PHILOSOPHICAL MAGAZINE A, 1999, VOL. 79, NO. 6, 1321–1333

Molecular dynamics study on the structural changes of the tilt grain boundary in aluminium

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[*Received 22 May 1997 and accepted 31 July 1998*]

ABSTRACT

The structure and physical properties of two Al tilt grain boundaries (GBs) at different temperatures have been studied using the molecular dynamics method. We find that, with increasing temperature, the GB structure changes by steps. Three characteristic temperatures T_0, T_1 and T_2 have been identified for the changes in the GB structure. A comparison with available experimental data has also been made.

§1. INTRODUCTION

Research into the grain-boundary (GB) structure has attracted the attentions of material scientists for a long time. The existence of special boundaries possessing low energies is experimentally confirmed. This fact, as well as the data of computer simulations of the structure of boundaries in Al and Cu, served as a base for the structural units model (Sutton and Vitek 1983, Sutton and Balluffi 1987). To a certain extent, the GB structure at low temperatures is consistent with this model. However, the GB structure at high temperatures is very disordered and far from understood. This can be particularly ascribed to the difficulties in the direct observation of its structure, since generally the boundary not only has a thin lateral dimension but also is a *buried* interface. The atomic simulation of GBs can avoid those difficulties, because it may provide very detailed information about the position and velocity of GB atoms. The atomic structure of a GB can be obtained and its physical properties can be calculated from the trajectories of atoms. Hence, one has turned to atomic simulations to investigate GB structures, and in particular the high-temperature structure of GB.

Many simulations on the structural changes of GBs have been performed in the last two decades (Broughton and Gilmer 1986, Nguyen *et al.* 1986, 1992, Lutsko *et al.* 1988). By a two-dimensional (2D) lattice gas model, Kikuchi and Cahn (1980) found that the boundary started to disorder when heated to about $0.50T_m$, and that the disordering progressed steadily as the temperature increased, culminating finally with boundary melting. In addition, by using the molecular dynamics and Lennard-Jones potential, Ciccotti *et al.* (1983) obtained results which appeared to be qualitatively similar to those of Kikuchi and Cahn. They found that the structure factor for the core region of the boundary began to decrease significantly at about $0.45T_m$; it then decreased smoothly at an accelerating rate until it apparently reached zero at T_m.

In contrast with these results, other researchers have found an apparent structural transition at temperatures as high as about $0.70T_m$. Deymier *et al.* (1987) have