advanced deformations and fracture intiation of viscoplastic materials, *Archives of Mechanics*, **35**, 257–277.
3. R.B. Pęcherski (1998). Macroscopic effects of micro-shear banding in plasticity of metals, *Acta Mechanica*, **131**, 203–224.
4. K. Nalepka, R.B. Pęcherski (2009). Modelling of the interatomic interactions in the Copper crystal applied in the structure (111) Cu || (0001) Al_2O_3, *Archives of Metallurgy and Materials*, **54**, 511–522.
5. K. Nalepka, J. Hoffman, S. Kret, P. Nalepka, Z. Szymanski (2014). Applied Physics A , DOI: 10.1007/s00339-014-8317-3, in press.
6. Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, J.D. Kress (2001). *Physical Review B*, **63**, 224106.
7. K. Nalepka (2012). *Computational Materials Science*, **56**, 100–107.
8. K. Nalepka (2013). *Bulletin of the Polish Academy of Sciences: Technical Sciences*, **61**, 441–450.