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

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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 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 (GBs), 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) \( P = sD_o \). Here \( s \) is the factor of GB segregation of diffusant\(^1\), \( \delta \) is the diffusion width of GB, \( D_o \) 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 \( \Sigma_5 \)-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 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 \( s = s_o \exp(-H_o/RT) \), where \( s_o \) is the pre-exponential factor and \( H_o \) is the enthalpy of GB segregation, then Arrhenius parameters found from the experiment are \( P_o = s_oD_o \) and \( H = H_o + H_D \). Here \( H_D \) and \( D_o \) are the parameters of the Arrhenius equation for \( D_o \). Note, that a validity of the complete identification of \( s \) with the equilibrium GB segregation factor is under question now [2].