Molecular Dynamics Modelling of Boundary Migration in Bicrystals under Nanoburnishing

Andrey I. Dmitriev*,†, Anton Yu. Nikonov*,†

*Institute of Strength Physics and Materials Science (ISPMS), Russian Academy of Science
Akademichesky pr. 2/4, 634021 Tomsk, Russia
e-mail: dmitr@ispms.tsc.ru, web page: http://www.ispms.ru/

†National Research Tomsk State University (TSU)
Lenin pr. 36, 634050 Tomsk, Russia
web page: http://www.tsu.ru

ABSTRACT

The operating characteristics of various machine parts are defined by the physical and mechanical properties of the surface layer. Unfortunately we still far from full understanding what parameters and mechanisms are responsible for certain surface modification. In this regards the methods of computer simulation can be considered as useful tools to investigate surface changing during contact interaction.

Many authors showed that nano-scale contact is ruled by atomistic phenomena and virtually always accompanied by plastic deformation in the form of dislocation nucleation at the surface or asperity flattening [1, 2]. With the exception of simple cases, such as nano indentation, these phenomena cannot be captured or understood using continuum mechanics because of their inherently discrete nature. In the paper we try to reproduce the details of burnishing process at nano-scale level with help of molecular dynamics simulation.

Early in [3] it was shown the migrations of symmetric tilt grain boundaries (STGB) under conditions of shear loading. To study the features of this effect under burnishing – like conditions the Cu bi-crystal [001] with STGB Σ5 (210) was modelled as a substrate. Results of our modelling are very close to the experimental observation.

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