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Effect of Diffusant Segregation on the Misorientation Dependences of the Characteristics of Grain-Boundary Diffusion: Ni and Au in Copper

S.I. Prokofjev

Institute of Solid State Physics, RU-142432 Chernogolovka, Moscow District, Russia

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Abstract. The diffusion of Ni along <100> symmetrical tilt boundaries in copper in misorientation range near Σ5(310) coincidence boundary is compared with that of Au. In both the cases the misorientation dependences of grain-boundary (*GB*) diffusion parameter (≡ the triple product) and activation parameters demonstrate narrow extrema at Σ5 misorientation. The characteristics of GB diffusion exhibit a step-like change on the borders of the Σ5-extrema. Such behaviour can be qualitatively described by Brandon's model. Within a framework of this approach, these steps are associated with a transition between near-coincidence and general GBs. The steps of the misorientation dependences have opposite signs for Ni and Au. A reason for this difference is likely a different sign of change in the GB segregation factors of Ni and Au in copper caused by the GB transformation. This is a consequence of opposite signs of the enthalpies of the GB segregation of Ni and Au in copper.

Introduction

Studies of diffusion along single grain boundaries (*GB*s), whose misorientation and orientation parameters are well-known, are of basic interest, since they make it possible to establish the correlation between characteristics of GB diffusion and GB structure [1]. Currently the measurements of GB diffusion along individual GBs are possible in the B-type kinetic regime only [1]. This makes it possible to determine the triple product (*GB diffusion parameter*) $P = s\delta D_b$. Here s is the factor of GB segregation of diffusant[1], δ is the diffusion width of GB, D_b is the GB diffusion coefficient. It has been found that the factor s depends on GB-structure, the comparison of diffusion of Cu, Au and Se in copper near Σ5(310) coincidence boundary has suggested a Σ5-minimum on the $s(\Theta)$ [2]. Thus, both $s(\Theta)$ and $D(\Theta)$ govern the behaviour of $P(\Theta)$. As result, a structural interpretation of the behaviour of $P(\Theta)$ becomes more complicated [3, 4]. Therefore, the knowledge of the effect of $s(\Theta)$ on the behaviour of $P(\Theta)$ is very important. However, such information is absent today.

The goal of the present paper is to compare the diffusion of Au [4, 5] and Ni [6-9] along <100> symmetrical tilt boundaries in copper in misorientation range close to Σ5(310) coincidence boundary. In both cases, the diffusion along <100> misorientation axis was studied. These studies were carried out on the bicrystals grown of copper of the same purity using identical technique [10, 11] to provide more reliable comparison. The effect of GB segregation factor of Ni (s^{Ni}) and Au (s^{Au}) in copper on the $P(\Theta)$ is considered on this basis. To conduct the comparison properly, a detailed analysis of the dependence $P^{Au}(\Theta)$ obtained in [4, 5] is carried out in the paper.

The analysis of concentration dependence of the GB surface tension in Cu(Ni) [12] and Cu(Au) [13, 14] alloys, study of GB diffusion of Au in copper in kinetic regimes of the B and C types [15], and computer simulation of GB segregation at Σ5(100) twist boundary in Cu(Ni) alloys

[1] If GB segregation is described by the Henry isotherm $s = s_o\exp(-H_S/RT)$, where s_o is the pre-exponential factor and H_S is the enthalpy of GB segregation, then Arrhenius parameters found from the experiment are $P_o = \delta s_o D_{bo}$ and $H = H_S + H_D$. Here H_D and D_{bo} are the parameters of the Arrhenius equation for D_b. Note, that a validity of the complete identification of s with the equilibrium GB segregation factor is under question now [2].