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Study of Grain-Boundary Diffusion of Au in Copper within Σ5 Misorientation Range in the Context of Structure of Grain Boundaries

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Abstract

^{195}Au and ^{64}Cu diffusion along <100> symmetric tilt boundaries in copper is studied in detail within a narrow range of misorientations around Σ5(310) coincidence boundary. The grain-boundary (GB) diffusion of ^{195}Au and ^{64}Cu is examined at temperatures of 661-1030 K for the former and 919 K for the latter. A narrow Σ5-minimum is found on misorientation dependences of the GB-diffusion parameter of ^{195}Au and ^{64}Cu. It is shown that this behaviour is governed by GB-structure rather than chemical factors. Such a behaviour qualitatively differs from predictions of the structural unit model. At the same time this behaviour agrees with predictions based on the model for GB-structure near coincidence misorientations advanced by Brandon. There is a some indication on structure transition at borders of Σ5-minimum between GB-structure governed by Σ5-misorientation and structure of general grain boundaries.

Introduction

Up to now a number of studies was conducted where misorientation dependences of grain-boundary (GB) diffusion characteristics were obtained [1]. They can be divided on two groups which results differ qualitatively [1,2]. In studies of the first group [3-7] sharp cusps at coincidence misorientations were observed. Such a behaviour agrees with the predictions [3-6] based on a model proposed by Brandon [8] (the CSL/SGBD model) to describe GB-structure in the vicinity of coincidence (CSL) misorientations. In second group of studies [2,9-11] "smooth" misorientation dependences were obtained those concords with the prediction [2,12] of the structural unit model [13]. Let us consider these GB-structure models and their predictions in some details.

According to the CSL/SGBD model GBs in the vicinity of CSL-misorientation (CSL-related GBs) consist from regions of low-energy CSL-structure divided by a network of secondary grain-boundary dislocations (SGBD). Their density **n** is determined by equation $|\Delta\Theta| = |\Theta - \Theta_{CSL}| = \mathbf{bn}$, where **b** is Burgers vector of SGBDs defined by the DSC-lattice [14]. Thus, the structure of CSL-related GBs *is completely defined by given CSL-misorientation.* Hence, on GB-phase diagram (for example, in Θ -