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Three Dimensional Structure of Grain Boundaries in Nanometals

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Grain boundaries (GBs) are important crystalline defects and the most widely existing interfaces in crystalline materials. The structure and behavior of GBs usually determine the mechanical as well as many physical properties of metals and alloys. Although considerable progress has been made in the last century in understanding GB structures and behaviors, most of the experiments relied on two-dimensional characterizations such as optical microscopy, electron back-scatter diffraction and transmission electron microscopy. Hence, studies of GBs in polycrystals are usually considered in terms of the overall GB geometry based on the crystallographic relationships between neighboring grains rather than detailed descriptions of interface structures. In addition, GB structures are largely dependent on temperature and other factors. For example, high-angle GBs are often thought to be composed of structural units with one-dimensional translational periodicity, however, under different circumstances with variation of temperature, stress or defects, GBs incline to undergo different structural transition and faceting. Therefore, the real structure of GBs in materials should be far more complex than the ideally flat GB proposed by classical grain boundary theory. In this work, we have studied structures of nanoporous gold fabricated by electrochemical dealloying method. In contrast to isolated nanoparticles or nanorods samples, ligaments in the nanoporous gold connect with each other and form a three-dimensional network. Electron tomography reconstruction was performed based on tilt series of high-angle annular dark-field scanning transmission electron microscopy images. We determine the three-dimensional structure of both high angle and low angle GBs. The high angle GBs are non-planar and lose translational periodicity in all directions. Based on the resolved grain boundary structures, the statistical distribution of GB coordination numbers and structural units are correlatively analyzed.

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